Extension of the Proximal Auxiliary Problem Method using Logarithmic-quadratic Distances

Convergence Theory and Numerical Investigations

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To my parents

Zusammenfassung

Variationsungleichungen bilden eine gemeinsame Grundlage, um die Theorie und Algorithmen zum Lösen verschiedener Probleme der mathematischen Physik, der Ökonomie und der Naturwissenschaften zu untersuchen. Als Problemklasse beinhalten sie nicht nur klassische nichtlineare Optimierungsprobleme, sondern auch Gleichgewichtsprobleme, Komplementaritätsprobleme, nichtlineare Gleichungssysteme und andere. Die aus Anwendungen stammenden Variationsungleichungen sind in den meisten Fällen schlecht gestellt. Beispielsweise führen kleine Störungen in den Eingangsdaten zu großen Abweichungen in der Lösung, oder es liegen nicht-eindeutige Lösungen vor. In diesen Fällen können Standard-Lösungsverfahren scheitern.

Aus diesem Grund gewinnen Regularisierungsverfahren an Bedeutung, da sie das Ausgangsproblem in eine Folge von gut gestellten Hilfsproblemen überführen, welche beispielsweise eine eindeutige Lösung und eine bessere Kondition besitzen. Ferner kann durch eine geeignete Wahl des Regularisierungsterms erreicht werden, dass die Hilfsprobleme unrestringiert sind und sogar zu Optimierungsproblemen äquivalent sind. Die Fortentwicklung solcher Verfahren ist Gegenstand aktueller Forschung, an der wir uns mit dieser Arbeit beteiligen.

So schlagen wir einen neuen, auf logarithmisch-quadratischer Regularisierung basierenden Algorithmus (LQPAP-Methode) vor, der die Vorteile des bekannten Proximal-Punkt Verfahrens mit dem sogenannten Auxiliary Problem Principle verbindet. Seine Untersuchung und Konvergenzanalyse ist eines der Hauptresultate der vorliegenden Dissertation.

Die LQPAP-Methode knüpft dabei an den aktuellen Entwicklungsstand von Regularisierungsverfahren zum Lösen von Variationsungleichungen an, indem sie verschiedene in der Literatur vorgestellte Techniken zur Verbesserung der numerischen Stabilität der Verfahren aufgreift. So entsteht durch die Verwendung einer logarithmisch-quadratischen Distanzfunktion ein Innerer-Punkt-Effekt, der es erlaubt, die Hilfsprobleme als unrestringiert zu betrachten. Ferner arbeiten wir mit äußeren Operatorapproximationen, was für die numerische Lösung von Variationsungleichungen mit mengenwertigen Operatoren von Wichtigkeit ist. Außerdem werden inexakte Lösungen der Hilfsprobleme betrachtet und entsprechende Fehlerbedingungen verwendet. Als weiteren Vorteil

der logarithmisch-quadratischen Distanz verifizieren wir, dass sie self-concordant ist (im Sinne von Nesterov/Nemirovskii), was die Anwendung der Newton Methode zum Lösen der Hilfsprobleme motiviert.

Im numerischen Teil der Arbeit wird die LQPAP-Methode auf linear restringierte, differenzierbare und nicht differenzierbare, konvexe Optimierungsprobleme, sowie auf nicht symmetrische Variationsungleichungen mit co-koerziven Operatoren angewendet. Ferner vergleichen wir die Ergebnisse mit einer entsprechenden Bregman-Distanz basierten Methode (BrPAP-Methode). Bei beiden Methoden lässt sich eine Diskrepanz zwischen der theoretischen Freiheit bei der Wahl der Regularisierungsparameter und dem numerischen Verhalten der Methode beobachten. Der Erfolg der Methode hängt wesentlich von einer passenden Wahl der Folge der Regularisierungsparameter ab. Probleme ergeben sich vor allem, wenn die Folge der Iterierten den Rand der zulässigen Menge erreicht, bevor sie in der Nähe der Optimallösung ist. Vor diesem Hintergrund stellen wir die Strategie der Unter-Relaxierung vor, mit deren Hilfe die LQPAP-Methode robustifiziert wird. Ein ähnlicher Erfolg kann bei der BrPAP-Methode nicht festgestellt werden. Ansonsten unterscheiden sich beide Methoden hinsichtlich ihrer Effektivität kaum.

Die Hilfsprobleme, die bei Anwenden der LQPAP-Methode auf differenzierbare, konvexe Optimierungsprobleme entstehen, werden mit der Newton Methode gelöst. Mit Testbeispielen werden verschiedene Experimente durchgeführt und ausgewertet, wie zum Beispiel eine adaptive Wahl des Start-Regularisierungsparameters und eine Kombination der Armijo- und Self-Concordanz-Schrittweite.

Testbeispiele für nicht-symmetrische Variationsungleichungsprobleme sind in der Literatur kaum zu finden. Daher präsentieren wir einen geometrischen und analytischen Zugang, um Testbeispiele mit bekannter Lösung oder sogar einer bekannten Lösungsmenge zu generieren.

Zur Lösung der Hilfsprobleme bei nicht-differenzierbaren, konvexen Optimierungsproblemen wird die bekannte Bundle-Technik angewendet. Dabei beschreiben wir detailliert die Vorgehensweise und gehen auf die Wahl der beteiligten Funktionen und Parameterfolgen ein. Solche Untersuchungen wurden bisher nur in Verbindung mit Bregman-Distanzen veröffentlicht. Die Effektivität dieses LQPAP-Bundle Verfahrens wird wiederum an akademischen Beispielen aus der Literatur getestet.

Unsere Arbeit schlägt somit eine Brücke zwischen theoretischen und numerischen Untersuchungen von Lösungsverfahren für Variationsungleichungen.

Contents

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Glossary

Abbreviations

VI	Variational Inequality
PPA	Proximal Point Algorithm
APP	Auxiliary Problem Principle
PAP	Proximal Auxiliary Problem
BrPPA	Bregman Proximal Point Algorithm
BrPAP	Bregman Proximal Auxiliary Problem
LQPPA	Logarithmic-Quadratic Proximal Point Algorithm
LQPAP	Logarithmic-Quadratic Proximal Auxiliary Problem
KKT	Karush-Kuhn-Tucker

Matrices

C^T	the transposed of a matrix C
$\widehat{C}$	the symmetric part of a matrix $C \in \mathbb{R}^{n\times n}$, i.e., $\widehat{C} = \frac{1}{2}\left(C + C^T\right)$
$\lambda_{\min}(C)$	the smallest eigenvalue of a matrix C
$\lambda_{\max}(C)$	the largest eigenvalue of a matrix C
$\mathrm{cond}(C)$	the condition number of a matrix C, i.e., $\mathrm{cond}(C) = \lambda_{\max}(C)/\lambda_{\min}(C)$
$\parallel C \parallel_2$	the Euclidean matrix norm of C, given by $\parallel C \parallel_2 = (\lambda_{\max}(C^T C))^{-1}$
$\mathrm{diag}(C)$	matrix consisting of the diagonal elements of C
$\mathrm{diag}(d_1, \ldots, d_n)$	diagonal matrix with diagonal entries $d_1, \ldots, d_n$

Symbols and Variables

A	$(p \times n)$ matrix of full column rank
a_i	i-th row of matrix A (considered as a column vector)
a	positive constant which fulfills $\parallel u \parallel_A \geq a \parallel u \parallel$ for all $u \in \mathbb{R}^n$
α_j	step size in the Newton method
$\alpha_{k,j}$	linearization error defined by $\alpha_{k,j} = \varphi(x^k) - \varphi(z^j) - \left\langle s^j, x^k - z^j \right\rangle$
$\tilde{\alpha}_k$	linearization error defined by $\tilde{\alpha}_k = \varphi(x^k) - \varphi^k(z^k) - \left\langle \tilde{s}^k, x^k - z^k \right\rangle$
b	vector in $\mathbb{R}^p$ defining a right hand side
β	modulus of strong monotonicity
γ	parameter of (weakened) co-coercivity

γ_1	parameter $\in (0,1)$ in the criterion for a serious step: $\tilde{\epsilon}_{k+1} \leq -\gamma_1 v^{k+1}$
γ_2	parameter in the adaptive update rule for χ_k with $0 < \gamma_2 < \gamma_1 < 1$
δ_k	error tolerance parameter
ϵ_k	enlargement parameter in $\mathcal{Q}_{\epsilon_k}$
$\tilde{\epsilon}_k$	accuracy value defined by $\tilde{\epsilon}_k = \varphi(z^k) - \varphi^k(z^k)$
e^{k+1}	error vector in scheme (P_e^k)
$\tilde{e}^{k+1}$	error vector in the LQPAP bundle method which fulfills $\tilde{e}^{k+1} \in \nabla\psi(x^k) + \partial\varphi^{k+1}(z^{k+1}) + \chi_k \nabla_I D(z^{k+1}, x^k)$
ϑ	parameter of self-concordance which fulfills $\lvert\mathcal{D}^3 F(x)[h,h,h]\rvert \leq \vartheta(\mathcal{D}^2 F(x)[h,h])^{3/2}$
θ	accuracy parameter in the stopping criterion: $\parallel x^k - x^{k+1} \parallel < \theta$
I_n	the $(n \times n)$ identity matrix
J^k	set of bundle indices, $J^k \subset \{1,\ldots,k\}$ and $k \in J^k$
κ	modulus of strong convexity
$\lambda(F,x)$	Newton decrement for a ϑ-self-concordant function F in x defined by $\lambda(F,x) = \frac{\vartheta}{2}\sqrt{(F'(x))^T[F''(x)]^{-1}F'(x)}$
L	Lipschitz constant
m	number of bundle elements given by $m = \lvert J^k\rvert$
n	number of columns in A, problem size
p^j	Newton direction
p	number of rows in A, number of restrictions
r	decreasing factor $\in (0,1)$ for the regularization parameter χ_k
r^+	positive part of $r \in \mathbb{R}$, defined by $r^+ = \max\{r, 0\}$
r^-	negative part of $r \in \mathbb{R}$, defined by $r^- = \min\{r, 0\}$
ρ_k	ratio between actual descent and predicted descent defined by $\rho_k = \frac{\varphi(z^{k+1}) - \varphi(x^k)}{\varphi^{k+1}(z^{k+1}) - \varphi(x^k)}$
S	(in Chapter 8) matrix with subgradients
t	under-relaxation parameter $\in (0,1)$, when used as a vector it denotes slack variables in the KKT system
T	the matrix $\mathrm{diag}(t_1,\ldots,t_{m+1})$
τ	step length in the primal-dual interior point method
τ_1, τ_2, τ_3	parameters in the adaptive update rule for χ_k
$\langle u, v\rangle$	Euclidean inner product $v^T u$ of two vectors $u, v \in \mathbb{R}^n$
$\parallel u \parallel$	Euclidean norm of a vector $u \in \mathbb{R}^n$
$\langle u, v\rangle_A$	inner product defined as $\langle u, v\rangle_A = \langle A^T A u, v\rangle$
$\parallel u \parallel_A$	vector norm defined as $\parallel u \parallel_A = \parallel Au \parallel$
$\mathcal{V}$	the matrix $\mathrm{diag}(\nu_1,\ldots,\nu_{m+1})$, where ν_i are Lagrange multipliers
χ_k	regularization parameter
$\underline{\chi}, \overline{\chi}$	lower and upper bound for the sequence $\{\chi_k\}$

Functions and Operators

$\partial_I D(x,y)$	the partial subdifferential of D with respect to the first argument
$\nabla_I D(x,y)$	the partial gradient of D with respect to the first argument
$\nabla_I^2 D(x,y)$	the partial Hesse matrix of D with respect to the first argument
f_∞	recession function of f
$f \circ l$	denotes function composition of f and l
$\mathcal{F}$	single-valued, monotone and continuous operator in a VI
I	identity operator $I : \mathbb{R}^n \to \mathbb{R}^n$, $I(x) = x$
log	the natural logarithm
$l(x)$	defined as $l(x) = b - Ax$
$l_i(x)$	defined as $l_i(x) = b_i - \langle a_i, x \rangle$
$\mathcal{L}^k$	k-th auxiliary operator
$l^k(x)$	aggregate affine function defined by $l^k(y) = \varphi^k(z^k) + \left\langle \tilde{e}^k - \chi_{k-1} \nabla_I D(z^k, x^{k-1}), y - z^k \right\rangle$
$\mathcal{N}_K$	normal cone operator of a set K
$\mathcal{Q}$	multi-valued, maximal monotone operator in a VI
$\mathcal{Q}_\epsilon$	ϵ-enlargement of $\mathcal{Q}$
$\mathcal{Q}^k$	outer approximation of $\mathcal{Q}$ which fulfills $\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k}$
$\nabla \mathcal{T}$	Jacobi-matrix of an operator $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$
$\partial \varphi$	the subdifferential of a convex function φ
$\partial_\epsilon \varphi$	the ϵ-subdifferential of a convex function φ
$\nabla \psi$	the gradient of a function ψ
$\nabla^2 \psi$	the Hesse matrix (Hessian) of a function ψ

Sets

$2^{\mathbb{R}^n}$	power set (set of all subsets) of $\mathbb{R}^n$
$\mathrm{bd}(K)$	the boundary of a set K
$\mathrm{cl}(K)$	the closure of a set K
$\mathrm{int}(K)$	the interior of a set K
$\mathrm{dom}(f)$	the effective domain of a function, given by $\mathrm{dom}(f) = \{x \in \mathbb{R}^n : f(x) < +\infty\}$
$\mathrm{ri}(\mathrm{dom}(f))$	the relative interior of $\mathrm{dom}(f)$
$\mathrm{dom}(\mathcal{T})$	the effective domain of an operator, given by $\mathrm{dom}(\mathcal{T}) = \{x \in \mathbb{R}^n : \mathcal{T}(x) \neq \emptyset\}$
$\mathrm{gph}(\mathcal{T})$	the graph of an operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$
$\mathrm{rge}(\mathcal{T})$	the range of an operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$
$\mathbb{R}^p_+$	the set of all vectors in $\mathbb{R}^p$ with nonnegative entries
$\mathbb{R}^p_{++}$	the set of all vectors in $\mathbb{R}^p$ with strictly positive entries

1. Introduction

Variational inequality problems (VIs) appear in a variety of mathematical applications like convex programming, game theory and economic equilibrium problems, but also in fluid mechanics, physics of solid bodies and others. As such, they constitute a common basis to investigate the theory and algorithms for many problems in mathematical physics, in economy as well as in natural and technical sciences. A selection of related works is Aubin/Ekeland [1], Ekeland/Témam [30], Facchinei/Pang [33], Kinderlehrer/Stampacchia [57], Patriksson [75], and Zeidler [91]. A growing interest in this field of research can be observed since VIs in infinite-dimensional spaces were introduced in the 1960s in connection with free boundary value problems (Fichera [36], Lions/Stampacchia [66]). As a parallel development, VIs in finite-dimensional space were first investigated as generalizations of nonlinear complementarity problems (Cottle [22]) and in the context of traffic equilibrium problems (Dafermos [25]).

In this thesis we will focus on VIs with maximal monotone operators in finite dimensional space: For a given maximal monotone and possibly multi-valued operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ and a closed, convex set $K \subset \mathbb{R}^n$, some $x^* \in K$ and an appropriate $t^* \in \mathcal{T}(x^*)$ have to be found such that

$$\langle t^*, x - x^* \rangle \geq 0 \quad \forall x \in K,$$

where $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product in $\mathbb{R}^n$. Since the theory about the existence and uniqueness of solutions of VIs is sufficiently developed (see, e.g., Rockafellar/Wets [83]), the current research is mainly devoted to the design and analysis of solution methods for different classes of VIs.

Many VIs arising from applications are ill-posed. This means, for example, that the solution is not unique, or that small deviations in the data can cause large deviations in the solution. In such a situation, standard solution methods, like Newton based methods or others (see Facchinei/Pang [33, 34]), converge very slowly or even fail. Moreover, they are not applicable on VIs with multi-valued operators.

In this case, so-called regularization methods are the methods of choice. They have the advantage that an ill-posed original problem is replaced by a sequence of well-posed auxiliary problems, which have better properties (like, e.g., a unique solution and a

better conditionality). Two important basic methods are the proximal point algorithm (going back to Martinet [70]) and the auxiliary problem principle (introduced by Cohen [17]). In Chapter 2 we present the history and current state of the existing regularization methods. Their further development is an active field of research.

In the last years the focus of attention was mainly to improve the numerical stability of regularization methods. As a first aspect with respect to numerical implementations it is important to treat inexact solutions of the auxiliary problems. This implies the development of appropriate stopping criteria (see, e.g., Eckstein [28], Kaplan/Tichatschke [49], Rockafellar [82], Solodov/Svaiter [87]). Secondly, approximations of the operator $\mathcal{T}$ based on the concept of the ϵ-enlargement are investigated (see, e.g., Burachik/Iusem/Svaiter [9]). This allows for example the application of bundle methods to solve the auxiliary problems. Finally, much research is devoted to the usage of generalized regularization terms in order to simplify the structure of the auxiliary problems. Especially, nonquadratic distances such as Bregman distances (Burachik/Iusem [8], Chen/Teboulle [15], Eckstein [27], Kaplan/Tichatschke [52], Solodov/Svaiter [87]), logarithmic-quadratic distances (Auslender/Teboulle/Ben-Tiba [6]) and ϕ-divergences (Teboulle [88]) constitute an interior point effect which allows to treat the auxiliary problems as unconstrained ones.

This thesis continues the recent developments. We suggest and investigate a logarithmic-quadratic proximal auxiliary problem (LQPAP) method that includes a new combination of the above techniques and methods. Its exploration and convergence analysis is one of the main results in this work. The LQPAP method uses a logarithmic-quadratic distance function and combines the advantages of the proximal-point algorithm and the auxiliary problem principle. To keep this scheme most general, we suppose that the operator $\mathcal{T}$ is splitted into $\mathcal{F} + \mathcal{Q}$, where $\mathcal{F}$ is single-valued, continuous and monotone, and $\mathcal{Q}$ is multi-valued and maximal monotone. Furthermore, we allow that the auxiliary problems are solved inexactly using a summable error criterion, and we utilize the ϵ-enlargement technique to approximate $\mathcal{Q}$. Related works are Auslender/Teboulle/Ben-Tiba [6] and Kaplan/Tichatschke [52]. In Auslender/Teboulle/Ben-Tiba [6], a logarithmic-quadratic distance is used in an inexact proximal-point framework, but without operator approximations and with an additional error criterion of Eckstein-type. The work of Kaplan/Tichatschke [52] is devoted to a proximal auxiliary problem (PAP) method together with Bregman distances. Here, inexact solutions as well as ϵ-enlargements are considered. These two papers gave us the main impulse to investigate the LQPAP method. As an advantage of the logarithmic-quadratic distance, no paramonotonicity assumption on $\mathcal{F} + \mathcal{Q}$ is needed in contrast to a Bregman PAP scheme. This allows to apply the LQPAP method on a broader class of problems. Only in special cases (e.g., for saddle point problems, or if $\mathcal{Q} = \partial\varphi$, or if $\mathcal{Q}$ is bounded) it is shown by Kaplan/Tichatschke [53] and Langenberg [62] that paramonotonicity of $\mathcal{F} + \mathcal{Q}$ can be replaced by other or weaker assumptions.

As a further advantage, the logarithmic-quadratic distance is self-concordant (as mentioned, e.g., in Auslender/Teboulle/Ben-Tiba [5]). It is shown by Nesterov/Nemirovskii [73] that the Newton method is especially efficient to minimize self-concordant functions. With respect to the numerical realization of the LQPAP method it is therefore of special interest to further investigate this connection.

Numerical results for the application of nonquadratic distances were hardly available in the past (one positive example is Auslender/Haddou [2] for ϕ-divergences). Few details were given how to solve the auxiliary problems numerically. Furthermore, only sparse information was published how to check the assumed properties of the involved operators, or how to ensure the convergence conditions for the controlling parameters. Only in the last decade, publications have started to include specific information about the implementation and numerical tests (see Hübner [44], Kiwiel [60], Langenberg [63], Xu/He/Yuan [90]). Therefore, our motivation is to fill the gap between theory and numerics by providing a deeper insight into all aspects that have to be regarded for an implementation and evaluation of the suggested LQPAP method.

Our numerical realization of the LQPAP method exploits the fact that for many VIs the resulting auxiliary problems are unconstrained, convex optimization problems. Three categories of original problems are distinguished, which emerge from special choices of the operators $\mathcal{F}$ and $\mathcal{Q}$: For the category of differentiable, convex optimization problems ($\mathcal{Q} = \nabla\psi$) we describe the implementation of the Newton method to solve the auxiliary problems and carry out different numerical experiments. For example, it is evaluated how the application of under-relaxation improves the results. As a second category, nonsymmetric VIs are considered, i.e., VIs where the operator $\mathcal{F}$ cannot be represented as the gradient of a convex function. Thus, it is not possible to formulate the VI as an optimization problem. Here, the LQPAP method has the advantage that those types of problems can yet be solved by means of optimization problems. The last category consists of nondifferentiable, convex optimization problems ($\mathcal{Q} = \partial\varphi$). We show how the auxiliary problems can be solved using the bundle-technique. As far as possible, our analysis is substantiated by new theoretical results. Furthermore, it will be explained in detail how the bundle auxiliary problems are solved with a primal-dual interior point method.

Our studies concerning the application of the bundle method differ from those in the related works of Hübner [44] and Auslender/Teboulle [4] as follows: Much of our investigation is inspired by Hübner [44], but in that work only Bregman functions are considered. Thus, a new convergence analysis for the logarithmic-quadratic distance function is needed. In Auslender/Teboulle [4] the bundle-technique is applied with a logarithmic-quadratic proximal method. But in contrast to our work, exact solutions of the bundle auxiliary problems are required and no operator $\mathcal{F}$ is included. Furthermore, no computational results are reported.

In our work, numerical results for all categories of problems are presented. Since paramonotonicity holds in the considered test problems, our solution method is competitive to the Bregman function based PAP method of Kaplan/Tichatschke [52]. We therefore extend our implementation to Bregman functions and compare the performance of both methods.

The present thesis is structured as follows:

Chapter 2 contains fundamental definitions and results. We introduce different notions of monotonicity for multi-valued operators, which will frequently be used in the convergence statements of the presented solution methods. The different problem classes covered by the general problem formulation of a VI are presented and a brief overview about existence and uniqueness results for solutions of VIs is given. Our main focus is dedicated to the history of the basic solution methods for VIs and the numerical methods which were recently developed. We attach particular importance to a structured presentation of the convergence conditions so that differences and similarities in the requirements on the data can easily be recognized. The different directions of development are clearly indicated and constitute the basis for our studies.

Chapters 3 to 8 contain own investigations and new results.

The main contribution of *Chapter 3* is the convergence analysis of the LQPAP method under standard assumptions on the problem data and parameters. Following the basic steps of a convergence proof, we first show that the method is well-defined, which includes a verification of the interior point effect (Theorem 3.3.1). Boundedness of the sequence of iterates is proved in a second step (Theorem 3.4.3) and, finally, the convergence of the iterates towards a solution of the given VI completes the analysis (Theorem 3.4.5).

In Theorem 4.2.3 and Lemma 4.2.5 of *Chapter 4* we give a proof that the logarithmic-quadratic distance function is strongly self-concordant but not a self-concordant barrier in the sense of Nesterov/Nemirovskii [73]. An efficient step size rule for the Newton method and the resulting quadratic convergence of the Newton decrements will be summarized.

The remaining chapters focus on the numerical realization of the LQPAP method.

Chapter 5 clarifies which types of LQPAP auxiliary problems are encountered when the LQPAP method is applied on certain categories of VIs. This gives us the basis to develop appropriate solution methods for the auxiliary problems. Furthermore, we analyze how to ensure the co-coercivity condition that is assumed in the convergence theorem of the LQPAP method (Lemmata 5.4.16 and 5.4.17). The standard choices for the auxiliary operator are discussed in Examples 5.4.18–5.4.20.

Chapter 6 describes the application of the LQPAP method to differentiable, convex optimization problems with linear constraints. The presented test problems also include some randomly generated examples. We will report the results of extensive numerical tests which, for instance, evaluate a step size rule based on self-concordance. Section 6.4 contains our achievements concerning the strategy of under-relaxation.

Chapter 7 primarily describes the construction of test examples for nonsymmetric VIs. We explain in Corollary 7.1.4 and Lemma 7.1.7 how to generate affine, nonsymmetric and co-coercive operators. Moreover, in Section 7.2 we present our ideas to generate test problems where the solution or even a solution set is known.

Finally, in *Chapter 8* the category of nondifferentiable, convex optimization problems is considered. We establish the LQPAP bundle method and prove its well-definedness and convergence in Theorem 8.1.2. The method is applied on several test examples from literature.

The Appendix contains additional material on convex functions and multi-valued operators, basic properties of logarithmic-quadratic distances, and some statements about the convergence of sequences of numbers. Moreover, most of the specific data for the test examples and the detailed results of our numerical tests are presented.

2. Variational Inequalities and Selected Solution Algorithms

Our investigation in the following chapters will focus on a new solution method for variational inequalities that is based on two classical algorithms, the proximal point algorithm and the auxiliary problem principle. In this chapter we describe the main ideas and important convergence results of these classical methods and point out advantages and disadvantages. Further, the proximal auxiliary problem principle will be presented as a method that combines the advantages of the basic algorithms. Finally, extensions of the basic methods include the usage of nonquadratic distance functions and enlargements of the operators. For example Bregman distances and logarithmic-quadratic distances lead to an interior point effect. The state of the art concerning these extensions will be summarized and relevant convergence conditions will be given.

Throughout this work we use the following notation. With $\langle \cdot, \cdot \rangle$ we refer to the canonical inner product in $\mathbb{R}^n$ with $\| \cdot \|$ as the associated Euclidean norm in $\mathbb{R}^n$. The power set of $\mathbb{R}^n$ is denoted with $2^{\mathbb{R}^n}$. $\mathbb{R}^n_{++}$ denotes the interior of the nonnegative orthant of $\mathbb{R}^n$. For a set $K \subset \mathbb{R}^n$ we denote with $\mathrm{int}(K)$ the interior of K, with $\mathrm{cl}(K)$ the closure of K, and with $\mathrm{bd}(K)$ the boundary of K. Further, $I : \mathbb{R}^n \to \mathbb{R}^n$ denotes the identity operator.

2.1 Preliminaries on monotone operators

We start with the main definitions and properties of monotone operators which are needed in our work. For more comprehensive information see [30, 57, 91].

Multi-valued/single-valued operator. A mapping $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is called a multi-valued operator, i.e., $\mathcal{T}$ maps a point $x \in \mathbb{R}^n$ to a set $\mathcal{T}(x) \subset \mathbb{R}^n$. An operator $\mathcal{T}$ is called single-valued if the image $\mathcal{T}(x)$ contains at most one element.

Effective domain, range, graph. For such operators the effective domain, the range, and the graph are defined, respectively, as

$$\begin{aligned}\mathrm{dom}(\mathcal{T}) &= \{x \in \mathbb{R}^n : \mathcal{T}(x) \neq \emptyset\},\\ \mathrm{rge}(\mathcal{T}) &= \bigcup_{x \in \mathrm{dom}(\mathcal{T})} \mathcal{T}(x),\\ \mathrm{gph}(\mathcal{T}) &= \{(x,u) \in \mathbb{R}^n \times \mathbb{R}^n : u \in \mathcal{T}(x), x \in \mathrm{dom}(\mathcal{T})\}.\end{aligned}$$

Inverse. The inverse operator $\mathcal{T}^{-1}$ of $\mathcal{T}$ is the multi-valued operator defined by the equivalence

$$x \in \mathcal{T}^{-1}(y) \Leftrightarrow y \in \mathcal{T}(x).$$

Obviously, it holds $\mathrm{dom}(\mathcal{T}^{-1}) = \mathrm{rge}(\mathcal{T})$.

Sum of operators. For two operators $\mathcal{T}_1, \mathcal{T}_2 : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ and two scalars $\alpha, \beta \in \mathbb{R}$ the operator $\alpha\mathcal{T}_1 + \beta\mathcal{T}_2$ is defined by

$$(\alpha\mathcal{T}_1 + \beta\mathcal{T}_2)(x) = \begin{cases} \alpha\mathcal{T}_1(x) + \beta\mathcal{T}_2(x) & \text{if } x \in \mathrm{dom}(\mathcal{T}_1) \cap \mathrm{dom}(\mathcal{T}_2) \\ \emptyset & \text{otherwise.} \end{cases}$$

Monotone/maximal monotone operators. A multi-valued operator $\mathcal{T}$ is called monotone if

$$\langle u - v, x - y \rangle \geq 0 \quad \forall x, y \in \mathbb{R}^n,\ \forall u \in \mathcal{T}(x),\ \forall v \in \mathcal{T}(y).$$

If $\mathcal{T}_1$, $\mathcal{T}_2$ are monotone then $\mathcal{T}_1^{-1}$, $\lambda\mathcal{T}_1$ with $\lambda \geq 0$, and $\mathcal{T}_1 + \mathcal{T}_2$ are monotone.

A monotone operator $\mathcal{T}$ is defined to be maximal monotone if $\mathrm{gph}(\mathcal{T})$ is not a proper subset of the graph of another monotone operator $\mathcal{T}' : \mathbb{R}^n \to 2^{\mathbb{R}^n}$.

If $\mathcal{T}$ is maximal monotone then $\mathcal{T}^{-1}$ and $\lambda\mathcal{T}$ with $\lambda > 0$ are maximal monotone. Further properties of a maximal monotone operator $\mathcal{T}$ are:

(a) $\mathcal{T}(x)$ is a convex and closed set for all $x \in \mathrm{dom}(\mathcal{T})$ [91, Proposition 32.6],

(b) $\mathrm{gph}(\mathcal{T})$ is closed [9, Proposition 1],

(c) $\mathrm{rge}(\mathcal{T}) = \mathbb{R}^n$ if $\mathrm{dom}(\mathcal{T})$ is bounded [91, Corollary 32.35],

(d) $\mathrm{cl}(\mathrm{dom}(\mathcal{T}))$, $\mathrm{ri}(\mathrm{dom}(\mathcal{T}))$, $\mathrm{cl}(\mathrm{rge}(\mathcal{T}))$, $\mathrm{ri}(\mathrm{rge}(\mathcal{T}))$ are convex sets [3, Proposition 6.4.1],

(e) $\mathcal{T}$ is locally bounded in $\mathrm{int}(\mathrm{dom}(\mathcal{T}))$ [79, Theorem 1],

(f) $\mathcal{T}$ is upper semicontinuous in $\mathrm{int}(\mathrm{dom}(\mathcal{T}))$ [3, Proposition 6.6.8]. Thus, a single-valued, maximal monotone operator is continuous in the interior of its domain.

Continuity and boundedness properties of multi-valued operators are defined in Appendix A.2.

Important examples of maximal monotone operators are:

(i) For a proper, lower semicontinuous, convex[1] function $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ the subdifferential $\partial\varphi : \mathbb{R}^n \to 2^{\mathbb{R}^n}$, which is defined as

$$\partial\varphi(x) = \{s \in \mathbb{R}^n : \varphi(y) \geq \varphi(x) + \langle s, y - x\rangle \quad \forall y \in \mathbb{R}^n\},$$

is a maximal monotone operator [83, Theorem 12.17].

(ii) Single-valued operators that are monotone and continuous are maximal monotone [91, Proposition 32.7].

(iii) An affine operator $\mathcal{T}(x) = Cx + d$ with $C \in \mathbb{R}^{n\times n}$ and $d \in \mathbb{R}^n$ is maximal monotone if $\frac{1}{2}(C + C^T)$ is positive semidefinite [83, Example 12.2].

(iv) The normal cone operator of a nonempty, closed, convex set $K \subset \mathbb{R}^n$, given by

$$\mathcal{N}_K(x) = \begin{cases} \{y \in \mathbb{R}^n : \langle y, u - x\rangle \leq 0 \quad \forall u \in K\} & \text{if } x \in K \\ \emptyset & \text{otherwise,} \end{cases}$$

is maximal monotone with $\mathrm{dom}(\mathcal{N}_K) = K$ [83, Corollary 12.18].

The sum of maximal monotone operators is not necessarily maximal monotone. Consider for example the case $\mathrm{dom}(\mathcal{T}_1) \cap \mathrm{dom}(\mathcal{T}_2) = \emptyset$, in which the graph of $\mathcal{T}_1 + \mathcal{T}_2$ is empty. Additional conditions are given in the following theorems.

Theorem 2.1.1 ([81], Theorem 1). *Let $\mathcal{T}_1$ and $\mathcal{T}_2$ be maximal monotone operators on $\mathbb{R}^n$ such that*

$$\mathrm{dom}(\mathcal{T}_1) \cap \mathrm{int}(\mathrm{dom}(\mathcal{T}_2)) \neq \emptyset.$$

Then $\mathcal{T}_1 + \mathcal{T}_2$ is maximal monotone.

Theorem 2.1.2 ([81], Theorem 3). *Let K be a nonempty, closed, convex subset of $\mathbb{R}^n$ and $\mathcal{T}$ be a single-valued monotone operator (not necessarily maximal) such that $K \subset \mathrm{dom}(\mathcal{T})$ and $\mathcal{T}$ is continuous along each line segment in K. Then $\mathcal{T} + \mathcal{N}_K$ is maximal monotone.*

We now recall some stronger notions of monotonicity for multi-valued operators because they will be frequently assumed in the analysis of solution methods for variational inequalities.

[1] Some basic definitions for convex functions are given in Appendix A.1.

Strictly/strongly monotone. A multi-valued operator $\mathcal{T}$ is strictly monotone if

$$\langle u - v, x - y \rangle > 0 \quad \forall x, y \in \mathbb{R}^n,\ x \neq y,\ \forall u \in \mathcal{T}(x),\ \forall v \in \mathcal{T}(y)$$

and strongly monotone if there exists a scalar $\beta > 0$ such that

$$\langle u - v, x - y \rangle \geq \beta \parallel x - y \parallel^2 \quad \forall x, y \in \mathbb{R}^n,\ \forall u \in \mathcal{T}(x),\ \forall v \in \mathcal{T}(y).$$

A strongly monotone operator is obviously strictly monotone. Two examples are:

(i) A continuously differentiable operator $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$ is strictly monotone if the Jacobi-matrix $\nabla\mathcal{T}(x)$ is positive definite for all $x \in \mathbb{R}^n$, and strongly monotone if $\nabla\mathcal{T}(x)$ is uniformly positive definite, i.e., $\langle \nabla\mathcal{T}(x)y, y \rangle \geq \alpha \parallel y \parallel^2$ for all $x, y \in \mathbb{R}^n$ with $\alpha > 0$. In particular, an affine operator $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$, $\mathcal{T}(x) = Cx + d$ with a positive definite matrix $C \in \mathbb{R}^{n \times n}$ and a vector $d \in \mathbb{R}^n$ is strongly and strictly monotone.

(ii) The subdifferential of a proper, lower semicontinuous, strictly (strongly) convex function is a strictly (strongly) monotone operator.

Paramonotone. A monotone operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is called paramonotone if for every $x, y \in \mathbb{R}^n$, $u \in \mathcal{T}(x)$, and $v \in \mathcal{T}(y)$ it holds

$$\langle u - v, x - y \rangle = 0 \quad \Rightarrow \quad u \in \mathcal{T}(y),\ v \in \mathcal{T}(x).$$

Strictly monotone operators are paramonotone. If $\mathcal{T}$ is the subdifferential of a proper, lower semicontinuous, convex function then $\mathcal{T}$ is paramonotone.

Co-coercive. Co-coercivity is a concept of generalized monotonicity for single-valued operators that lies strictly between simple and strong monotonicity. A single-valued operator $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$ is co-coercive on a set $K \subset \mathbb{R}^n$ with modulus $\gamma > 0$ if

$$\langle \mathcal{T}(x) - \mathcal{T}(y), x - y \rangle \geq \gamma \parallel \mathcal{T}(x) - \mathcal{T}(y) \parallel^2 \quad \forall x, y \in K.$$

Another name for this concept is Dunn-property [26]. The sum of co-coercive operators is co-coercive, and co-coercivity is preserved under affine transformations [93, Proposition 2.2].

A co-coercive operator $\mathcal{T}$ with modulus γ is monotone and Lipschitz continuous with constant $1/\gamma$. Although the converse is not true in general, it is valid in $\mathbb{R}^1$, where a function is co-coercive on an interval if and only if it is monotone (increasing) and Lipschitz continuous on that interval.

Co-coercive operators are paramonotone but not necessarily strongly monotone. Consider for example a constant operator, which is co-coercive with arbitrary $\gamma > 0$ but neither strongly nor even strictly monotone.

Further, co-coercivity of an operator $\mathcal{T}$ is equivalent to the strong monotonicity of the possibly multi-valued operator $\mathcal{T}^{-1}$ [92, Proposition 3.3]. A more detailed treatment of co-coercive operators will follow in Section 5.4.1.

Coercive/weakly coercive. Notions that describe the behavior of a monotone operator at infinity are useful to get statements about the solvability of a variational inequality. According to [91, Definition 25.2] an operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is said to be coercive if

$$\lim_{\|x\|\to\infty} \frac{\inf_{u\in\mathcal{T}(x)} \langle u, x\rangle}{\| x \|} = +\infty,$$

and weakly coercive if

$$\lim_{\|x\|\to\infty} \inf_{u\in\mathcal{T}(x)} \| u \| = +\infty,$$

with $\inf \emptyset = +\infty$. It is clear that coercive operators are weakly coercive, and that a bounded effective domain of $\mathcal{T}$ is sufficient for $\mathcal{T}$ to be coercive. Further, strongly monotone operators are weakly coercive.

2.2 Variational inequalities and related problems

A variational inequality is a problem formulation that includes several other mathematical problems like convex optimization problems, nonlinear equation systems, complementarity problems, and saddle point problems. Historically, the variational inequality problem was introduced in the 1960s in the context of optimal control theory and in connection with the solution of free boundary value problems in mathematical physics. These applications in infinite-dimensional spaces are described, e.g., in [57]. The research on finite-dimensional variational inequalities is motivated by discretizations of infinite-dimensional variational inequalities. As a parallel impulse, which is not related to the infinite-dimensional version, Dafermos [25] recognized in the 1980s that the traffic equilibrium problem can be formulated as a finite-dimensional variational inequality. For a detailed survey of the history of variational inequality problems we refer to [40] and the corresponding books [33, 34].

Definition of a variational inequality problem. For a given multi-valued operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ and a closed, convex set $K \subset \mathbb{R}^n$ the general problem formulation of a variational inequality is

$$\begin{aligned} \mathrm{VI}(\mathcal{T}, K): \quad & \text{Find } x^* \in K \text{ and } t^*(x^*) \in T(x^*) \text{ with} \\ & \langle t^*(x^*), x - x^* \rangle \geq 0 \quad \forall x \in K. \end{aligned}$$

In the case that $\mathcal{T}$ is a single-valued operator, $t^*(x^*)$ is replaced with $T(x^*)$.

With the help of the normal cone operator $\mathcal{N}_K$, problem VI($\mathcal{T}, K$) can be equivalently formulated as an inclusion problem

$$\begin{aligned} \text{IP}(\mathcal{T}, K): \quad & \text{Find } x^* \in \mathbb{R}^n \text{ with} \\ & 0 \in \mathcal{T}(x^*) + \mathcal{N}_K(x^*). \end{aligned}$$

Many applications in mathematical physics result in variational inequality problems with operators that can be splitted into the sum of a maximal monotone, multi-valued operator $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ and a single-valued, monotone, continuous operator $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$. For example the Signorini-problem, which describes a unilateral contact of an elastic body and a rigid support, and the Bingham problem, which describes the flow of a viscous plastic fluid in a cylindrical pipe, can be formulated as variational inequalities where the operator in splitted into $\mathcal{F} + \mathcal{Q}$. The considered problem then has the form

$$\begin{aligned} \text{VI}(\mathcal{F}, \mathcal{Q}, K): \quad & \text{Find } x^* \in K \text{ and } q^*(x^*) \in \mathcal{Q}(x^*) \text{ with} \\ & \langle \mathcal{F}(x^*) + q^*(x^*), x - x^* \rangle \geq 0 \quad \forall\ x \in K. \end{aligned}$$

It is not intended to explain further details about the Signorini or the Bingham problem in this work. We refer the reader to [57] for more information.

The solution method presented in our work solves problems of the form VI($\mathcal{F}, \mathcal{Q}, K$). This keeps the scheme most general because with the setting $\mathcal{F} = 0$ (or $\mathcal{Q} = 0$) the general case of a multi-valued (or single-valued) variational inequality is included.

The equivalent formulation of VI($\mathcal{F}, \mathcal{Q}, K$) as an inclusion problem is

$$\begin{aligned} \text{IP}(\mathcal{F}, \mathcal{Q}, K): \quad & \text{Find } x^* \in \mathbb{R}^n \text{ with} \\ & 0 \in \mathcal{F}(x^*) + \mathcal{Q}(x^*) + \mathcal{N}_K(x^*). \end{aligned}$$

Related problems. A large variety of problem classes is included in the problem formulation VI($\mathcal{F}, \mathcal{Q}, K$). In this work, convex optimization problems are of special interest regarding to numerical tests. Setting $\mathcal{F} = \nabla\psi$ with $\psi : \mathbb{R}^n \to \mathbb{R}$ convex and differentiable, and $\mathcal{Q} = \partial\varphi$ with $\varphi : \mathbb{R}^n \to \mathbb{R}$ convex and nondifferentiable, VI($\mathcal{F}, \mathcal{Q}, K$) describes the necessary and sufficient optimality conditions for the point x^* to be a local minimizer of the convex nonsmooth optimization problem

$$\begin{aligned} \text{OP}(\psi + \varphi, K): \quad & \min\ \{\psi(x) + \varphi(x)\} \\ & \text{s.t.}\ \ x \in K. \end{aligned}$$

The reformulation of a monotone variational inequality as an optimization problem enables the usage of solution methods developed for convex problems. However, the description of an arbitrary operator $\mathcal{F}$ as the gradient of a convex function is not possible in all cases. A necessary and sufficient condition contains Theorem 2.2.1.

Theorem 2.2.1 ([33], Theorem 1.3.1). *Assume that $\mathcal{F} : U \to \mathbb{R}^n$ is continuously differentiable on the open, convex set $U \subset \mathbb{R}^n$. Then the following statements are equivalent:*

(i) There exists a function $\psi : \mathbb{R}^n \to \mathbb{R}$ with $\mathcal{F}(x) = \nabla\psi(x)$ for all $x \in U$.

(ii) The Jacobian $\nabla\mathcal{F}(x)$ is symmetric for all $x \in U$.

The function ψ that fulfills (i) of Theorem 2.2.1 is given by

$$\psi(x) = \int_0^1 \mathcal{F}(x^0 + t(x - x^0))^T (x - x^0) dt,$$

where x^0 is an arbitrary fixed vector in $\mathbb{R}^n$. Operators having the property of Theorem 2.2.1 are called symmetric operators, otherwise nonsymmetric. As a generalization, a variational inequality problem $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ where

$$\exists \psi, \varphi : \mathbb{R}^n \to \mathbb{R} \text{ convex with } \mathcal{F} = \nabla\psi, \mathcal{Q} = \partial\varphi$$

is called symmetric. Otherwise, the variational inequality is called nonsymmetric.

Other problem classes arise from $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ if the restriction set and/or the operators are of a special structure. If $K = \mathbb{R}^n$ and $\mathcal{F} = 0$ the problem reduces to finding a zero of the multi-valued operator $\mathcal{Q}$ because in that case $\mathcal{N}_K(x) = \{0\}$ for all x. If $K = \mathbb{R}^n$ and $\mathcal{Q} = 0$ then $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ is equivalent to a nonlinear equation system

$$\mathrm{NEQ}(\mathcal{F}): \quad \text{Find } x^* \in \mathbb{R}^n \text{ with } \mathcal{F}(x^*) = 0.$$

A complementarity problem is included in $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ if K is a cone because then the problem can be reformulated as

$$\begin{aligned} \mathrm{CP}(\mathcal{F}, \mathcal{Q}, K): \quad & \text{Find } x^* \in K \text{ and } q^*(x^*) \in \mathcal{Q}(x^*) \text{ with} \\ & q^*(x^*) + \mathcal{F}(x^*) \in K^* \text{ and } \langle q^*(x^*) + \mathcal{F}(x^*), x^* \rangle = 0. \end{aligned}$$

Here, $K^* = \{d \in \mathbb{R}^n : \langle d, x \rangle \geq 0 \ \forall x \in K\}$ denotes the dual cone of K. If $K = \mathbb{R}^n_+$ then $K^* = \mathbb{R}^n_+$, and with $\mathcal{Q} = 0$ we get the classical nonlinear complementarity problem

$$\begin{aligned} \mathrm{NCP}(\mathcal{F}, K): \quad & \text{Find } x^* \in \mathbb{R}^n \text{ with } x^* \geq 0 \text{ and } \mathcal{F}(x^*) \geq 0 \text{ and} \\ & x_i(\mathcal{F}(x^*))_i = 0 \quad \forall i = 1, \ldots, n. \end{aligned}$$

If $\mathcal{F}(x)$ is affine, i.e., $\mathcal{F}(x) = Cx + d$ for a matrix $C \in \mathbb{R}^{n \times n}$ and a vector $d \in \mathbb{R}^n$, problem $\mathrm{NCP}(\mathcal{F}, K)$ reduces to a linear complementarity problem.

Finally, we introduce the saddle point problem as being included in $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$. Let $N \subset \mathbb{R}^n$ and $M \subset \mathbb{R}^m$ be two nonempty, closed sets and $L : N \times M \to \mathbb{R}$ be a function

of two arguments (called a saddle function in this context). The saddle point problem is given as

$$\begin{aligned} \mathrm{SPP}(L, N \times M): \quad & \text{Find } (x^*, y^*) \in N \times M \text{ with} \\ & L(x^*, y) \leq L(x^*, y^*) \leq L(x, y^*) \quad \forall (x, y) \in N \times M. \end{aligned}$$

If L is convex in x and concave in y, and N, M are convex sets, the saddle point problem can be formulated as a $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{F} = 0$,

$$\mathcal{Q}(x, y) = \partial_x L(x, y) \times \partial_y[-L](x, y), \quad \text{and} \quad K = N \times M.$$

Existence and uniqueness of solutions. We now come to existence and uniqueness results needed to prove the well-definedness of our solution method.

Since $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ is equivalent to an inclusion problem $\mathrm{IP}(\mathcal{T}, K)$ with operator $\mathcal{T} = \mathcal{F} + \mathcal{Q} + \mathcal{N}_K$, existence and uniqueness results for inclusion problems can easily be transferred to variational inequalities. It is clear that an inclusion problem $\mathrm{IP}(\mathcal{T}, K)$ is solvable if and only if

$$0 \in \mathrm{rge}(\mathcal{T}).$$

Hence, conditions on $\mathcal{T}$ ensuring that $\mathrm{rge}(\mathcal{T}) = \mathbb{R}^n$ are sufficient for the existence of a solution. For example:

Theorem 2.2.2 ([91], Corollary 32.35). *Let $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ be a maximal monotone and weakly coercive operator. Then* $\mathrm{rge}(\mathcal{T}) = \mathbb{R}^n$.

Special inclusion problems with operators of the type $\mathcal{T} + \partial\varphi$, where $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is a maximal monotone operator and $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is a proper, lower semicontinuous, convex function, will occur in our work. An important existence result in this context is

Theorem 2.2.3 ([8], Proposition 3). *Let $\mathcal{T}\colon \mathbb{R}^n \to 2^{\mathbb{R}^n}$ be a monotone operator and $\varphi\colon \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ a proper, lower semicontinuous, convex function. Suppose further that the following conditions are satisfied:*

(a) $\mathrm{dom}(\mathcal{T}) \cap \mathrm{dom}(\partial\varphi) \neq \emptyset$ *and* $\mathrm{rge}(\partial\varphi) = \mathbb{R}^n$,

(b) $\mathcal{T} + \partial\varphi$ is maximal monotone.

Then $\mathrm{rge}(\mathcal{T} + \partial\varphi) = \mathbb{R}^n$.

The last theorem does not ensure uniqueness of the solution. Uniqueness is guaranteed if the operator $\mathcal{T} + \partial\varphi$ is strictly monotone as follows directly from the definition. Strongly monotone operators are strictly monotone and weakly coercive and therefore ensure both existence and uniqueness.

Theorem 2.2.4 ([83], Proposition 12.54). *For a maximal monotone and strongly monotone operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ the inclusion problem $\mathrm{IP}(\mathcal{T}, K)$ has a unique solution.*

2.3 Basic solution algorithms

A survey of the theory, algorithms, and applications for finite-dimensional variational inequalities with single-valued operators is given in [40]. For the multi-valued case a suitable monograph is not existent and we refer to the papers cited within this section for more information.

The *proximal point algorithm* (PPA) and the *auxiliary problem principle* (APP) are the main topic of this section. We explain the ideas behind these solution methods for variational inequalities, present corresponding algorithms, and mention selected convergence results to get familiar with standard convergence conditions. Moreover, the *proximal auxiliary problem method* (PAP method) is described, which combines the advantages of the PPA and the APP.

2.3.1 Proximal point algorithm (PPA)

The proximal point algorithm was first developed by Martinet [70] as a solution method for inclusion problems $\mathrm{IP}(\mathcal{T}, \mathbb{R}^n)$ with a maximal monotone, multi-valued operator $\mathcal{T}$. It is based on a fixed-point iteration for the resolvent operator

$$J_{\chi\mathcal{T}} = \left(I + \frac{1}{\chi}\mathcal{T}\right)^{-1}, \quad \chi > 0,$$

which is single-valued and nonexpansive [81, Proposition 1]. Fixed-points of $J_{\chi\mathcal{T}}$ are solutions of $\mathrm{IP}(\mathcal{T}, \mathbb{R}^n)$ [34, Proposition 12.3.5]. The inexact version of the PPA, which allows some error in the calculation of $J_{\chi\mathcal{T}}$ and a varying parameter χ, was investigated by Rockafellar [82]. For a variational inequality (i.e., $\mathcal{T} = \mathcal{Q} + \mathcal{N}_K$ with $\mathcal{Q}$ multi-valued, maximal monotone and $K \subset \mathbb{R}^n$ closed, convex) the corresponding inexact PPA is presented in Algorithm 2.1. For its convergence the following conditions on the data and the parameters are needed:

Conditions (PPA): *(see Rockafellar [82])*

(1) $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ *maximal monotone,* $K \subset \mathbb{R}^n$ *closed, convex,* $\mathrm{VI}(\mathcal{Q}, K)$ *solvable,*

(2) $0 < \chi_k \leq \overline{\chi} < \infty$, $\forall k \in \mathbb{N}_0$, $\sum_{k=0}^{\infty} \delta_k < \infty$.

Algorithm 2.1: Inexact proximal point algorithm (PPA)

1. *(Initialization)* Choose an initial point $x^0 \in K$, a parameter $\chi_0 > 0$, and an error parameter $\delta_0 \geq 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem VI$(\mathcal{Q}, K)$ then stop.
3. *(Auxiliary problem)* Find $x^{k+1} \in K$ and $e^{k+1} \in \mathbb{R}^n$ such that

$$e^{k+1} \in \mathcal{Q}(x^{k+1}) + \chi_k(x^{k+1} - x^k) + \mathcal{N}_K(x^{k+1})$$

   and $\| e^{k+1} \| \leq \delta_k \chi_k$.
4. *(Update)* Choose new parameters $\chi_{k+1} > 0$ and $\delta_{k+1} \geq 0$. Set $k := k + 1$ and go to step 2.

The PPA has the advantage that the auxiliary problems have better properties than the original problem: The operator

$$\mathcal{Q}(\cdot) + \chi_k(I(\cdot) - x^k)$$

is strongly monotone for each $\chi_k > 0$, which leads to uniquely solvable subproblems. This is of special importance when dealing with ill-posed problems.

Ill-posed problems. According to Hadamard [38] a problem is said to be ill-posed if at least one of the following properties is not fulfilled: solvability of the problem, uniqueness of the solution, continuous dependency of the solution on the input parameters. If a problem has multiple solutions the convergence rate of standard methods can be poor. If the solution depends in a discontinuous way on the data then small errors can create large deviations. Proximal point methods are regularization methods which means that they replace an ill-posed variational inequality problem by a sequence of well-posed problems. Furthermore, the regularization parameter χ_k does not have to tend to zero which ensures numerical stability of the regularized problems.

We illustrate the regularizing effect of the PPA in the case of a minimization problem. Take $\mathcal{Q} = \partial\varphi$ with a convex function $\varphi : \mathbb{R}^n \to \mathbb{R}$ that has multiple minima and/or a small curvature. Then the PPA generates auxiliary problems that are equivalent to the solution of

$$\min_{x \in K} \left\{ \varphi(x) + \frac{\chi_k}{2} \| x - x^k \|^2 \right\},$$

which is a better conditioned, uniquely solvable, strongly convex optimization problem.

Remark 2.3.1 (On the schemes (P_e^k) and (P_δ^k)). *We close this section with a comment on the types of auxiliary problems. The auxiliary problems presented in this section will either be given in form of an inclusion problem or in form of a variational*

inequality. To point out the relationship, consider a variational inequality $\mathrm{VI}(\mathcal{T}, K)$ *and the following examples of (inexact) auxiliary problems, where* $\mathcal{H}(\cdot,\cdot)$ *denotes a certain auxiliary operator (specified in the sequel):*

$$
\begin{aligned}
(P_e^k): \quad & \textit{Find } x^{k+1} \in K \textit{ and } e^{k+1} \in \mathbb{R}^n \textit{ such that} \\
& e^{k+1} \in \mathcal{T}(x^{k+1}) + \chi_k \mathcal{H}(x^{k+1}, x^k) + \mathcal{N}_K(x^{k+1}) \\
& \textit{and } \parallel e^{k+1} \parallel \leq \delta_k,
\end{aligned}
$$

$$
\begin{aligned}
(P_\delta^k): \quad & \textit{Find } x^{k+1} \in K \textit{ and } t(x^{k+1}) \in \mathcal{T}(x^{k+1}) \textit{ such that} \\
& \left\langle t(x^{k+1}) + \chi_k \mathcal{H}(x^{k+1}, x^k), x - x^{k+1} \right\rangle \geq -\delta_k \parallel x - x^{k+1} \parallel \quad \forall x \in K.
\end{aligned}
$$

It is easy to see that a solution x^{k+1} *of the inclusion problem* (P_e^k) *is also a solution of the variational inequality* (P_δ^k) *by the definition of the normal cone operator and the Cauchy-Schwarz inequality. Schemes* (P_e^k) *and* (P_δ^k) *are obviously equivalent if exact solutions are required, i.e.,* $e^{k+1} = 0$ *and* $\delta_k = 0$ *for all* k*. It can also be shown that* (P_e^k) *and* (P_δ^k) *are equivalent if the iterates* $\{x^k\}$ *belong to the interior of* K *(see Lemma 3.4.1).*

2.3.2 Auxiliary problem principle (APP)

Cohen [17] introduced the auxiliary problem principle to unify the convergence analysis of gradient and subgradient optimization algorithms as well as some decomposition algorithms. In [19] this approach is applied to solve variational inequalities. The auxiliary problem principle has proved its usefulness in a variety of areas. Contributions were not only made to the field of optimization [17, 20] but also, for example, to the field of stochastic optimization [24], Nash equilibria [18], and variational inequalities [35, 49].

The convergence analysis of the APP differentiates the case where the given operator of the variational inequality is single-valued from the case where it is multi-valued.

Single-valued case. We first describe the method for variational inequality problems $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{Q} = 0$.

The idea is to introduce a sequence of single-valued, strongly monotone auxiliary operators $\{\Omega^k\}_{k\in\mathbb{N}_0}$ and a sequence $\{\chi_k\}_{k\in\mathbb{N}_0}$ of positive parameters so that $\mathcal{F}$ is approximated in iteration k by $\{\chi_k\Omega^k\}$. The error made by approximating $\mathcal{F}$ is taken into account by adding the error term $\mathcal{F}(x^k) - \chi_k\Omega^k(x^k)$. Thus, in iteration k, $\mathcal{F}$ is replaced by the operator $\mathcal{F}(x^k) + \chi_k(\Omega^k(\cdot) - \Omega^k(x^k))$. Algorithm 2.2 summarizes the classical auxiliary problem principle.

Algorithm 2.2: Classical auxiliary problem principle (APP)

1. *(Initialization)* Choose an initial point $x^0 \in K$, an auxiliary operator Ω^0, and a parameter $\chi_0 > 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem VI$(\mathcal{F}, K)$ then stop.
3. *(Auxiliary problem)* Find $x^{k+1} \in K$ such that

$$\left\langle \mathcal{F}(x^k) + \chi_k(\Omega^k(x^{k+1}) - \Omega^k(x^k)), x - x^{k+1} \right\rangle \geq 0 \quad \forall x \in K.$$

4. *(Update)* Choose a new auxiliary operator Ω^{k+1} and a parameter $\chi_{k+1} > 0$. Set $k := k + 1$ and go to step 2.

In the first version of the auxiliary problem method for variational inequalities, Cohen takes symmetric auxiliary operators and sets

$$\Omega^k = \Omega = \nabla h \quad \text{and} \quad \chi_k = \chi \quad \forall k \in \mathbb{N}_0,$$

where $h : \mathbb{R}^n \to \mathbb{R}$ is some continuously differentiable function. In this case the auxiliary problems reduce to

$$\begin{aligned} &\text{Find } x^{k+1} \in K \text{ such that} \\ &\left\langle \mathcal{F}(x^k) + \chi(\nabla h(x^{k+1}) - \nabla h(x^k)), x - x^{k+1} \right\rangle \geq 0 \quad \forall x \in K, \end{aligned} \tag{2.1}$$

which is equivalent to solving the optimization problem

$$\min_{x \in K} \left\{ \chi h(x) + \left\langle \mathcal{F}(x^k) - \chi \nabla h(x^k), x - x^k \right\rangle \right\}. \tag{2.2}$$

This equivalence is one of the advantages of the auxiliary problem principle. Since the operator $\mathcal{F}$ is fixed at the current iterate, even variational inequalities with nonsymmetric operators can be reduced to solving a sequence of optimization problems.

For the convergence of the iterates $\{x^k\}$ towards a solution of VI$(\mathcal{F}, K)$, Cohen requires in [19, Theorem 2.2] the following conditions:

Conditions (APP, case: $\Omega^k = \Omega = \nabla h$, $\mathcal{F}$ strongly monotone): *(see Cohen [19])*

(1) $K \subset \mathbb{R}^n$ *closed, convex,*

(2) $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ *is strongly monotone with modulus* β_1 *and Lipschitz continuous with constant* L *(thus,* $\mathcal{F}$ *is co-coercive with modulus* β_1/L^2*),*

(3) $h : \mathbb{R}^n \to \mathbb{R}$ *is convex and* ∇h *is strongly monotone with modulus* β_2*, and*

(4) $\frac{L^2}{2\beta_1\beta_2} < \chi < +\infty$.

If $\mathcal{F}$ is not strongly monotone but only monotone, a convergence result can be given in the case that $\mathcal{F}$ is symmetric. In [17, Theorem 2.1], Cohen proves that every limit point of the sequence $\{x^k\}$ is a solution if

Conditions (APP, case: $\Omega^k = \Omega = \nabla h$, $\mathcal{F} = \nabla\psi$ monotone): *(see Cohen [17])*

(1) $K \subset \mathbb{R}^n$ *closed, convex,*

(2) $\mathcal{F} = \nabla\psi$ *with* $\psi : \mathbb{R}^n \to \mathbb{R}$ *convex and weakly coercive, and* $\nabla\psi$ *Lipschitz continuous with constant* L*,*

(3) $h : \mathbb{R}^n \to \mathbb{R}$ *is convex, and* ∇h *is strongly monotone with modulus* β *and Lipschitz continuous with constant* L_h*, and*

(4) $\frac{L}{2\beta} < \chi < +\infty$*.*

Monotonicity of $\mathcal{F}$ without any additional condition is not sufficient for convergence if $\mathcal{F}$ is nonsymmetric. This can be illustrated with the rotation operator

$$\mathcal{F}(x_1, x_2) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad \forall (x_1, x_2)^T \in \mathbb{R}^2,$$

which geometrically rotates every point in $\mathbb{R}^2$ by $90°$. Thus, it is clear that the scalar product $\langle \mathcal{F}(x) - \mathcal{F}(y), x - y \rangle$ is zero for all $x, y \in \mathbb{R}^2$. This shows that $\mathcal{F}$ is monotone but neither strongly monotone nor co-coercive. $\mathrm{VI}(\mathcal{F}, \mathbb{R}^2)$ is equivalent to finding the unique zero $x^* = (0,0)^T$ of $\mathcal{F}$. If Ω is chosen as the identity operator on $\mathbb{R}^2$, (2.1) is equivalent to $x^{k+1} = x^k - \frac{1}{\chi}\mathcal{F}(x^k)$, respectively

$$x_1^{k+1} = x_1^k + \frac{1}{\chi} x_2^k, \quad x_2^{k+1} = x_2^k - \frac{1}{\chi} x_1^k.$$

Hence

$$\| x^{k+1} \|^2 = (1 + (1/\chi)^2) \| x^k \|^2 .$$

Starting with $x^0 \neq x^*$, the norm of the iterates strictly increases with k for every $\chi > 0$. Thus, the iterates cannot converge towards x^*.

The strong monotonicity assumption on $\mathcal{F}$ for nonsymmetric variational inequalities was weakened by Zhu/Marcotte [93, Theorem 3.2] by assuming only co-coercivity of $\mathcal{F}$, and by El Farouq [31, Theorem 4.1] who proves the convergence of the sequence $\{x^k\}$ to a solution under a pseudo Dunn property.

Zhu/Marcotte also discuss the case of approximate solutions of the auxiliary problems. They consider the scheme

Find $x^{k+1} \in K$ with
$\left\langle \mathcal{F}(x^k) + \chi(\nabla h(x^{k+1}) - \nabla h(x^k)), x - x^{k+1} \right\rangle \geq -\rho_k \quad \forall x \in K',$

where $\rho_k > 0$ and K' is a bounded set. If K itself is bounded one can set $K' = K$. Otherwise, one defines $K' = K \cap \{x : \| x \| \leq R\}$, where R is a suitable large constant. In [93, Theorem 3.5] convergence is proved under the error conditions

$$\rho_k \geq 0, \ \forall k \in \mathbb{N}_0, \quad \sum_{k=0}^{\infty} \rho_k < \infty.$$

An extension to nonsymmetric auxiliary operators is presented by Zhu/Marcotte [93, Section 4]. They consider a scheme as in Algorithm 2.2 with $\chi_k = \chi$ and

$$\Omega^k = \chi^{-1}\mathcal{L} + \nabla h \quad \forall k \in \mathbb{N}_0, \tag{2.3}$$

where $\mathcal{L} : \mathbb{R}^n \to \mathbb{R}^n$ is a continuous, monotone operator and $h : \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable, convex function. In [93, Theorem 4.1] they prove the convergence of the sequence $\{x^k\}$ to a solution of $\mathrm{VI}(\mathcal{F}, K)$ under the following assumptions:

Conditions (APP, case: $\Omega^k = \chi^{-1}\mathcal{L} + \nabla h$): *(see Zhu/Marcotte [93])*

(1) $K \subset \mathbb{R}^n$ *closed, convex,* $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ *continuous, monotone,* $\mathrm{VI}(\mathcal{F}, K)$ *solvable*

(2) $\mathcal{F} - \mathcal{L}$ *is co-coercive with modulus* γ*,*

(3) $\mathcal{L}$ *is continuous and monotone,*

(4) ∇h *is strongly monotone with modulus* β *and Lipschitz continuous with constant* L_h*,*

(5) $\frac{1}{2\beta\gamma} < \chi < +\infty$.

Note that for a given auxiliary operator Ω that is strongly monotone with modulus β, a decomposition like in (2.3) can be obtained in a natural way by setting $h(x) = (\beta/2) \| x \|^2$ and $\mathcal{L}(x) = \chi(\Omega(x) - \beta x)$.

So far only schemes with fixed auxiliary operator Ω and fixed parameter χ where described. The possibility that the auxiliary operator can change at each iteration makes the method more flexible with regard to special applications. Salmon/Nguyen/Strodiot [84] introduce a variant of the auxiliary problem principle that covers the use of nonsymmetric auxiliary operators of the type

$$\Omega^k = \chi_k^{-1}\mathcal{L}^k + \nabla h, \tag{2.4}$$

where $\mathcal{L}^k : \mathbb{R}^n \to \mathbb{R}^n$ is continuous and monotone and $h : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and convex. In most applications $\mathcal{L}^k$ depends explicitly on the iterate x^k. Therefore, to describe the operators $\mathcal{L}^k$, one uses a family of operators $\mathcal{L}_y$ parameterized by $y \in K$ and defines $\mathcal{L}^k = \mathcal{L}_{y|y=x^k}$. The proof of [84, Theorem 2.1] implies that the

iterates of Algorithm 2.2 with Ω^k as in (2.4) converge to a solution of $\mathrm{VI}(\mathcal{F}, K)$ if the following conditions are valid:

Conditions (APP, case: $\Omega^k = \chi_k^{-1}\mathcal{L}^k + \nabla h$): *(see Salmon/Nguyen/Strodiot [84])*

(1) $K \subset \mathbb{R}^n$ *closed, convex,* $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ *continuous, monotone,* $\mathrm{VI}(\mathcal{F}, K)$ *solvable,*

(2) $\mathcal{F} - \mathcal{L}_y$ *fulfills the weakened co-coercivity condition that there exists* $\gamma > 0$ *with*

$$\langle \mathcal{F}(y) - \mathcal{L}_y(y) + \mathcal{L}_y(x), y - x\rangle \geq \gamma \parallel \mathcal{F}(y) - \mathcal{L}_y(y) - \mathcal{F}(x) + \mathcal{L}_y(x) \parallel^2$$

for all $x, y \in \mathbb{R}^n$ *with* $\langle \mathcal{F}(x), y - x\rangle \geq 0$,

(3) $\{\mathcal{L}_y\}$ *is a family of monotone and uniformly Lipschitz continuous operators,*

(4) ∇h *is strongly monotone with modulus* β *and Lipschitz continuous with constant* L_h,

(5) $\frac{1}{2\beta\gamma} < \underline{\chi} \leq \chi_k \leq \chi_{k+1} \leq \overline{\chi} < +\infty$, $\forall k \in \mathbb{N}_0$.

Summarizing the preceding aspects one can say that the convergence results for the auxiliary problem principle are of two types if the operator of the given variational inequality is single-valued and nonsymmetric. On the one hand, if the auxiliary operators are symmetric then $\mathcal{F}$ is required to be strongly monotone or to have the (pseudo) Dunn property. On the other hand, if the auxiliary operators are nonsymmetric then the operator $\mathcal{F}$ and the sequence Ω^k have to be linked by some kind of co-coercivity condition. Further, the sequence of parameters $\{\chi_k\}$ is supposed to be bounded (or constant) and strict greater than some number that depends on the strong monotonicity and co-coercivity moduli. In each case the conditions ensure that the auxiliary operators are maximal monotone and strongly monotone such that the auxiliary problems are uniquely solvable.

Multi-valued case. We briefly consider the case that the given operator of the variational inequality is multi-valued, i.e., $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{F} = 0$. Then, the auxiliary problems in Algorithm 2.2 have to be modified by taking one element $q(x^k) \in \mathcal{Q}(x^k)$ instead of $\mathcal{F}(x^k)$. In this case the auxiliary operators are generally taken to be symmetric. In [19], Cohen assumes that $\mathcal{Q}$ is strongly monotone and fulfills a growth condition to prove convergence. Concerning the sequence $\{\chi_k\}$ it is required that

$$\chi_k > 0, \ \forall k \in \mathbb{N}_0, \quad \sum_{k=0}^{\infty} \frac{1}{\chi_k} = +\infty, \quad \sum_{k=0}^{\infty} \frac{1}{\chi_k^2} < +\infty,$$

which implies that the sequence increases with k but not too fast. This is a typical requirement for the step sizes $\lambda_k = 1/\chi_k$ of a subgradient method (see [76, Chapter 5]).

Included methods. The second advantage of the APP scheme is that with special choices of the auxiliary operators well-known descent methods are covered. As examples we present the gradient and the Newton method for the minimization of a sufficiently smooth, convex function $\psi : \mathbb{R}^n \to \mathbb{R}$.

- Gradient method: With $\mathcal{F} = \nabla\psi$, $\Omega^k = I$ and $K = \mathbb{R}^n$ the auxiliary problem in Algorithm 2.2 is equivalent to finding $x^{k+1} \in \mathbb{R}^n$ with

$$\left\langle \nabla\psi(x^k) + \chi_k(x^{k+1} - x^k), x - x^{k+1} \right\rangle \geq 0 \quad \forall x \in \mathbb{R}^n,$$

  which results in the calculation of x^{k+1} as

$$x^{k+1} = x^k - \frac{1}{\chi_k}\nabla\psi(x^k).$$

  Note, if $K \subsetneqq \mathbb{R}^n$ the scheme yields the gradient projection method.

- Newton method: Choosing $\mathcal{F} = \nabla\psi$, $\Omega^k(x) = \nabla^2\psi(x^k)x$, and $K = \mathbb{R}^n$ the auxiliary problem

$$\left\langle \nabla\psi(x^k) + \chi_k(\nabla^2\psi(x^k)x^{k+1} - \nabla^2\psi(x^k)x^k), x - x^{k+1} \right\rangle \geq 0 \quad \forall x \in \mathbb{R}^n$$

  is obtained, which is equivalent to

$$x^{k+1} = x^k - [\nabla^2\psi(x^k)]^{-1}\nabla\psi(x^k).$$

For the gradient method the auxiliary operator is chosen independently of $\mathcal{F}$, whereas $\mathcal{F}(x)$ is linearly approximated by $\nabla\mathcal{F}(x^k)x$ to retrieve the Newton method. Other linear approximation methods are given by

$$\Omega^k(x) = D(x^k)x \quad \forall k \in \mathbb{N}_0,\ \forall x \in \mathbb{R}^n,$$

where $D(x^k) \in \mathbb{R}^{n\times n}$ is a not necessarily symmetric, positive definite matrix that depends on x^k. This establishes auxiliary problems of the form

$$\begin{aligned} &\text{Find } x^{k+1} \in K \text{ with} \\ &\left\langle \mathcal{F}(x^k) + \chi_k D(x^k)(x^{k+1} - x^k), x - x^{k+1} \right\rangle \geq 0 \quad \forall x \in K, \end{aligned}$$

and for example the following methods are included:

- Projection method: $D(x^k) = B$, where B is a symmetric, positive definite matrix,
- Quasi Newton method: $D(x^k) \approx \nabla\mathcal{F}(x^k)$,
- Jacobi method: $D(x^k) = \operatorname{diag}(\nabla\mathcal{F}(x^k))$,

- Successive over-relaxation (SOR): $D(x^k) = l(\nabla\mathcal{F}(x^k)) + \frac{1}{\omega}\mathrm{diag}(\nabla\mathcal{F}(x^k))$,

where $\mathcal{F}$ is supposed to be continuously differentiable (if necessary), $\mathrm{diag}(B)$ is the diagonal part of B, $l(B)$ denotes the lower triangular part of B, and $\omega \in (0, 2)$. We refer to [74] for more details.

Besides the mentioned descent methods, also the proximal point method for a single-valued operator is included in the APP scheme by taking $\Omega^k = \chi_k^{-1}\mathcal{L} + \nabla h$ with $h(x) = \frac{1}{2} \parallel x \parallel^2$ and $\mathcal{L}(x) = \mathcal{F}(x)$. Then, the corresponding convergence conditions reduce to requiring that $\mathcal{F}$ is monotone and continuous (thus maximal monotone) and $\{\chi_k\}$ is a bounded sequence.

Decomposition. Since the operator $\mathcal{F}$ of the given variational inequality appears only as a fixed value $\mathcal{F}(x^k)$ in the auxiliary problems, it is possible to build up decomposition algorithms with the APP scheme. Parallel decomposition can be achieved if the restriction set K is the product of N sets K_j, $j = 1, \ldots, N$, and an additive auxiliary operator

$$\Omega^k(x) = \sum_{j=1}^{N} \Omega_j^k(x_j), \quad x_j \in K_j$$

is chosen. Then, the auxiliary problems in step 3 of Algorithm 2.2 can be splitted up into N independent variational inequalities. We do not intend to go further into detail here and refer to [16] and [17], where such kinds of algorithms are studied.

2.3.3 Proximal auxiliary problem (PAP) method

The solution methods PPA and APP both have their advantages: The PPA only requires monotonicity of the given operator, whereas in the APP the operator has to possess some monotonicity reserve (e.g., be strongly monotone). On the other hand, the auxiliary problems of the APP can be solved as optimization problems even if the given operator is not symmetric, whereas the structure of the auxiliary problems in the PPA is the same as in the original problem. Furthermore, with special choices of the auxiliary operator, the APP scheme leads to well-known descent methods such as the Newton method, and existing solution software can be used. Both methods regularize the given problem by generating uniquely solvable auxiliary problems. Moreover, there exist convergence proofs for the inexact versions under certain error summability criteria.

It is obviously worthwhile to establish a method that combines the positive properties of the PPA and the APP. In [48], Kaplan/Tichatschke investigate the so-called proximal auxiliary problem method, which is especially interesting if the given operator of the variational inequality can be splitted into $\mathcal{F} + \mathcal{Q}$ as described in $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$. They

propose an iterative scheme where $\mathcal{F}$ is fixed in the current iterate x^k like in the APP and $\mathcal{Q}$ is considered in the unknown next iterate x^{k+1} as in the PPA. Further, auxiliary operators of the type $\mathcal{L}^k + \chi_k \nabla h$ are used like in (2.4). The PAP method can be seen as an extension of the APP or a combination of PPA and APP. Its basic form is described in Algorithm 2.3.

Algorithm 2.3: Proximal auxiliary problem method (PAP)

---

1. *(Initialization)* Choose an initial point $x^0 \in K$, an auxiliary operator $\mathcal{L}^0$, a parameter $\chi_0 > 0$, and an error parameter $\delta_k \geq 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ then stop.
3. *(Auxiliary problem)* Find $x^{k+1} \in K$ and $q(x^{k+1}) \in \mathcal{Q}(x^{k+1})$ such that

$$\begin{aligned}&\left\langle \mathcal{F}(x^k) + q(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k(\nabla h(x^{k+1}) - \nabla h(x^k)), x - x^{k+1} \right\rangle \\ &\geq -\delta_k \parallel x - x^{k+1} \parallel \quad \forall x \in K.\end{aligned}$$

4. *(Update)* Choose a new auxiliary operator $\mathcal{L}^{k+1}$ and new parameters $\chi_{k+1} > 0$, $\delta_{k+1} \geq 0$. Set $k := k + 1$ and go to step 2.

The splitting in $\mathcal{F} + \mathcal{Q}$ is flexible, even one of the operators can be zero. For example, operator $\mathcal{F}$ can describe single-valued (nonsymmetric) operators that have a certain monotonicity reserve. Other (multi-valued) operators without monotonicity reserve can be included into $\mathcal{Q}$. More details are presented in Chapter 5.

The PAP method includes the APP as a special case if $\mathcal{Q} = 0$ and $\Omega^k = \chi_k^{-1}\mathcal{L}^k + \nabla h$. The PPA is covered as well with the choice $\mathcal{F} = 0$, $\mathcal{L} = 0$, and $h = \frac{1}{2} \parallel \cdot \parallel^2$.

Kaplan/Tichatschke describe in [49] and [51] different extensions of the basic form of the PAP method in a Hilbert space, which include approximations of the operator $\mathcal{Q}$ and the set K. It can be extracted from [51, Theorem 3.1] that the following conditions are needed for the convergence of the basic form described in Algorithm 2.3:

Conditions (PAP): *(see Kaplan/Tichatschke [51])*

(1) General conditions on the data $\mathcal{F}, \mathcal{Q}, K$:
$K \subset \mathbb{R}^n$ *closed, convex,* $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ *maximal monotone,* $\mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K) \neq \emptyset$, $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ *single-valued, continuous,* $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ *solvable.*

(2) Special conditions on $\mathcal{F}$, $\mathcal{Q}$, $\{\mathcal{L}_y\}$, and h:

(a) The operator

$$\mathcal{Q}_K : y \mapsto \begin{cases} \mathcal{Q}(y) & \text{if } y \in K \\ \emptyset & \text{otherwise} \end{cases}$$

is locally hemi-bounded at each point of $\mathrm{dom}(\mathcal{Q}) \cap K$,

(b) $\{\mathcal{L}_y\}$ *is a family of monotone and Lipschitz continuous operators with a common Lipschitz constant* L,

(c) $\mathcal{F} - \mathcal{L}_y$ *fulfills the condition that there exists* $\gamma > 0$ *with*

$$\begin{aligned} &\langle \mathcal{F}(y) - \mathcal{L}_y(y) + \mathcal{L}_y(x) + q(x), y - x \rangle \\ &\geq \gamma \parallel \mathcal{F}(y) - \mathcal{L}_y(y) - \mathcal{F}(x) + \mathcal{L}_y(x) \parallel^2 \end{aligned} \tag{2.5}$$

forall $x, y \in \mathbb{R}^n$ *and* $q(x) \in \mathcal{Q}(x)$ *with* $\langle \mathcal{F}(x) + q(x), y - x \rangle \geq 0$,

(d) h *is convex and* ∇h *is Lipschitz continuous with constant* L_h,

(e) for a given linear, continuous, and monotone operator $\mathcal{B} : \mathbb{R}^n \to \mathbb{R}^n$ *that has the symmetry property* $\langle \mathcal{B}x, y \rangle = \langle \mathcal{B}y, x \rangle$ *it holds*

$$\langle q(x) - q(y), x - y \rangle \geq \langle \mathcal{B}(x - y), x - y \rangle$$

for all $x, y \in \mathrm{dom}(\mathcal{Q}) \cap K$, *for all* $q(x) \in \mathcal{Q}(x), q(y) \in \mathcal{Q}(y)$,

(f) for given constants $\tilde{\chi} > 0$, $\kappa > 0$ *the inequality*

$$\frac{1}{2}\tilde{\chi} \langle \mathcal{B}(x - y), x - y \rangle + h(x) - h(y) - \langle \nabla h(y), x - y \rangle \geq \kappa \parallel x - y \parallel^2$$

is valid for all $x, y \in K$.

(3) Conditions on the sequences $\{\chi_k\}$ *and* $\{\delta_k\}$*:*

(a) $0 < \underline{\chi} \leq \chi_k \leq \chi_{k+1} \leq \overline{\chi} < +\infty$, $\forall k \in \mathbb{N}_0$,

(b) $\frac{1}{4\gamma\kappa} < \underline{\chi}$, $2\tilde{\chi}\overline{\chi} < 1$,

(c) $\sum_{k=0}^{\infty} \delta_k < \infty$.

We close this section with some comments on the Conditions (PAP).

Local hemi-boundedness of $\mathcal{Q}_K$ is needed to provide the following implication with a fixed $\bar{x} \in \mathrm{dom}(\mathcal{Q}) \cap K$: If for all $x \in \mathrm{dom}(\mathcal{Q}) \cap K$ there exists $q(x) \in \mathcal{Q}(x)$ with $\langle \mathcal{F}(\bar{x}) + q(x), x - \bar{x} \rangle \geq 0$ then $\bar{x}$ is a solution of $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$. This is needed to show that each limit point of the sequence $\{x^k\}$ is a solution of $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$.

Condition (2.5) on the operators $\mathcal{F} - \mathcal{L}_y$ is certainly fulfilled if they are co-coercive with a common modulus $\gamma > 0$. In [51] an example is presented where (2.5) is fulfilled but

the considered operator is not co-coercive. It is also interesting to note that condition (2.5) does not force the operator $\mathcal{F}$ to be monotone. Thus, the given operator $\mathcal{F} + \mathcal{Q}$ does not necessarily have to be monotone as distinct to the PPA and the APP scheme.

Compared to the APP scheme, the standard assumption on the strong convexity of the auxiliary function h is weakened by exploiting some monotonicity reserve of the operator $\mathcal{Q}$. If $\mathcal{Q}$ is strongly monotone then $\mathcal{B}$ can be taken as the identity operator, which implies that h only has to be convex. The other extreme is to have $\mathcal{B} = 0$ and $\mathcal{Q}$ only monotone. Then h must be strongly convex.

Finally, ill-posed problems can be handled with the PAP scheme because the convergence conditions allow that the solution set of $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ is unbounded. Moreover, in comparison to the inexact scheme of the APP described by Zhu/Marcotte, the restriction set K does not have to be compact because the error term $-\delta_k \parallel x - x^{k+1} \parallel$ allows K to be unbounded.

2.4 Extensions of the basic solution algorithms

There are different extensions of the basic methods introduced in the last years to solve variational inequalities or variants of this problem formulation. A selection of works is [6, 8, 9, 14, 28, 88] for proximal-like methods, [32, 51, 52, 75] for auxiliary problem principle based methods.

Of special interest in this work are extensions that have the aim to simplify the numerical realization of the auxiliary problems. Besides the possibility of inexact solutions of the auxiliary problems, there are two further aspects that are currently focused on in the literature. On the one hand, nonquadratic distances are investigated that establish an interior point effect by forcing the iterates to stay strictly feasible. On the other hand, the given multi-valued operator is approximated from outside such that an evaluation of this operator does not have to be done exactly. This results in the discussion of so-called enlargements of operators. Both techniques - interior point idea and enlargements - will be presented in this section.

2.4.1 Bregman function based PPA and PAP

Motivation of Bregman functions. Algorithms based on Bregman functions were investigated as extensions of the basic solution algorithms with the idea to get unrestricted auxiliary problems by means of an interior point effect. In this context, it is generally assumed that $\mathrm{int}(K) \neq \emptyset$.

For a motivation we reformulate the PAP scheme of Algorithm 2.3 in a more general setting with auxiliary problems of the form

$$\begin{aligned}&\text{Find } x^{k+1} \in K \text{ and } q(x^{k+1}) \in \mathcal{Q}(x^{k+1}) \text{ such that}\\&\left\langle \mathcal{F}(x^k) + q(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k \nabla_I D_h(x^{k+1}, x^k), x - x^{k+1} \right\rangle \\&\geq -\delta_k \parallel x - x^{k+1} \parallel \quad \forall x \in K.\end{aligned} \tag{2.6}$$

Here, $D_h : K \times \text{int}(K) \to \mathbb{R}$ is a nonquadratic function defined as

$$D_h(x, y) = h(x) - h(y) - \langle \nabla h(y), x - y \rangle \tag{2.7}$$

and $h : \mathbb{R}^n \to \mathbb{R}$ is (at least) strictly convex and continuous on K and continuously differentiable on $\text{int}(K)$. Then

$$\nabla_I D_h(x, y) = \nabla h(x) - \nabla h(y)$$

is the gradient of D_h with respect to the first vector argument. For every strictly convex function h it is further obvious that $D_h(x, y) \geq 0$, and that $D_h(x, y) = 0$ if and only if $x = y$. The source of definition (2.7) becomes clear if $h = \frac{1}{2} \parallel \cdot \parallel^2$. Then it is easy to see that

$$D_{\frac{1}{2}\|\cdot\|^2}(x, y) = \frac{1}{2} \parallel x - y \parallel^2,$$

which is the standard quadratic distance function. However, in contrast to the squared Euclidean distance, D_h is in general not symmetric and does not obey the triangle inequality. For that reason, it is called a generalized distance or distance-like function. Geometrically, $D_h(x, y)$ is the difference between $h(x)$ and the value at x of the linear approximation of h at y as illustrated in Figure 2.1.

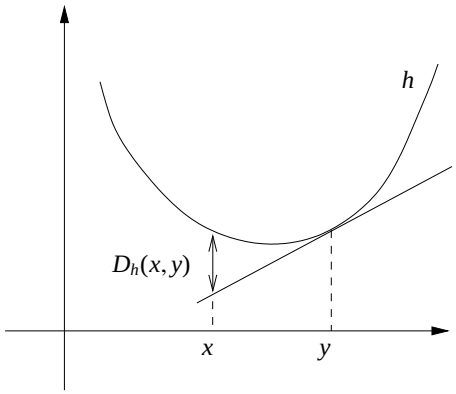

Figure 2.1. Generalized distance D_h.

The idea is to impose additional properties on h such that the distance function D_h acts as a barrier at the boundary of K and forces the sequence $\{x^k\}$ of iterates (with

$x^0 \in \text{int}(K)$) to remain in the interior of K. Further, unique solvability of the auxiliary problems should be guaranteed. These goals can be achieved for example by Bregman functions, a notion that goes back to Bregman [7].

Definition of Bregman functions. The following definition of a Bregman function is given in [87] and is seen to be minimal relative to the different definitions used in literature.

Let $K \subset \mathbb{R}^n$ be a closed, convex set with $\text{int}(K) \neq \emptyset$. A function $h : K \to \mathbb{R}$ is a Bregman function with zone $\text{int}(K)$ if

(B1) h is strictly convex and continuous on K,

(B2) h is continuously differentiable on $\text{int}(K)$,

(B3) for all $x \in K$ and all constants $\eta \in \mathbb{R}$ the set

$$L(x, \eta) = \{y \in \text{int}(K) : D_h(x, y) \leq \eta\}$$

is bounded,

(B4) for a sequence $\{x^k\} \subset \text{int}(K)$ converging to x it holds

$$\lim_{k\to\infty} D_h(x, x^k) = 0.$$

If h is a Bregman function then D_h is called a Bregman distance.

Solodov/Svaiter showed in [87, Theorem 2.4] that the so-called convergence consistence property, i.e.,

(B5) if $\{x^k\} \subset K$ and $\{y^k\} \subset \text{int}(K)$ are sequences such that $\{x^k\}$ is bounded, $\lim_{k\to\infty} y^k = \bar{y}$, and $\lim_{k\to\infty} D_h(x^k, y^k) = 0$ then $\lim_{k\to\infty} x^k = \bar{y}$,

is a consequence of (B1) and (B2).

If in addition to (B1)–(B4) h also satisfies the following condition

(B6) $\nabla h(\text{int}(K)) = \mathbb{R}^n$, i.e., $\forall y \in \mathbb{R}^n \; \exists x \in \text{int}(K) : \nabla h(x) = y$,

then h is a so-called zone coercive (or full-range) Bregman function. Further, a Bregman function h is said to be boundary coercive if

(B7) for every sequence $\{y^k\} \subset \text{int}(K)$ it holds: if $\lim_{k\to\infty} y^k = \bar{y} \in \text{bd}(K)$ then $\left\langle \nabla h(y^k), x - y^k \right\rangle \to -\infty \; \forall x \in \text{int}(K)$.

It is proved in [14, Corollary 6] that zone coerciveness implies boundary coerciveness. Since boundary coerciveness implies divergence of ∇h on $\mathrm{bd}(K)$, this property links K and h by

$$\mathrm{dom}(\nabla h) = \mathrm{int}(K).$$

This also implies that the auxiliary problems cannot have solutions on the boundary of K – an interior point effect that leads to essentially unconstrained auxiliary problems.

Examples of Bregman functions. Examples of zone coercive Bregman functions for different polyhedral sets can be found, e.g., in [8, 14]. A selection of examples is

(a) $K = \mathbb{R}^n$, $h(x) = \frac{1}{2} \parallel x \parallel^2$, $D_h(x,y) = \frac{1}{2} \parallel x - y \parallel^2$,

(b) $K = \mathbb{R}^n_+$, $h(x) = \sum_{j=1}^n x_j \log x_j$ with the convention that $0 \log 0 = 0$, $D_h(x,y) = \sum_{j=1}^n \left(x_j \log \frac{x_j}{y_j} - x_j + y_j \right)$, which is the so-called Kullback-Leibler relative entropy distance functional [65].

(c) $K = [a_1, b_1] \times \cdots \times [a_n, b_n]$ with $a_j < b_j \ \forall j = 1, \ldots, n$,
$h(x) = \sum_{j=1}^n [(x_j - a_j) \log(x_j - a_j) + (b_j - x_j) \log(b_j - x_j)]$,
$D_h(x,y) = \sum_{j=1}^n \left[(x_j - a_j) \log \left(\frac{x_j - a_j}{y_j - a_j} \right) + (b_j - x_j) \log \left(\frac{b_j - x_j}{b_j - y_j} \right) \right]$,

(d) $K = \{x \in \mathbb{R}^n : Ax \leq b\}$ with $A \in \mathbb{R}^{p \times n}$, $p \geq n$, $\mathrm{rank}(A) = n$, $b \in \mathbb{R}^n$, $h(x) = \sum_{i=1}^p (b_i - \langle a_i, x \rangle) \log(b_i - \langle a_i, x \rangle)$, where a_i denotes the i-th row of A, $i = 1, \ldots, p$, $D_h(x,y) = \sum_{i=1}^p \left(l_i(x) \log \frac{l_i(x)}{l_i(y)} - l_i(x) + l_i(y) \right)$, $l_i(x) = b_i - \langle a_i, x \rangle$, $i = 1, \ldots, p$.

Bregman-*like* functions can be defined for nonpolyhedral sets as demonstrated in Kaplan/Tichatschke [55], where the concept of Bregman functions is modified by using a more general convergence sensing condition as in (B4).

Bregman-PPA. Eckstein [27] and Chen/Teboulle [15] were the first who introduced Bregman functions to extend the PPA. Further contributions include [8, 14, 28, 45, 87]. In [28], Eckstein considers inexact solutions of the auxiliary problems and gives appropriate error tolerance criteria. To solve $\mathrm{VI}(\mathcal{Q}, K)$ with a multi-valued, maximal monotone operator $\mathcal{Q}$, Algorithm 2.4 is used with h as a zone coercive Bregman function with zone $\mathrm{int}(K)$. As a consequence of the interior point effect, the auxiliary problems can be written as inclusion problems omitting the normal cone operator since $\mathcal{N}_K(x^{k+1}) = \{0\}$.

The convergence theorem [28, Theorem 1] for BrPPA requires the following conditions:

Algorithm 2.4: Inexact Bregman proximal point algorithm (BrPPA)

1. *(Initialization)* Choose an initial point $x^0 \in \text{int}(K)$, a parameter $\chi_0 > 0$, and an error parameter $\delta_0 \geq 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem $\text{VI}(\mathcal{Q}, K)$ then stop.
3. *(Auxiliary problem)* Find $x^{k+1} \in K$ and $e^{k+1} \in \mathbb{R}^n$ such that

$$e^{k+1} \in \mathcal{Q}(x^{k+1}) + \chi_k(\nabla h(x^{k+1}) - \nabla h(x^k))$$

   and $\| e^{k+1} \| \leq \delta_k$.
4. *(Update)* Choose new parameters $\chi_{k+1} > 0$ and $\delta_{k+1} \geq 0$. Set $k := k + 1$ and go to step 2.

Conditions (BrPPA): *(see Eckstein [28])*

(1) $K \subset \mathbb{R}^n$ *closed, convex,* $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ *maximal monotone,* $\text{dom}(\mathcal{Q}) \cap \text{int}(K) \neq \emptyset$, $\text{VI}(\mathcal{Q}, K)$ *solvable.*

(2) One of the following situations hold:

(a) $\text{int}(K) \supseteq \text{cl}(\text{dom}(\mathcal{Q}))$,

(b) $\mathcal{Q}$ *is the subdifferential of some proper, lower semicontinuous, convex function,*

(c) $\mathcal{Q}$ *is paramonotone, and if* $\{x^k\} \subset \text{int}(K)$, $y^k \in \mathcal{Q}(x^k)$, *and* $\{x^k\}$ *is convergent then* $\{y^k\}$ *has a limit point.*

(3) h *is a zone coercive Bregman function with zone* $\text{int}(K)$.

(4) For the sequences $\{\chi_k\}$, $\{\delta_k\}$, *and* $\{e^k\}$ *it holds:*

$$0 < \chi_k \leq \overline{\chi} < \infty, \forall k \in \mathbb{N}_0, \tag{2.8}$$

$$\sum_{k=0}^{\infty} \delta_k < \infty, \tag{2.9}$$

$$\sum_{k=1}^{\infty} \langle e^k, x^k \rangle \text{ exists and is finite.} \tag{2.10}$$

Paramonotonicity of $\mathcal{Q}$ is needed to exploit the following property (see [9, Proposition 10]): If $\mathcal{Q}$ is paramonotone and x^* is a solution of $\text{VI}(\mathcal{Q}, K)$, then $\bar{x}$ is also a solution of $\text{VI}(\mathcal{Q}, K)$ if and only if there exists $v \in \mathcal{Q}(\bar{x})$ such that $\langle v, x^* - \bar{x} \rangle \geq 0$.

The requirement on $\{\langle e^k, x^k \rangle\}$ to be summable turns out to be difficult to verify in practice because it involves the sequence of iterates, which is not known before using the algorithm. Only if for example K is bounded and therefore $\{x^k\}$ is a bounded sequence, this condition is automatically fulfilled as a consequence of (2.9).

In [54], Kaplan/Tichatschke prove convergence of the iterates of the BrPPA without condition (2.10) but under the assumption that the distance function fulfills a so-called cone condition:

(B8) For arbitrary $x \in K$ there exist constants $\alpha(x) > 0$ and $c(x) \in \mathbb{R}$ such that

$$D_h(x, y) + c(x) \geq \alpha(x) \parallel x - y \parallel \quad \forall y \in \text{int}(K).$$

In [54] it is shown that most of the known Bregman functions and so-called logarithmic-quadratic distance functions (see Section 2.4.2 below) fulfill the cone condition.

Bregman-PAP. The question arises if an interior point effect can be achieved not only in a proximal point method but also in the APP or PAP scheme by choosing h as a Bregman function. This is not immediately possible since in both schemes h must have a Lipschitz continuous gradient which is contradictory to the requested boundary coercivity of the Bregman functions. Also complications emerge because of the nondifferentiability of a Bregman function h on the boundary of K. Therefore, a modified analysis is needed. Kaplan/Tichatschke present in [52] a convergence analysis for Algorithm 2.5 where D_h is a Bregman distance.

Algorithm 2.5: Bregman proximal auxiliary problem (BrPAP) method

1. *(Initialization)* Choose an initial point $x^0 \in \text{int}(K)$, an auxiliary operator $\mathcal{L}^0$, a parameter $\chi_0 > 0$, and an error parameter $\delta_k \geq 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem VI$(\mathcal{F}, \mathcal{Q}, K)$ then stop.
3. *(Auxiliary problem)* Find $x^{k+1} \in K$ and $q(x^{k+1}) \in \mathcal{Q}(x^{k+1})$ such that

$$\begin{aligned} &\langle \mathcal{F}(x^k) + q(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k \nabla_I D_h(x^{k+1}, x^k), x - x^{k+1} \rangle \\ &\geq -\delta_k \parallel x - x^{k+1} \parallel \quad \forall x \in K. \end{aligned}$$

4. *(Update)* Choose a new auxiliary operator $\mathcal{L}^{k+1}$ and new parameters $\chi_{k+1} > 0$, $\delta_{k+1} \geq 0$. Set $k := k + 1$ and go to step 2.

Compared to the assumptions for the PAP scheme on pages 24–25 the following additional properties or modifications are needed:

Conditions (BrPAP): *(compared to Conditions (PAP), see Kaplan/Tichatschke [52])*

(1) Standard conditions on the data $\mathcal{F}, \mathcal{Q}, K$ as in (PAP)(1).

(2) Special conditions on $\mathcal{F}$, $\mathcal{Q}$, $\{\mathcal{L}_y\}$, and h:

- *Condition (PAP)(2)(a) is extended by requiring that one of the following assumptions is valid:*

  (a) $\operatorname{int}(K) \supseteq \operatorname{cl}(\operatorname{dom}(\mathcal{Q}))$, *and the operator*

$$\mathcal{Q}_K : y \mapsto \begin{cases} \mathcal{Q}(y) & \text{if } y \in K \\ \emptyset & \text{otherwise} \end{cases}$$

  is locally hemi-bounded at each point of $\operatorname{dom}(\mathcal{Q}) \cap K$,

  (b) $\mathcal{F} = \nabla\psi$, $\mathcal{Q} = \partial\varphi$, *where ψ is a convex, continuously differentiable function and $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is a proper, lower semicontinuous, convex function,*

  (c) $\mathcal{F} + \mathcal{Q}$ *is paramonotone, and the situation $\{x^k\} \in \operatorname{int}(K) \cap \operatorname{dom}(\mathcal{Q})$, $y^k \in \mathcal{Q}(x^k)$, $\lim_{k\to\infty} x^k = \bar{x}$ implies that $\{y^k\}$ is a bounded sequence.*

- *The uniform Lipschitz continuity of $\{\mathcal{L}_y\}$ in (PAP)(2)(b) is weakened by assuming that for any convergent sequence $\{y^k\} \subset \operatorname{int}(K)$ it holds*

$$\mathcal{L}_{y^k}(y^{k+1}) - \mathcal{L}_{y^k}(y^k) \to 0 \text{ as } k \to \infty.$$

- *The co-coercivity like condition on $\mathcal{F} - \mathcal{L}_y$ in (PAP)(2)(c) (with modulus γ) remains the same.*

- *Conditions (PAP)(2)(d), (PAP)(2)(e), and (PAP)(2)(f) are replaced by requiring that h is a* ***strongly*** *convex (with modulus κ) and zone coercive Bregman function with zone* $\operatorname{int}(K)$. *Note that for a strongly convex function h property (B3) is automatically fulfilled.*

(3) Conditions on the sequences $\{\chi_k\}$ and $\{\delta_k\}$:

(a) $0 < \underline{\chi} \le \chi_k \le \overline{\chi} < \infty$, $\forall k \in \mathbb{N}_0$, $\sum_{k=0}^{\infty} \max\{0, \chi_k - \chi_{k+1}\} < \infty$,

(b) $\underline{\chi} > \frac{1}{4\kappa\gamma}$,

(c) $\sum_{k=0}^{\infty} \delta_k < \infty$.

Paramonotonicity assumption. The assumption on $\mathcal{F}+\mathcal{Q}$ to be paramonotone restricts the usage of the PAP scheme with Bregman functions. Excluded are for example variational inequalities that characterize saddle points of Lagrangians associated with constrained convex programming problems. It is shown in [46] that the Lagrangian of a smooth convex programming problem is paramonotone only in special cases when, in fact, all constraints are not active. For saddle point problems Kaplan/Tichatschke [53] prove convergence of a Bregman function based proximal scheme under an additional strict complementarity condition, but without paramonotonicity.

Recently, Langenberg [61] established the convergence of a Bregman function based proximal-like method without a paramonotonicity assumption but requiring the weaker property that the operator is pseudomonotone* (see [23] for a definition). Paramonotone and pseudomonotone* operators are known to have the cutting plane property (see [64] for a definition and corresponding references). As discussed in [53, Remark 1.2] this property cannot be expected in the context of saddle-point problems of the Lagrangian of a convex optimization problem. For that reason, Langenberg [64] investigates the BrPPA without assuming the cutting plane property and shows that it is sufficient that the restriction set has some special nonlinear structure like a ball. Also for the PAP scheme as presented in [52], Langenberg [62] analyzes how the restrictive assumption of paramonotonicity can be weakened. He shows that in the case $\mathcal{Q}=\partial\varphi$ the assumption of paramonotonicity can be replaced by a quite natural hypothesis on $\mathcal{F}$ that in view of (2.5) holds true when $\mathcal{L}_y$ is co-coercive (which is the case for many commonly used symmetric $\mathcal{L}_y$). For bounded $\mathcal{Q}$ he describes how the assumption that $\mathcal{F}+\mathcal{Q}$ is paramonotone can be replaced by paramonotonicity of $\mathcal{Q}$ only.

2.4.2 Logarithmic-quadratic function based PPA

Following the interior point idea established by using nonquadratic distance functions in proximal point methods, Auslender/Teboulle/Ben-Tiba [4]–[6] investigate logarithmic-quadratic distance functions as alternatives to Bregman distances. Their aim is to describe an interior proximal method that is convergent to a solution of the given variational inequality under the only assumption that the set of solutions is nonempty. Thus, the restrictive assumption of paramonotonicity in Bregman based algorithms is avoided. But their concept only works for polyhedral restriction sets.

For that purpose, they consider $\mathrm{VI}(\mathcal{Q},K)$ with a multi-valued, maximal monotone operator $\mathcal{Q}$ and a polyhedral restriction set

$$K=\{x\in\mathbb{R}^n\colon Ax\le b\},\tag{2.11}$$

where $A\in\mathbb{R}^{p\times n}$, $p\ge n$, $\operatorname{rank}(A)=n$, $b\in\mathbb{R}^p$, and $\operatorname{int}(K):=\{x\in\mathbb{R}^n\colon Ax<b\}\neq\emptyset$. As a special case, the nonlinear complementarity problem is covered by choosing $K=\mathbb{R}^n_+$.

The condition on A to have full column rank is especially fulfilled if the variables have lower or upper bounds. For brevity, the notation

$$\begin{aligned} l_i(x) &= b_i - \langle a_i, x \rangle, \quad i = 1, \ldots, p, \\ l(x) &= (l_1(x), \ldots, l_p(x))^T = b - Ax \end{aligned}$$

is used, where a_i denotes the i-th row of A. Then $K = \{x \in \mathbb{R}^n : l(x) \geq 0\}$.

Logarithmic-quadratic distances. For parameters $\nu > \mu > 0$ a logarithmic-quadratic regularization term tailored for $K = \mathbb{R}^p_+$ is defined as

$$\begin{aligned} &d_{LQ}^{\nu,\mu} : \mathbb{R}^p \times \mathbb{R}^p_{++} \to \mathbb{R} \cup \{+\infty\}, \\ &d_{LQ}^{\nu,\mu}(u,v) := \begin{cases} \sum_{i=1}^p \frac{\nu}{2}(u_i - v_i)^2 + \mu \left(v_i^2 \log \frac{v_i}{u_i} + u_i v_i - v_i^2 \right) & \text{if } u \in \mathbb{R}^p_{++} \\ +\infty & \text{otherwise.} \end{cases} \end{aligned} \tag{2.12}$$

It is straightforward to show that for every $v \in \mathbb{R}^p_{++}$ function $d_{LQ}^{\nu,\mu}(\cdot, v)$ is a nonnegative, proper, lower semicontinuous, convex function with $\mathrm{dom}(d_{LQ}^{\nu,\mu}(\cdot, v)) = \mathbb{R}^p_{++}$, and that $d_{LQ}^{\nu,\mu}(u,v) = 0$ if and only if $u = v$ (see Appendix, Lemma A.3.1). However, no symmetry property and no triangle inequality are valid. Thus, $d_{LQ}^{\nu,\mu}$ is called a distance-*like* function. Obviously, for fixed $v \in \mathbb{R}^p_{++}$, $d_{LQ}^{\nu,\mu}(\cdot, v)$ is differentiable at any $u \in \mathbb{R}^p_{++}$.

To simplify the presentation we set

$$\nu = 2, \quad \mu = 1$$

and calculate that $d_{LQ}^{\nu,\mu}$ can be written as

$$d_{LQ}(u,v) := \begin{cases} \sum_{i=1}^p u_i^2 - u_i v_i - v_i^2 \log \frac{u_i}{v_i} & \text{if } u \in \mathbb{R}^p_{++} \\ +\infty & \text{otherwise.} \end{cases} \tag{2.13}$$

The logarithmic-quadratic distance function for a general polyhedral set K is given by

$$\begin{aligned} &D_{LQ} : \mathbb{R}^n \times \mathrm{int}(K) \to \mathbb{R} \cup \{+\infty\}, \\ &D_{LQ}(x,y) := d_{LQ}(l(x), l(y)). \end{aligned} \tag{2.14}$$

With $\partial_I D_{LQ}(\cdot, y)$ we denote the subdifferential with respect to the first vector argument. For $x \in \mathrm{int}(K)$ it holds that $l(x) \in \mathbb{R}^p_{++}$. Thus, for fixed $y \in \mathrm{int}(K)$, $D_{LQ}(\cdot, y)$ is differentiable at every $x \in \mathrm{int}(K)$. Therefore,

$$\partial_I D_{LQ}(x,y) = \{\nabla_I D_{LQ}(x,y)\} \quad \forall x \in \mathrm{int}(K),$$

where $\nabla_I D_{LQ}(x,y)$ denotes the partial gradient with respect to the first vector argument. For $x \in \mathrm{int}(K)$ and $y \in \mathrm{int}(K)$ the latter is obtained as

$$\nabla_I D_{LQ}(x,y) = -\sum_{i=1}^p a_i \left(2l_i(x) - l_i(y) - \frac{l_i(y)^2}{l_i(x)} \right). \tag{2.15}$$

Logarithmic-quadratic PPA. Logarithmic-quadratic distance functions are not Bregman function based because the mixed term $l_i(y)^2/l_i(x)$ in (2.15) contradicts a representation of the form $\nabla_I D_{LQ}(x,y) = \nabla h(x) - \nabla h(y)$ with a function h. Thus, the logarithmic-quadratic proximal point algorithm (LQPPA) presented in Algorithm 2.6 is different to the BrPPA in Algorithm 2.4.

Algorithm 2.6: Inexact logarithmic-quadratic proximal point algorithm (LQPPA)

1. *(Initialization)* Choose an initial point $x^0 \in \operatorname{int}(K)$, a parameter $\chi_0 > 0$, and an error parameter $\delta_0 \geq 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem $\mathrm{VI}(\mathcal{Q}, K)$ then stop.
3. *(Auxiliary problem)* Use D_{LQ} as defined in (2.14) and find $x^{k+1} \in K$ and $e^{k+1} \in \mathbb{R}^n$ such that

$$e^{k+1} \in \mathcal{Q}(x^{k+1}) + \chi_k \nabla_I D_{LQ}(x^{k+1}, x^k)$$

   and $\| e^{k+1} \| \leq \delta_k$.
4. *(Update)* Choose new parameters $\chi_{k+1} > 0$ and $\delta_{k+1} \geq 0$. Set $k := k+1$ and go to step 2.

In [6, Proposition 1] it is proved that the sequence $\{x^k\}$ of iterates generated by the LQPPA belongs to $\operatorname{int}(K)$. To show that $\{x^k\}$ converges to a solution of $\mathrm{VI}(\mathcal{Q}, K)$, Auslender/Teboulle/Ben-Tiba require in [6, Theorem 1] typical error criteria known from the BrPPA and a typical boundedness criterion for the sequence $\{\chi_k\}$. The overall conditions are:

Conditions (LQPPA): *(see Auslender/Teboulle/Ben-Tiba [6])*

(1) $K = \{x \in \mathbb{R}^n \colon Ax \leq b\}$, $A \in \mathbb{R}^{p \times n}$, $p \geq n$, $\operatorname{rank}(A) = n$, $b \in \mathbb{R}^p$, $\operatorname{int}(K) \neq \emptyset$, $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ *maximal monotone,* $\operatorname{dom}(\mathcal{Q}) \cap \operatorname{int}(K) \neq \emptyset$, $\mathrm{VI}(\mathcal{Q}, K)$ *solvable.*

(2) For the sequences $\{\chi_k\}$, $\{\delta_k\}$, *and* $\{e^k\}$ *it holds:*

$$0 < \chi_k \leq \overline{\chi} < \infty, \ \forall k \in \mathbb{N}_0, \tag{2.16}$$

$$\sum_{k=0}^{\infty} \frac{1}{\chi_k} \delta_k < \infty, \tag{2.17}$$

$$\sum_{k=1}^{\infty} \frac{1}{\chi_k} \left\langle e^k, x^k \right\rangle \ \textit{exists and is finite.} \tag{2.18}$$

Concerning condition (2.18) it was mentioned in the previous section that logarithmic-quadratic distance functions fulfill the cone condition (B6). This makes condition (2.18) redundant as shown in [54].

In comparison to the BrPPA no paramonotonicity assumption is needed for the convergence of the LQPPA. On the other hand, only variational inequalities with polyhedral restriction sets K can be solved. The reason is that others than linear restrictions $l(x)$ would not result in a convex distance function $D_{LQ}(\cdot, y)$ because of the term $l_i(y)^2 \log \frac{l_i(y)}{l_i(x)}$ in $D_{LQ}(l(x), l(y))$ (see (2.12)). An extension of the LQPPA to the case of polyhedral sets with additional unrestricted variables is presented in [6, Section 4]. The idea is to treat the unrestricted variables as in the usual quadratic proximal method. This extension is of particular interest if a convex constrained optimization problem is considered and the LQPPA is applied to the corresponding saddle point problem for the Lagrange function. This approach is further described in [5].

ϕ-divergences. For the sake of completeness we briefly present ϕ-divergences as a third type of nonquadratic distance functions providing an interior point effect. They are analyzed in [88] in the context of proximal-like algorithms for convex minimization problems or variational inequalities with restriction set $K = \mathbb{R}^p_+$. A ϕ-divergence is defined as

$$d_\phi(x, y) = \sum_{i=1}^{p} y_i \phi\left(\frac{x_i}{y_i}\right), \quad x, y \in \mathbb{R}^p_{++}, \tag{2.19}$$

where $\phi : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is a proper, lower semicontinuous, convex function with $\mathrm{dom}(\phi) \subseteq [0, +\infty)$ and with the following properties:

(i) ϕ is twice continuously differentiable on $\mathrm{int}(\mathrm{dom}(\phi))$,

(ii) ϕ is strictly convex on $\mathrm{dom}(\phi)$,

(iii) $\lim_{t \to 0^+} \phi'(t) = -\infty$,

(iv) $\phi(1) = \phi'(1) = 0$, and $\phi''(1) > 0$.

Properties (ii) and (iv) imply that $\phi(t) \geq 0$ for all t, and $\phi(t) = 0$ if and only if $t = 1$. Thus, d_ϕ is a distance-like function satisfying $d_\phi(x, y) \geq 0$, and $d_\phi(x, y) = 0$ if and only if $x = y$.

Except for the case that $\phi(t) = t \log t - t + 1$, where the ϕ-divergence coincides with the Kullback-Leibler relative entropy functional (see page 29), ϕ-divergences are not Bregman function based. This is due to the fact that the three-point-lemma [15, Lemma 3.1], which holds for Bregman distances, does not hold in general for d_ϕ.

A convergence result is established in [88, Theorem 5.1] for a ϕ-divergence based proximal method which solves VI($\mathcal{Q}, K$) with $K = \mathbb{R}^p_+$, but only ergodic convergence can be shown, i.e., every limit point of the averaged sequence of iterates is a solution.

Motivation of logarithmic-quadratic distances. In our work, ϕ-divergences will not be focused on. But it is interesting to see that the definition of logarithmic-quadratic distances can be given by a slight modification of (2.19): Defining for $v \in \mathbb{R}^p_{++}$

$$\tilde{d}_\phi(u, v) = \sum_{i=1}^{p} v_i^2 \phi\left(\frac{u_i}{v_i}\right) \tag{2.20}$$

and setting

$$\phi(t) = \begin{cases} \frac{\nu}{2}(t-1)^2 + \mu(t - \log t - 1) & \text{if } t > 0 \\ +\infty & \text{otherwise,} \end{cases} \tag{2.21}$$

we obtain the logarithmic-quadratic distance function (2.12). The motivation of taking in (2.20) a square in the second variable, which is the difference to (2.19), is to get a homogeneous function of second order (i.e., $\tilde{d}_\phi(\alpha x, \alpha y) = \alpha^2 \tilde{d}_\phi(x, y)$ for all $\alpha > 0$). This provides better convergence properties of corresponding interior proximal methods as presented in Auslender/Teboulle/Ben-Tiba [5]. In their work, distance functions of type (2.20) with different kernels ϕ fulfilling (i)–(iv) (on page 36) are analyzed in the context of convex optimization problems. We refer to [5, Section 7] for a source of logarithmic-quadratic distance functions and for a detailed study of the properties of the kernel (2.21). Rewriting (2.20) with (2.21) as

$$d_{LQ}(u, v) = \frac{\nu}{2} \parallel u - v \parallel^2 + \mu \sum_{i=1}^{p} v_i^2 \left(\frac{u_i}{v_i} - \log \frac{u_i}{v_i} - 1\right) \tag{2.22}$$

presents the motivation behind logarithmic-quadratic distance functions: The first term is the standard quadratic regularization term used in proximal methods. It is combined with a logarithmic term that builds up an interior point effect and forces the iterates to stay in the strict positive orthant $\mathbb{R}^p_{++}$. The parameters ν and μ provide the possibility to explicitly control the balance between the interior point effect versus the regularization effect.

2.4.3 Methods using enlargements of monotone operators

Definition and properties of the ϵ-enlargement. To solve the auxiliary problems in Algorithm 2.4 and Algorithm 2.6 numerically, we have to know the explicit structure

of the set $\mathcal{Q}(x)$ for every $x \in K$, since it is required to find $e^{k+1} \in \mathbb{R}^n$ and $x^{k+1} \in K$ with

$$e^{k+1} \in \mathcal{Q}(x^{k+1}) + \nabla_I D(x^{k+1}, x^k),$$

where D is either the Bregman distance D_h or the logarithmic-quadratic distance D_{LQ}. In order to avoid an exact calculation of $\mathcal{Q}(x)$, which is only possible in special cases, a concept is needed that allows us to approximate $\mathcal{Q}(x)$ for every $x \in \mathrm{dom}(\mathcal{Q})$ by a set with manageable structure.

A motivation comes from the field of convex optimization, where the usage of the ϵ-subdifferential is a well-known concept.

ϵ-subdifferential. Let $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a proper, convex function and $\epsilon \geq 0$. The ϵ-subdifferential of φ in a point $x \in \mathrm{dom}(\varphi)$ is defined as

$$\partial_\epsilon \varphi(x) = \{s \in \mathbb{R}^n : \varphi(y) - \varphi(x) - \langle s, y - x\rangle \geq -\epsilon \quad \forall y \in \mathbb{R}^n\}.$$

Obviously, the inclusion

$$\partial\varphi(x) \subseteq \partial_\epsilon \varphi(x) \quad \forall \epsilon \geq 0,\ \forall x \in \mathrm{dom}(\partial\varphi)$$

is valid. It shows that the ϵ-subdifferential is an outer approximation for $\partial\varphi$ in every point of its domain. If $\partial\varphi$ is replaced by $\partial_\epsilon\varphi$ in an algorithm, the convergence properties of the method are preserved if ϵ is chosen adequately (see [58]). Further, such methods get more robust since exact computations are not possible in numerical tests. Some properties of the subdifferential respectively ϵ-subdifferential are given in Appendix A.1.

ϵ-enlargement. Analogously, an outer approximation of a monotone operator can be introduced. Recall that an operator $\mathcal{Q}$ is monotone if and only if $\langle u - v, x - y\rangle \geq 0$ for all $x, y \in \mathbb{R}^n$, and all $u \in \mathcal{Q}(x)$, $v \in \mathcal{Q}(y)$. For a monotone operator $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ and $\epsilon \geq 0$ the ϵ-enlargement of $\mathcal{Q}$ is defined as

$$\mathcal{Q}_\epsilon : \mathbb{R}^n \to 2^{\mathbb{R}^n},\ \mathcal{Q}_\epsilon(x) = \{u \in \mathbb{R}^n : \langle u - v, x - y\rangle \geq -\epsilon \quad \forall (y, v) \in \mathrm{gph}(\mathcal{Q})\}.$$

The following theorem contains some of the main properties of the ϵ-enlargement.

Theorem 2.4.1 ([9], Propositions 1, 2, and 5). *Let $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ be monotone. Then the following statements are valid:*

(a) $\mathcal{Q}_{\epsilon_1}(x) \subset \mathcal{Q}_{\epsilon_2}(x)$ *for all* $0 \leq \epsilon_1 \leq \epsilon_2$ *and all* $x \in \mathbb{R}^n$.

(b) $\mathcal{Q}_{\epsilon_1}(x) + \mathcal{G}_{\epsilon_2}(x) \subset (\mathcal{Q} + \mathcal{G})_{\epsilon_1+\epsilon_2}(x)$ *for all* $\epsilon_1, \epsilon_2 \geq 0$, $x \in \mathbb{R}^n$, $\mathcal{G} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ *monotone.*

(c) $\mathcal{Q}_\epsilon(x)$ *is convex and closed for all* $\epsilon \geq 0$ *and all* $x \in \mathbb{R}^n$.

(d) If $\epsilon_k \to \bar{\epsilon}$, $\bar{\epsilon} \geq 0$, $x^k \to \bar{x}$, $u^k \to \bar{u}$, *with* $u^k \in \mathcal{Q}_{\epsilon_k}(x^k)$ *for all* $k \in \mathbb{N}$, *then* $\bar{u} \in \mathcal{Q}_{\bar{\epsilon}}(\bar{x})$.

If additionally $\mathcal{Q}$ *is maximal monotone, it holds:*

(e) $\mathcal{Q}_0(x) = \mathcal{Q}(x)$, *thus, in view of (a),* $\mathcal{Q}(x) \subset \mathcal{Q}_\epsilon(x)$ *for all* $\epsilon \geq 0$ *and all* $x \in \mathbb{R}^n$.

(f) If $\mathrm{dom}(\mathcal{Q})$ *is closed then* $\mathrm{dom}(\mathcal{Q}) = \mathrm{dom}(\mathcal{Q}_\epsilon)$ *for all* $\epsilon \geq 0$.

(g) If $\mathrm{dom}(\mathcal{Q})$ *is closed then, for all* $\epsilon \geq 0$, $\mathcal{Q}_\epsilon$ *is bounded on bounded sets.*

In the special case $\mathcal{Q} = \partial\varphi$, where $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is a proper, lower semicontinuous, convex function, $\partial_\epsilon\varphi$ and $(\partial\varphi)_\epsilon$ are related as described in the following two lemmata.

Lemma 2.4.2 ([9], Proposition 3). *Let* $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ *be a proper, lower semicontinuous, convex function. For all* $\epsilon \geq 0$ *it holds*

$$\partial_\epsilon\varphi(x) \subset (\partial\varphi)_\epsilon(x) \quad \forall x \in \mathbb{R}^n.$$

Lemma 2.4.3 ([50], Lemma A.2). *Let* $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ *be a proper, lower semicontinuous, convex function. If* φ *is positive homogen, i.e.,* $\varphi(\lambda x) = \lambda\varphi(x)$ *for all* $\lambda \geq 0$, *then*

$$\partial_\epsilon\varphi(x) = (\partial\varphi)_\epsilon(x) \quad \forall x \in \mathbb{R}^n,\ \forall \epsilon \geq 0.$$

We give an example (see [9, Example 1]) that the equality $\partial_\epsilon\varphi(x) = (\partial\varphi)_\epsilon(x)$ does not hold in general. Consider $\varphi : \mathbb{R} \to \mathbb{R}$, $\varphi(x) = \frac{1}{2}x^2$. It holds

$$\partial_\epsilon\varphi(x) = [x - \sqrt{2\epsilon}, x + \sqrt{2\epsilon}], \quad (\partial\varphi)_\epsilon(x) = [x - 2\sqrt{\epsilon}, x + 2\sqrt{\epsilon}] \quad \forall x \in \mathbb{R}^n$$

and thus $(\partial\varphi)_\epsilon(x) = \partial_{2\epsilon}\varphi(x)$ for all $x \in \mathbb{R}^n$. In Figure 2.2 the corresponding graphs of the subdifferential, the ϵ-subdifferential, and the ϵ-enlargement are presented. On the other hand, $\varphi : \mathbb{R} \to \mathbb{R}$, $\varphi(x) = |x|$ is positive homogen, and we get as a consequence of Lemma 2.4.3

$$\partial_\epsilon\varphi(x) = (\partial\varphi)_\epsilon(x) = \begin{cases} [-1, -1 - \frac{\epsilon}{x}] & \text{if } x < -\frac{\epsilon}{2} \\ [-1, 1] & \text{if } |x| \leq \frac{\epsilon}{2} \\ [1 - \frac{\epsilon}{x}, 1] & \text{if } x > \frac{\epsilon}{2}. \end{cases}$$

Figure 2.3 illustrates the corresponding graphs.

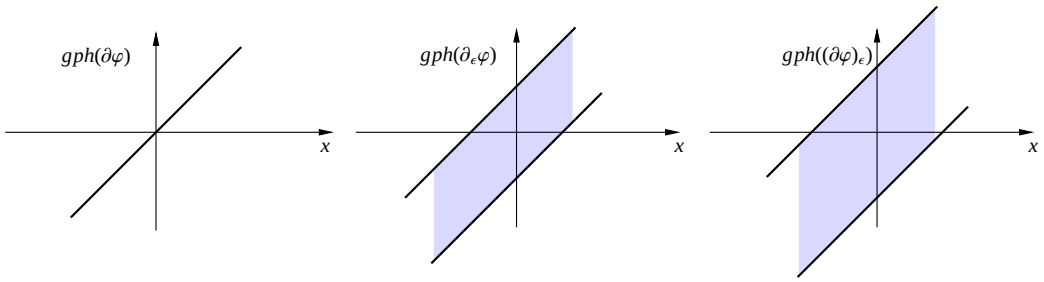

Figure 2.2. Subdifferential, ϵ-subdifferential, and ϵ-enlargement of $\varphi(x) = \frac{1}{2}x^2$.

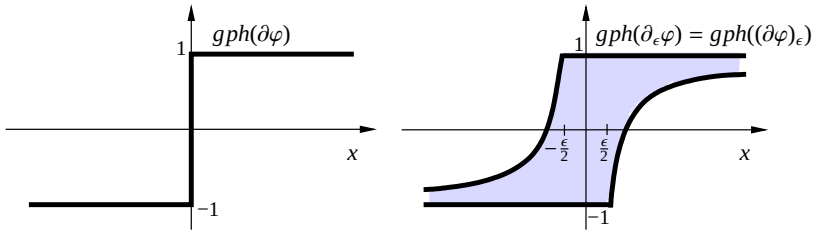

Figure 2.3. Subdifferential and ϵ-subdifferential/ϵ-enlargement of $\varphi(x) = |x|$.

BrPPA using enlargements. Enlargements of monotone operators were introduced by Burachik/Iusem/Svaiter [9] and applied in a Bregman function based proximal point method which is presented in Algorithm 2.7.

Algorithm 2.7: Bregman proximal point algorithm using enlargements (enl-BrPPA)

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1. *(Initialization)* Choose an initial point $x^0 \in \operatorname{int}(K)$, a parameter $\chi_0 > 0$, and an enlargement parameter $\epsilon_0 \geq 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem $\mathrm{VI}(\mathcal{Q}, K)$ then stop.
3. *(Auxiliary problem)* Find $x^{k+1} \in K$ such that

$$0 \in \mathcal{Q}_{\epsilon_k}(x^{k+1}) + \chi_k(\nabla h(x^{k+1}) - \nabla h(x^k)).$$

4. *(Update)* Choose new parameters $\chi_{k+1} > 0$ and $\epsilon_{k+1} \geq 0$. Set $k := k + 1$ and go to step 2.

Convergence of the sequence $\{x^k\}$ generated by enl-BrPPA towards a solution of $\mathrm{VI}(\mathcal{Q}, K)$ is proved in [9, Theorem 3] under the following conditions. In condition (enl-BrPPA)(5) we point out the additional assumptions needed in comparison to the BrPPA scheme without enlargements.

Conditions (enl-BrPPA): *(see Burachik/Iusem/Svaiter [9])*

(1) General assumptions on the data $\mathcal{Q}$ *and* K*:* $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ *maximal monotone,* $K \subset \mathbb{R}^n$ *closed, convex with* $\operatorname{int}(K) \neq \emptyset$*,* $\operatorname{VI}(\mathcal{Q}, K)$ *solvable.*

(2) h *is a Bregman function with zone* $\operatorname{int}(K)$ *and either*

(a) h *is zone coercive, or*

(b) h *is boundary coercive and the gap-function*

$$q_{\mathcal{Q},K}(x) = \sup\{\langle v, x - y\rangle : y \in K, v \in \mathcal{Q}(y)\}$$

is finite for all $x \in K$*.*

(3) $\mathcal{Q}$ *is paramonotone.*

(4) For the sequence $\{\chi_k\}$ *it holds:* $0 < \chi_k \leq \overline{\chi} < \infty$*,* $\forall k \in \mathbb{N}_0$*.*

(5) Special assumptions needed for the enlargement technique:

(a) $\operatorname{dom}(\mathcal{Q})$ *is closed,*

(b) $\operatorname{int}(\operatorname{dom}(\mathcal{Q})) \supset K$*,*

(c) $0 < \underline{\chi} \leq \chi_k$*,* $\forall k \in \mathbb{N}_0$*, and*

(d) $\{\epsilon_k\} \subset \mathbb{R}_{++}$ *with* $\sum_{k=0}^{\infty} \epsilon_k < \infty$*.*

The advantage of taking an outer operator approximation is obvious. Since $\mathcal{Q}(x) \subset \mathcal{Q}_\epsilon(x)$ for all $\epsilon \geq 0$, it can be expected that each auxiliary problem is easier to solve.

In [12] more theoretical properties of $\mathcal{Q}_\epsilon$, like local Lipschitz continuity, local boundedness, a transportation formula and a Brønsted-Rockafellar property are established.

BrPAP using enlargements. It is now interesting to see how all discussed techniques, which lead to theoretical or numerical improvements in the solution methods for variational inequalities, work together. We therefore consider in Algorithm 2.8

- the combination of PPA and APP in the PAP scheme,
- the usage of auxiliary operators $\mathcal{L}^k$,
- the application of Bregman functions,
- the idea of enlargements, and
- the possibility of inexact solutions in the auxiliary problems.

Algorithm 2.8: BrPAP method using enlargements (enl-BrPAP)

1. *(Initialization)* Choose an initial point $x^0 \in \text{int}(K)$, an auxiliary operator $\mathcal{L}^0$, a parameter $\chi_0 > 0$, an enlargement parameter $\epsilon_0 \geq 0$, and an error parameter $\delta_0 \geq 0$. Set $k := 0$.
2. *(Stopping criterion)* If x^k solves problem $\text{VI}(\mathcal{F}, \mathcal{Q}, K)$ then stop.
3. *(Auxiliary problem)* Find $x^{k+1} \in K$ and $q^k(x^{k+1}) \in \mathcal{Q}^k(x^{k+1})$ such that

$$\begin{aligned}&\left\langle \mathcal{F}(x^k) + q^k(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k(\nabla h(x^{k+1}) - \nabla h(x^k)), x - x^{k+1} \right\rangle \\ &\geq -\delta_k \parallel x - x^{k+1} \parallel \quad \forall x \in K,\end{aligned}$$

   where h is a strongly convex, zone coercive Bregman function with zone $\text{int}(K)$ and $\mathcal{Q}^k$ satisfies $\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k}$.
4. *(Update)* Choose a new auxiliary operator $\mathcal{L}^{k+1}$ and new parameters $\chi_{k+1} > 0$, $\epsilon_{k+1} \geq 0$, $\delta_{k+1} \geq 0$. Set $k := k + 1$ and go to step 2.

A convergence theorem for enl-BrPAP is given in [52, Theorem 2]. We already discussed the convergence assumptions for the BrPAP method without enlargements (see page 32). It is therefore sufficient to mention the additional assumptions needed to work with an operator $\mathcal{Q}^k$ which approximates $\mathcal{Q}$ and satisfies the chain of inclusions

$$\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k}. \tag{2.23}$$

Conditions (enl-BrPAP): *(in addition to BrPAP, see Kaplan/Tichatschke [52])*

(1) $\text{dom}(\mathcal{Q}) \cap K$ *is closed.*

(2) $\{\epsilon_k\} \subset \mathbb{R}_{++}$ *with* $\sum_{k=0}^{\infty} \epsilon_k < \infty$.

The enlargement technique is interesting to deal with computational errors when solving the auxiliary problems numerically. However, the question arises how to calculate an element in $\mathcal{Q}_{\epsilon_k}(x)$ or how to verify if a given point belongs to $\mathcal{Q}_{\epsilon_k}(x)$ for a given $x \in \mathbb{R}^n$. The transportation formula in [12, Theorem 3.11] shows how to use convex sums of elements from the graph of $\mathcal{Q}$ to describe elements in some $\hat{\epsilon}$-enlargement of $\mathcal{Q}$, where $\hat{\epsilon}$ is calculated a posteriori. So, for a given $\epsilon_k \geq 0$ it is unclear which elements in the graph of $\mathcal{Q}$ have to be chosen to construct an element in the graph of $\mathcal{Q}_{\epsilon_k}$.

In [11], Burachik/Sagastizábal/Svaiter describe how to obtain a polyhedral approximation of $\mathcal{Q}_{\epsilon_k}$ by using the transportation formula together with bundle-techniques. They describe an implementable algorithm to solve an inclusion problem with a maximal monotone operator which also involves projection ideas. But numerical results are not reported.

In general it is difficult or even impossible to have a full knowledge of $\mathcal{Q}_{\epsilon_k}$. It therefore seems to be important to work with operators $\mathcal{Q}^k$ that are close to the ϵ_k-enlargement in the sense of (2.23) and that are easier to handle with respect to a numerical solution of the auxiliary problems.

In [52], Kaplan/Tichatschke present some ideas to construct operators $\mathcal{Q}^k$ that inherit the continuity properties of the ϵ_k-enlargement, but whose treatment is much simpler than that of $\mathcal{Q}_{\epsilon_k}$. For example, let $\mathcal{Q} = \mathcal{Q}_1 + \mathcal{Q}_2$, where $\mathcal{Q}_1$ is single-valued, continuous and monotone, and $\mathcal{Q}_2$ is multi-valued and maximal monotone. Then

$$\mathcal{Q}^k = \mathcal{Q}_1 + (\mathcal{Q}_2)_{\epsilon_k}$$

fulfills $\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k}$. For the special case $\mathcal{Q} = \partial g$, where g is a convex function that can be splitted into the sum of a differentiable, convex function ψ and a nondifferentiable, convex function φ, the setting

$$\mathcal{Q}^k = \nabla\psi + \partial_{\epsilon_k}\varphi$$

fulfills $\mathcal{Q} \subset \mathcal{Q}^k \subset \partial_{\epsilon_k} g \subset (\partial g)_{\epsilon_k}$. Furthermore, in the case that $\mathcal{Q}$ has a block-diagonal structure, this structure can be transmitted to $\mathcal{Q}^k$ as shown in [52, Section 3.3], although $\mathcal{Q}_{\epsilon_k}$ does not possess this property.

In our work, the case $\mathcal{Q} = \partial\varphi$ and $\mathcal{Q}^k = \partial_{\epsilon_k}\varphi$ will be of special interest because a concrete implementation using bundle-techniques can be given (see Chapter 8) to solve the corresponding auxiliary problems. Other numerically meaningful approximations of multivalued operators are not known to us.

3. Logarithmic-quadratic Proximal Auxiliary Problem Method

The described extensions of the PPA and APP schemes given in the previous chapter show that the application of logarithmic-quadratic distance functions in the PAP scheme might as well be interesting as an alternative to the BrPAP and an extension of the LQPPA. Until now this extension has not been investigated.

This chapter presents a full convergence analysis of the suggested *logarithmic-quadratic proximal auxiliary problem method* (LQPAP method). The underlying problem formulation is a variational inequality

$$\begin{aligned} \mathrm{VI}(\mathcal{F}, \mathcal{Q}, K): \quad & \text{Find } x^* \in K \text{ and } q^*(x^*) \in \mathcal{Q}(x^*): \\ & \langle \mathcal{F}(x^*) + q^*(x^*), x - x^* \rangle \geq 0 \quad \forall\, x \in K, \end{aligned} \tag{3.1}$$

where $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is a maximal monotone, multi-valued operator and $\mathcal{F} : K \to \mathbb{R}^n$ is a single-valued, continuous operator that has a certain monotonicity property described below. The restriction set K is given by

$$K = \{x \in \mathbb{R}^n \colon Ax \leq b\}, \tag{3.2}$$

where $A \in \mathbb{R}^{p \times n}$, $p \geq n$, $\mathrm{rank}(A) = n$, $b \in \mathbb{R}^p$, and $\mathrm{int}(K) := \{x \in \mathbb{R}^n \colon Ax < b\} \neq \emptyset$. Since A has full column rank, $B := A^T A$ is symmetric and positive definite. Hence, $\langle u, v \rangle_B := \langle Bu, v \rangle = \langle A^T Au, v \rangle$ defines an inner product on $\mathbb{R}^n$ with associated norm $\| u \|_B := \sqrt{\langle u, u \rangle_B} = \sqrt{\langle Au, Au \rangle} = \| Au \|$. For short, we use the notation

$$\begin{aligned} \langle u, v \rangle_A &:= \langle Au, Av \rangle \\ \| u \|_A &:= \| Au \| . \end{aligned}$$

Since all norms in $\mathbb{R}^n$ are equivalent, there exists a constant $a > 0$ such that

$$\| u \|_A \geq a \, \| u \| \quad \forall u \in \mathbb{R}^n. \tag{3.3}$$

3.1 Definition and properties of the logarithmic-quadratic distance function

As introduced in Section 2.4.2, the logarithmic-quadratic distance function that is tailored to the set K is defined by

$$D : \mathbb{R}^n \times \operatorname{int}(K) \to \mathbb{R} \cup \{+\infty\}$$
$$D(x,y) = \begin{cases} \sum_{i=1}^{p} l_i(x)^2 - l_i(x)l_i(y) - l_i(y)^2 \log \frac{l_i(x)}{l_i(y)} & \text{if } x \in \operatorname{int}(K) \\ +\infty & \text{otherwise.} \end{cases} \tag{3.4}$$

We recall that D can be expressed in terms of the distance function d (see (2.12)) as

$$D(x,y) = d(l(x), l(y)), \text{ with } d : \mathbb{R}^p \times \mathbb{R}^p_{++} \to \mathbb{R} \cup \{+\infty\},$$
$$d(u,v) = \begin{cases} \sum_{i=1}^{p} u_i^2 - u_i v_i - v_i^2 \log \frac{u_i}{v_i} & \text{if } u \in \mathbb{R}^p_{++} \\ +\infty & \text{otherwise.} \end{cases} \tag{3.5}$$

The subscript LQ is omitted for better writing because only logarithmic-quadratic distance functions are considered in the following. Note that D is only well-defined if $\operatorname{int}(K) \neq \emptyset$. We further recall that $D(\cdot, y)$ is differentiable at $x \in \operatorname{int}(K)$ for any $y \in \operatorname{int}(K)$. Thus, $\partial_I D(\cdot, y)$ and $\nabla_I D(\cdot, y)$ coincide on $\operatorname{int}(K)$. For $x, y \in \operatorname{int}(K)$ it holds

$$\nabla_I D(x,y) = -\sum_{i=1}^{p} a_i \left(2l_i(x) - l_i(y) - \frac{l_i(y)^2}{l_i(x)} \right). \tag{3.6}$$

Moreover, for fixed $y \in \operatorname{int}(K)$, the second derivative of $D(\cdot, y)$ at $x \in \operatorname{int}(K)$ is obtained as

$$\nabla_I^2 D(x,y) = A^T \begin{pmatrix} 2 + \frac{l_1(y)^2}{l_1(x)^2} & & 0 \\ & \ddots & \\ 0 & & 2 + \frac{l_p(y)^2}{l_p(x)^2} \end{pmatrix} A. \tag{3.7}$$

We now show important properties of $D(\cdot, y)$ that will be exploited in the upcoming convergence analysis.

Lemma 3.1.1. *Let $y \in \operatorname{int}(K)$. Then $D(\cdot, y) : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is a proper, lower semicontinuous, convex function, and for all $x_1, x_2 \in \operatorname{int}(K)$*

$$\langle \nabla_I D(x_1, y) - \nabla_I D(x_2, y), x_1 - x_2 \rangle \geq 2 \parallel x_1 - x_2 \parallel_A^2 .$$

Hence, $D(\cdot, y)$ is strongly convex on $\operatorname{int}(K)$ with modulus $2a$, where a fulfills (3.3).

Proof. We can write $D(\cdot, y) = d(\cdot, l(y)) \circ l \colon \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$. As already mentioned, $d(\cdot, v) : \mathbb{R}^p \to \mathbb{R} \cup \{+\infty\}$ is a proper, lower semicontinuous, convex function for all $v \in \mathbb{R}^p_{++}$. Since l is a linear function, it follows that $D(\cdot, y)$ is lower semicontinuous and convex. For all $x \in \operatorname{int}(K)$, $D(x, y)$ is obviously finite. Thus, $D(\cdot, y)$ is a proper function. We rewrite (see (2.22)) $d(u, v)$ for $u, v \in \mathbb{R}^p_{++}$ as

$$d(u,v) = \| u - v \|^2 + \sum_{i=1}^{p} v_i^2 \left(\frac{u_i}{v_i} - \log \frac{u_i}{v_i} - 1 \right). \tag{3.8}$$

For $u, v \in \mathbb{R}^p_{++}$ it holds that

$$\nabla_I^2 d(u,v) = \begin{pmatrix} 2 + \frac{v_1^2}{u_1^2} & & 0 \\ & \ddots & \\ 0 & & 2 + \frac{v_p^2}{u_p^2} \end{pmatrix}. \tag{3.9}$$

It is now evident that $d(\cdot, v)$ is strongly convex on $\mathbb{R}^p_{++}$ with modulus $\kappa = 2$. Thus, for $y \in \operatorname{int}(K)$, $d(\cdot, l(y))$ is strongly convex on $\mathbb{R}^p_{++}$. Since A is of full column rank, it follows that $D(\cdot, y) = d(\cdot, l(y)) \circ l$ is strongly convex on $\operatorname{int}(K)$ with modulus $2a$. In detail, it holds for every $x_1, x_2 \in \operatorname{int}(K)$:

$$\begin{aligned}
&\langle \nabla_I D(x_1, y) - \nabla_I D(x_2, y), x_1 - x_2 \rangle \\
&= \langle \nabla_I (d(\cdot, l(y)) \circ l)(x_1) - \nabla_I (d(\cdot, l(y)) \circ l)(x_2), x_1 - x_2 \rangle \\
&= \left\langle -A^T \nabla_I d(l(x_1), l(y)) - (-A^T) \nabla_I d(l(x_2), l(y)), x_1 - x_2 \right\rangle \\
&= \left\langle (-A^T)(\nabla_I d(l(x_1), l(y)) - \nabla_I d(l(x_2), l(y))), x_1 - x_2 \right\rangle \\
&= \langle (\nabla_I d(l(x_1), l(y)) - \nabla_I d(l(x_2), l(y))), (b - Ax_1) - (b - Ax_2) \rangle \\
&= \langle (\nabla_I d(l(x_1), l(y)) - \nabla_I d(l(x_2), l(y))), l(x_1) - l(x_2) \rangle \\
&\geq 2 \| l(x_1) - l(x_2) \|^2 \\
&= 2 \| x_1 - x_2 \|_A^2 \\
&\geq 2a \| x_1 - x_2 \|^2 .
\end{aligned}$$

□

Corollary 3.1.2. *Let $y \in \operatorname{int}(K)$. Then $\partial_I D(\cdot, y) : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is maximal monotone and $\operatorname{dom}(\partial_I D(\cdot, y)) = \operatorname{int}(K)$.*

Proof. Maximal monotonicity of $\partial_I D(\cdot, y)$ follows from Lemma 3.1.1 and [83, Theorem 12.17]. The inclusion $\operatorname{dom}(\partial_I D(\cdot, y)) \supset \operatorname{int}(K)$ is obvious, because $D(x, y)$ is differentiable for all $x \in \operatorname{int}(K)$. To show that $\operatorname{dom}(\partial_I D(\cdot, y)) \subset \operatorname{int}(K)$, suppose that $\partial_I D(\bar{x}, y) \neq \emptyset$ holds for some $\bar{x} \notin \operatorname{int}(K)$. Let $s \in \partial_I D(\bar{x}, y)$. Then, according to the definition of the subdifferential, the inequality

$$D(x, y) \geq D(\bar{x}, y) + \langle s, x - \bar{x} \rangle$$

holds true for all $x \in \mathbb{R}^n$. However, according to the definition of D, $D(\bar{x}, y) = +\infty$ and $D(x, y) < +\infty$ for all $x \in \operatorname{int}(K)$. This is a contradiction. Hence, $\partial_I D(\bar{x}, y) = \emptyset$. □

The next step is to obtain that $\nabla_I D(\cdot, y) : \mathrm{int}(K) \to \mathbb{R}^n$ is onto. For that purpose, the definition of the recession function as given, e.g., in [41, Definition IV.3.2.3] is needed.

Definition 3.1.3. *Let $f : \mathbb{R}^p \to \mathbb{R} \cup \{+\infty\}$ be a proper, lower semicontinuous, convex function. The recession function f_∞ is defined by*

$$s \mapsto f_\infty(s) := \lim_{t \to +\infty} \frac{f(x^0 + ts) - f(x^0)}{t},$$

where x^0 is arbitrary in $\mathrm{dom}(f)$.

The value of f_∞ at s is independent of x^0 [41, Theorem I.2.3.1] and can be interpreted as something like a "slope at infinity" in the direction s. It is well-known that the epigraph of f_∞ is equal to the asymptotic cone of $\mathrm{epi}(f)$, i.e., $\mathrm{epi}(f_\infty) = (\mathrm{epi} f)_\infty$ [41, Proposition IV.3.2.2].

The next proposition presents a class of functions whose gradient maps are onto.

Proposition 3.1.4 ([6], Proposition 2). *Let $f : \mathbb{R}^p \to \mathbb{R} \cup \{+\infty\}$ be a function with the following properties:*

(i) f is proper, lower semicontinuous, convex with $\mathrm{dom}(f)$ open,

(ii) f is differentiable on $\mathrm{dom}(f)$, and

(iii) $f_\infty(s) = +\infty$ for all $s \neq 0$.

Then

(1) the gradient map ∇f is onto, i.e., $\nabla f(\mathrm{dom}(f)) = \mathbb{R}^p$.

(2) Let $A \in \mathbb{R}^{p \times n}$ be a matrix with $p \geq n$ and rank$(A) = n$, $b \in \mathbb{R}^p$, $l \colon \mathbb{R}^n \to \mathbb{R}^p$ with $l(x) = b - Ax$ and $(b - A(\mathbb{R}^n)) \cap \mathrm{dom}(f) \neq \emptyset$. Then $\nabla(f \circ l)$ is onto, i.e., $\nabla(f \circ l)((b - A(\mathbb{R}^n)) \cap \mathrm{dom}(f)) = \mathbb{R}^n$.

Now, we take a fixed $y \in \mathrm{int}(K)$ and define for $u \in \mathbb{R}^p$

$$f_y(u) = \begin{cases} \sum_{i=1}^p u_i^2 - u_i l_i(y) - l_i(y)^2 \log \frac{u_i}{l_i(y)} & \text{if } u \in \mathbb{R}^p_{++} \\ +\infty & \text{otherwise.} \end{cases} \tag{3.10}$$

Then $f_y(u) = d(u, l(y))$. We aim to apply Proposition 3.1.4 to f_y and therefore prove the following statement.

Lemma 3.1.5. *Function f_y as defined in (3.10) fulfills properties (i)–(iii) of Proposition 3.1.4.*

Proof. It is clear that f_y is a proper, lower semicontinuous, convex function (see Appendix, Lemma A.3.1) with $\mathrm{dom}(f) = \mathbb{R}^p_{++}$ open, and that f_y is differentiable on $\mathbb{R}^p_{++}$. Thus, for arbitrary $u \in \mathbb{R}^p_{++}$ it holds

$$\begin{aligned}(f_y)_\infty(s) &= \lim_{t\to+\infty} \frac{f_y(u+ts) - f_y(u)}{t} \\ &\geq \lim_{t\to+\infty} \frac{f_y(u) + t\left\langle \nabla f_y(u), s\right\rangle - f_y(u)}{t} \\ &= \left\langle \nabla f_y(u), s\right\rangle,\end{aligned}$$

where

$$\nabla f_y(u) = \sum_{i=1}^{p} \left(2u_i - l_i(y) - \frac{l_i(y)^2}{u_i}\right).$$

For every $s \neq 0$ it is possible to define a sequence $\{u^k\} \subset \mathbb{R}^p_{++}$ such that the behavior of the sequence $\{u_i^k\}$ depends on the sign of the entry s_i in the following way: If $s_i < 0$ then let $u_i^k \to 0$ for $k \to \infty$, if $s_i > 0$ then let $u_i^k \to +\infty$ for $k \to \infty$, and if $s_i = 0$ then set $u_i^k = 1$ for all k. Since at least one entry of s is not equal to zero it is clear that

$$\lim_{k\to\infty} \left\langle \nabla f_y(u^k), s\right\rangle = +\infty,$$

which shows that $(f_y)_\infty(s) = +\infty$. □

With this result we can now establish that $\nabla_I D(\cdot, y)$ is onto.

Corollary 3.1.6. *Let $y \in \mathrm{int}(K)$. Then, for all $z \in \mathbb{R}^n$ there exists $x \in \mathrm{int}(K)$ with*

$$\nabla_I D(x, y) = z.$$

In other words, the operator $\nabla_I D(\cdot, y) : \mathrm{int}(K) \to \mathbb{R}^n$ is onto.

Proof. In view of Lemma 3.1.5 the assertion follows directly from Proposition 3.1.4(2) applied to $D(\cdot, y) = d(\cdot, l(y)) \circ l = f_y \circ l$. □

A crucial step in the upcoming convergence analysis is to estimate the scalar product $\langle \nabla_I D(x, y), z - y\rangle$ for $x, y \in \mathrm{int}(K), z \in K$ from above. In this context the following lemma concerning positive/nonnegative numbers is helpful.

Lemma 3.1.7 ([6], Lemma 2). *For any $s > 0, t > 0$, and $u \geq 0$ it holds*

$$(t-u)\left(2t - s - \frac{s^2}{t}\right) \geq \frac{3}{2}((u-t)^2 - (u-s)^2) + \frac{1}{2}(t-s)^2 \tag{3.11}$$

$$\geq \frac{3}{2}((u-t)^2 - (u-s)^2) \tag{3.12}$$

and

$$(t-u)\left(2t-s-\frac{s^2}{t}\right)\geq(s-t)(3u-2t-s). \tag{3.13}$$

Now, the key property of the logarithmic-quadratic distance function reads as follows (see also [5, Lemma 3.4]).

Lemma 3.1.8. *For any $x,y\in\operatorname{int}(K)$ and $z\in K$ it holds*

$$\langle\nabla_I D(x,y),z-x\rangle\leq\frac{3}{2}(\parallel z-y\parallel_A^2-\parallel z-x\parallel_A^2). \tag{3.14}$$

Proof. For any $x,y\in\operatorname{int}(K)$ and $z\in K$ we get

$$\begin{aligned}\langle-\nabla_I D(x,y),z-x\rangle&=\left\langle\sum_{i=1}^{p}a_i\left(2l_i(x)-l_i(y)-\frac{l_i(y)^2}{l_i(x)}\right),z-x\right\rangle\\&=\sum_{i=1}^{p}\left(2l_i(x)-l_i(y)-\frac{l_i(y)^2}{l_i(x)}\right)\langle a_i,z-x\rangle\\&=\sum_{i=1}^{p}\left(2l_i(x)-l_i(y)-\frac{l_i(y)^2}{l_i(x)}\right)(l_i(x)-l_i(z)).\end{aligned}$$

Application of (3.12) with $t=l_i(x), s=l_i(y)$, and $u=l_i(z)$ results in

$$\begin{aligned}\langle-\nabla_I D(x,y),z-x\rangle&\geq\sum_{i=1}^{p}\frac{3}{2}((l_i(z)-l_i(x))^2-(l_i(z)-l_i(y))^2)\\&=\frac{3}{2}\sum_{i=1}^{p}(\langle a_i,x-z\rangle^2-\langle a_i,y-z\rangle^2)\\&=\frac{3}{2}(\parallel A(x-z)\parallel^2-\parallel A(y-z)\parallel^2)\\&=\frac{3}{2}(\parallel z-x\parallel_A^2-\parallel z-y\parallel_A^2).\end{aligned}$$

□

3.2 LQPAP iteration scheme and convergence assumptions

We are now ready to present the LQPAP scheme for solving $\mathrm{VI}(\mathcal{F},\mathcal{Q},K)$. The scheme includes the following techniques and methods:

- PAP scheme with auxiliary operators $\mathcal{L}^k$,
- the application of logarithmic-quadratic distance functions,
- the idea of enlargements, and
- the possibility of inexact solutions in the auxiliary problems.

This combination has so far not been investigated.

First, we introduce some preliminary requirements for the involved operators and controlling parameters. As usual, a family of monotone operators $\{\mathcal{L}_y\}$ parameterized by $y \in K$ is used and $\mathcal{L}^k$ is defined by setting $\mathcal{L}^k = \mathcal{L}_{y|y=x^k}$. Following the technique of ϵ-enlargements, the operators $\mathcal{Q}^k$ represent an outer approximation of the multi-valued operator $\mathcal{Q}$ satisfying

$$\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k} \quad \forall k \in \mathbb{N}_0, \tag{3.15}$$

where $\{\epsilon_k\}$ is a sequence with

$$\epsilon_k \geq 0 \quad \forall k \in \mathbb{N}_0 \quad \text{and} \quad \lim_{k\to\infty} \epsilon_k = 0, \tag{3.16}$$

and $\mathcal{Q}_{\epsilon_k}$ denotes the ϵ_k-enlargement of the operator $\mathcal{Q}$. Ideas for the construction of $\mathcal{Q}^k$ were presented on page 43. The sequence $\{\chi_k\}$ of regularization parameters and the sequence $\{\delta_k\}$ of error tolerance parameters are supposed to satisfy

$$0 < \underline{\chi} \leq \chi_k \leq \overline{\chi} < \infty \quad \forall k \in \mathbb{N}_0, \tag{3.17}$$

and

$$\delta_k \geq 0 \quad \forall k \in \mathbb{N}_0 \quad \text{and} \quad \lim_{k\to\infty} \delta_k = 0. \tag{3.18}$$

Now, the LQPAP scheme can be described as follows.

LQPAP iteration scheme (S): *Given a current iterate* x^k *(*$x^0 \in \operatorname{int}(K)$ *arbitrarily chosen), at step* $(k+1)$ *iterate* x^{k+1} *is calculated by solving the problem*

$$\begin{aligned}(\boldsymbol{P}^{\boldsymbol{k}}_{\boldsymbol{\delta}}) : \text{Find } & x^{k+1} \in K,\ q^k(x^{k+1}) \in \mathcal{Q}^k(x^{k+1}): \\ & \langle \mathcal{F}(x^k) + q^k(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k \nabla_I D(x^{k+1}, x^k), x - x^{k+1}\rangle \\ & \geq -\delta_k \parallel x - x^{k+1} \parallel \quad \forall\ x \in K.\end{aligned}$$

The LQPAP method will be studied under the following general assumptions.

Conditions (LQPAP):

(A1) The solution set $\mathrm{SOL}(\mathcal{F}, \mathcal{Q}, K)$ of $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ is nonempty.

(A2) $K = \{x \in \mathbb{R}^n \colon Ax \leq b\}$ with $A \in \mathbb{R}^{p\times n}$, $p \geq n$, $\mathrm{rank}(A) = n$, $b \in \mathbb{R}^p$, and $\mathrm{int}(K) \neq \emptyset$.

(A3) $\mathcal{Q} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is maximal monotone and $\mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K) \neq \emptyset$.

(A4) $\mathcal{F} : K \to \mathbb{R}^n$ is continuous on K.

(A5) $\mathrm{dom}(\mathcal{Q}) \cap K$ is a nonempty and closed set.

(A6) $\{\mathcal{L}_y\}$, with $\mathcal{L}_y : K \to \mathbb{R}^n$, is a family of monotone and continuous operators.

(A7) There exists $\gamma > 0$ (independent of x, y) such that for $x, y \in K$ the inequality

$$\langle \mathcal{F}(y) - \mathcal{L}_y(y) - \mathcal{F}(x) + \mathcal{L}_y(x), y - x\rangle \geq \gamma \parallel \mathcal{F}(y) - \mathcal{L}_y(y) - \mathcal{F}(x) + \mathcal{L}_y(x) \parallel^2$$

is valid.

(A8) For any convergent sequence $\{y^k\} \subset \mathrm{dom}(\mathcal{Q}) \cap K$ it holds

$$\mathcal{L}_{y^k}(y^{k+1}) - \mathcal{L}_{y^k}(y^k) \to 0 \quad \text{as} \quad k \to \infty.$$

Let us comment on some assumptions. With the aim to present an interior point method it is obvious to require $\mathrm{int}(K) \neq \emptyset$ in (A2). Condition $\mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K) \neq \emptyset$ in (A3) ensures that $\mathcal{Q} + \mathcal{N}_K$ maximal monotone. The closedness of $\mathrm{dom}(\mathcal{Q}) \cap K$ in (A5) is needed to exploit properties of the ϵ-enlargement of $\mathcal{Q}$. Assumption (A7) is certainly fulfilled if for all $y \in K$ the operators $\mathcal{F} - \mathcal{L}_y$ are co-coercive on K with a common modulus $\gamma > 0$:

$$\begin{aligned}\langle \mathcal{F}(v) - \mathcal{L}_y(v) - \mathcal{F}(x) + \mathcal{L}_y(x), v - x\rangle \\ \geq \gamma \parallel \mathcal{F}(v) - \mathcal{L}_y(v) - \mathcal{F}(x) + \mathcal{L}_y(x) \parallel^2 \quad \forall x, v \in K.\end{aligned}$$

The weakening in (A7) is to require the above inequality only for $v = y$. A consequence of condition (A7) is

$$\begin{aligned}\langle \mathcal{F}(y) - \mathcal{L}_y(y) + \mathcal{L}_y(x^*) + q^*(x^*), y - x^*\rangle \\ \geq \gamma \parallel \mathcal{F}(y) - \mathcal{L}_y(y) - \mathcal{F}(x^*) + \mathcal{L}_y(x^*) \parallel^2,\end{aligned}$$

where $x^* \in \mathrm{SOL}(\mathcal{F}, \mathcal{Q}, K)$, $y \in K$, and the element $q^*(x^*) \in \mathcal{Q}(x^*)$ is chosen such that

$$\langle \mathcal{F}(x^*) + q^*(x^*), x - x^* \rangle \geq 0 \quad \forall x \in K.$$

Since the operators $\mathcal{L}_y$ are monotone, it follows from (A7) that $\mathcal{F}$ is monotone and thus $\mathcal{F} + \mathcal{Q}$ is monotone due to (A3). (A8) is surely fulfilled if we have the uniform Lipschitz continuity of the operators $\mathcal{L}_y$ in $y \in K$. None of the present assumptions is new in the context of the solution methods described in Chapter 2. (A1), (A2), and (A3) are familiar from the Conditions (LQPPA) (see page 35), whereas the other assumptions already occurred in the Conditions (enl-BrPAP) (see pages 32 and 42).

3.3 Solvability of the auxiliary problems and interior point effect

The scope of this section is to verify that the LQPAP iteration scheme (S) is well-defined. This includes two aspects. First, we prove that for each k the auxiliary problem (P_δ^k) is solvable. Second, it has to be shown that the iterates $\{x^k\}$ belong to $\mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K)$.

Let us explain the background of the second aspect. Surely, if (P_δ^k) is solvable, iterate x^{k+1} belongs to $\mathrm{dom}(\mathcal{Q}^k)$. However, it is important to have $x^{k+1} \in \mathrm{dom}(\mathcal{Q})$ in order to stop the iteration process at an approximate solution of the original problem. Further, it is necessary that the iterates belong $\mathrm{int}(K)$ because $D(x, \cdot)$ is only defined on $\mathrm{int}(K)$. Moreover, only if $x^{k+1} \in \mathrm{int}(K)$ one can write $\nabla_I D(x^{k+1}, x^k)$ instead of $\partial_I D(x^{k+1}, x^k)$. Finally, the second aspect constitutes the interior point effect of our method. As a consequence, the restriction set K can be omitted and the auxiliary problems can be considered as unconstrained ones.

Now, turn to the first aspect. To prove the existence of a solution of problem (P_δ^k), we consider the case of *exact* solutions. Let (P_0^k) denote problem (P_δ^k) with $\delta_k = 0$ and $\mathcal{Q}^k = \mathcal{Q}$, i.e.,

$(\boldsymbol{P_0^k})$: Find $x^{k+1} \in K,\ q(x^{k+1}) \in \mathcal{Q}(x^{k+1})$ such that for all $x \in K$:

$$\langle \mathcal{F}(x^k) + q(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k \nabla_I D(x^{k+1}, x^k), x - x^{k+1} \rangle \geq 0.$$

Using the normal cone operator this can equivalently be written as

Find $x^{k+1} \in K$:

$$0 \in \mathcal{F}(x^k) + \mathcal{Q}(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \mathcal{N}_K(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k). \quad (3.19)$$

If problem (P_0^k) has an exact solution, this solution obviously solves the inexact problem (P_δ^k), where $\delta_k \geq 0$ and $\mathcal{Q} \subset \mathcal{Q}^k$. Of course, other solutions of (P_δ^k) may exist since some error is admitted and some outer approximation of $\mathcal{Q}$ is used.

Theorem 3.3.1. *Let Assumptions (A2), (A3), (A5), (A6) and relations (3.15)–(3.18) be valid. Then*

(i) problem (P_0^k) has a unique solution for each k, and

(ii) the sequence $\{x^k\}$ generated by the LQPAP iteration scheme (S) belongs to $\mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K)$.

In other words, the LQPAP iteration scheme (S) is well-defined.

Proof. To prove the existence of a solution x^{k+1} of problem (P_0^k), we use Theorem 2.2.3. Let $x^k \in \mathrm{int}(K)$. We define the operator $\mathcal{G}^k : K \to 2^{\mathbb{R}^n}$ by

$$\mathcal{G}^k(y) = \mathcal{F}(x^k) + Q(y) + \mathcal{L}^k(y) - \mathcal{L}^k(x^k) + \mathcal{N}_K(y).$$

The values $\mathcal{F}(x^k)$ and $\mathcal{L}^k(x^k)$ are constant in this context. Because of (A6), operator $\mathcal{L}^k$ is finite, single-valued, monotone, and continuous on $\mathrm{dom}(\mathcal{L}^k) = K$. In view of (A2), it follows from Theorem 2.1.2 that $\mathcal{L}^k + \mathcal{N}_K : K \to \mathbb{R}^n$ is maximal monotone with $\mathrm{dom}(\mathcal{L}^k + \mathcal{N}_K) = K$. Due to Theorem 2.1.1 and Assumption (A3), maximal monotonicity of $\mathcal{Q} + \mathcal{L}^k + \mathcal{N}_K$ on K is obtained. Hence, $\mathcal{G}^k$ is maximal monotone on K with $\mathrm{dom}(\mathcal{G}^k) = \mathrm{dom}(\mathcal{Q}) \cap K$. As shown in Corollary 3.1.2, $\partial_I D(\cdot, x^k)$ is maximal monotone and $\mathrm{dom}(\partial_I D(\cdot, x^k)) = \mathrm{int}(K)$. By Assumption (A3) and relation (3.17), it follows that

$$\mathcal{G}^k + \chi_k \partial_I D(\cdot, x^k) \text{ is maximal monotone.}$$

According to Corollary 3.1.6, $\mathrm{rge}(\chi_k \partial_I D(\cdot, x^k)) = \mathbb{R}^n$. Therefore, Theorem 2.2.3 implies

$$\mathrm{rge}(\mathcal{G}^k + \chi_k \partial_I D(\cdot, x^k)) = \mathbb{R}^n.$$

Consequently, there exists a solution $x^{k+1} \in \mathrm{dom}(\mathcal{G}^k + \chi_k \partial_I D(\cdot, x^k)) = \mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K)$ for problem (P_0^k). Since $\partial_I D(\cdot, x^k)$ and $\nabla_I D(\cdot, x^k)$ coincide on $\mathrm{int}(K)$, we will speak of the operator $\nabla_I D(\cdot, x^k)$ instead of $\partial_I D(\cdot, x^k)$ in the sequel. In view of the monotonicity of $\mathcal{G}^k$ and the strict monotonicity of $\chi_k \nabla_I D(\cdot, x^k)$ on $\mathrm{int}(K)$, we conclude that the solution x^{k+1} is unique.

Now, let us turn to the inexact scheme (P_δ^k). From $\mathrm{dom}(\nabla_I D(\cdot, x^k)) = \mathrm{int}(K)$ it follows for a solution x^{k+1} of (P_δ^k) that

$$x^{k+1} \in \mathrm{dom}(\mathcal{Q}^k) \cap \mathrm{int}(K).$$

In order to prove $x^{k+1} \in \mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K)$, it suffices to show that

$$\mathrm{dom}(\mathcal{Q}^k) \cap K = \mathrm{dom}(\mathcal{Q}) \cap K.$$

Because of the inclusion $\mathcal{Q} \subset \mathcal{Q}^k$, one immediately gets

$$\mathrm{dom}(\mathcal{Q}) \cap K \subset \mathrm{dom}(\mathcal{Q}^k) \cap K.$$

To establish the reverse inclusion, we consider the choice of $\mathcal{Q}^k$ in (3.15) and make use of some properties of the ϵ-enlargement. Theorem 2.4.1(b) yields

$$\mathcal{Q}_{\epsilon_k} + \mathcal{N}_K \subset (\mathcal{Q} + \mathcal{N}_K)_{\epsilon_k},$$

which implies

$$\mathrm{dom}(\mathcal{Q}_{\epsilon_k} + \mathcal{N}_K) \subset \mathrm{dom}((\mathcal{Q} + \mathcal{N}_K)_{\epsilon_k}).$$

Because of Assumption (A5), $\mathrm{dom}(\mathcal{Q} + \mathcal{N}_K)$ is closed. Hence, Theorem 2.4.1(f) can be applied to get

$$\mathrm{dom}((\mathcal{Q} + \mathcal{N}_K)_{\epsilon_k}) = \mathrm{dom}(\mathcal{Q} + \mathcal{N}_K).$$

Together with (3.15) this yields

$$\begin{aligned}
\mathrm{dom}(\mathcal{Q}^k) \cap K &\subset \mathrm{dom}(\mathcal{Q}_{\epsilon_k}) \cap K \\
&= \mathrm{dom}(\mathcal{Q}_{\epsilon_k} + \mathcal{N}_K) \\
&\subset \mathrm{dom}((\mathcal{Q} + \mathcal{N}_K)_{\epsilon_k}) \\
&= \mathrm{dom}(\mathcal{Q} + \mathcal{N}_K) \\
&= \mathrm{dom}(\mathcal{Q}) \cap K.
\end{aligned}$$

Choosing $x^0 \in \mathrm{int}(K)$ it now follows that the entire sequence $\{x^k\}$ generated by the LQPAP iteration scheme (S) belongs to $\mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K)$. □

3.4 Convergence analysis of the LQPAP method

We start with a reformulation of the auxiliary problems as nonlinear equation systems.

The interior point effect proved in Theorem 3.3.1 ensures that the solution of (P_0^k) belongs to $\mathrm{int}(K)$. Since $\mathcal{N}_K(x) = \{0\}$ for all $x \in \mathrm{int}(K)$, we can formulate problem (3.19) as a nonlinear equation system of the form

$$\begin{aligned}
&\text{Find } x^{k+1} \in K,\ q(x^{k+1}) \in \mathcal{Q}(x^{k+1}): \\
&0 = \mathcal{F}(x^k) + q(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k \nabla_I D(x^{k+1}, x^k).
\end{aligned}$$

Furthermore, the interior point effect can be exploited to analogously reformulate the inexact auxiliary problems (P_δ^k) as nonlinear equation systems of the form

$$\begin{aligned}
(\boldsymbol{P_e^k}):\ &\text{Find } x^{k+1} \in K,\ q^k(x^{k+1}) \in \mathcal{Q}^k(x^{k+1}),\ \text{and } e^{k+1} \in \mathbb{R}^n: \\
&e^{k+1} = \mathcal{F}(x^k) + q^k(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k \nabla_I D(x^{k+1}, x^k) \\
&\text{and } \ \| e^{k+1} \| \leq \delta_k.
\end{aligned}$$

Equivalence of the two schemes (P_δ^k) and (P_e^k) is proved in the following lemma.

Lemma 3.4.1. *Let $x^k \in \operatorname{int}(K)$ be a current iterate. Then the schemes (P_e^k) and (P_δ^k) are equivalent, i.e., a solution x^{k+1} of (P_e^k) is also a solution of (P_δ^k) and vice versa.*

Proof. For abbreviation we set $\mathcal{T}^k(x) := \mathcal{F}(x^k) + \mathcal{Q}^k(x) + \mathcal{L}^k(x) - \mathcal{L}^k(x^k)$. Let $x^{k+1} \in \operatorname{int}(K)$ be a solution of (P_e^k). Then $0 = t^k(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k) - e^{k+1}$ with a suitable $t^k(x^{k+1}) \in \mathcal{T}^k(x^{k+1})$. This is equivalent to

$$\left\langle t^k(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k) - e^{k+1}, x - x^{k+1} \right\rangle \geq 0 \quad \forall x \in \mathbb{R}^n.$$

Rearranging terms and applying the Cauchy-Schwarz inequality yields

$$\left\langle t^k(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k), x - x^{k+1} \right\rangle \geq - \parallel e^{k+1} \parallel \parallel x - x^{k+1} \parallel \quad \forall x \in \mathbb{R}^n.$$

Due to $\parallel e^{k+1} \parallel \leq \delta_k$, it follows that

$$\left\langle t^k(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k), x - x^{k+1} \right\rangle \geq -\delta_k \parallel x - x^{k+1} \parallel \quad \forall x \in \mathbb{R}^n.$$

Thus, x^{k+1} is a solution of (P_δ^k).

Now, let $x^{k+1} \in \operatorname{int}(K)$ and $t^k(x^{k+1}) \in \mathcal{T}^k(x^{k+1})$ fulfill scheme (P_δ^k). Define

$$e^{k+1} := t^k(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k).$$

Since $x^{k+1} \in \operatorname{int}(K)$, there exists $\tau > 0$ such that

$$\bar{x} := x^{k+1} - \tau e^{k+1} \in K.$$

The inequality of scheme (P_δ^k) reduces for $x = \bar{x}$ to

$$\left\langle e^{k+1}, -\tau e^{k+1} \right\rangle \geq -\delta_k \parallel -\tau e^{k+1} \parallel .$$

The case $e^{k+1} = 0$ is trivial. For $e^{k+1} \neq 0$ we can conclude that $\parallel e^{k+1} \parallel \leq \delta_k$. Hence, x^{k+1} is a solution of scheme (P_e^k). □

Now, the complete LQPAP algorithm, which uses scheme (P_e^k), is formulated in Algorithm 3.1.

The convergence of Algorithm 3.1 is proved under the following conditions on the nonnegative controlling parameters:

$$0 < \underline{\chi} \leq \chi_k \leq \overline{\chi} < \infty, \ \forall k \in \mathbb{N}_0, \tag{3.20}$$

$$\underline{\chi} > \frac{1}{2a^2\gamma}, \text{ with } a \text{ as in (3.3)}, \gamma \text{ as in (A7)}, \tag{3.21}$$

$$\sum_{k=0}^{\infty} \delta_k < +\infty, \tag{3.22}$$

$$\sum_{k=0}^{\infty} \epsilon_k < +\infty. \tag{3.23}$$

Algorithm 3.1: Inexact logarithmic-quadratic proximal auxiliary problem method (LQPAP)

1. Let $x^0 \in \operatorname{int}(K)$. Choose scalars $\delta_0 \geq 0$, $\chi_0 > 0$, $\epsilon_0 \geq 0$, an auxiliary operator $\mathcal{L}^0$, and an operator $\mathcal{Q}^0$ with $\mathcal{Q} \subset \mathcal{Q}^0 \subset \mathcal{Q}_{\epsilon_0}$. Set $k := 0$.
2. If x^k solves the problem $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ then stop.
3. Calculate $x^{k+1} \in K$, $q^k(x^{k+1}) \in \mathcal{Q}^k(x^{k+1})$, and $e^{k+1} \in \mathbb{R}^n$ such that
$$e^{k+1} = \mathcal{F}(x^k) + q^k(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) + \chi_k \nabla_I D(x^{k+1}, x^k)$$
with $\| e^{k+1} \| \leq \delta_k$.
4. Choose $\delta_{k+1} \geq 0$, $\chi_{k+1} > 0$, $\epsilon_{k+1} \geq 0$, $\mathcal{L}^{k+1}$, and $\mathcal{Q}^{k+1}$. Set $k := k + 1$ and go to step 2.

Due to $\| e^{k+1} \| \leq \delta_k$, condition (3.22) implies

$$\sum_{k=0}^{\infty} \| e^{k+1} \| < +\infty. \tag{3.24}$$

All conditions are standard in the context of (interior) proximal auxiliary problem methods (see Conditions (PAP) (page 24) and Conditions (enl-BrPAP) (page 42)). The special requirement (3.21) for the lower bound of the sequence of regularization parameters results from the estimates needed in the convergence proof.

We start with a preliminary result that exploits the weakened co-coercivity condition (A7). The gained estimate is crucial for the subsequent theorem. A similar idea can be found in the proof of [93, Theorem 3.2].

Lemma 3.4.2. *Let Assumption (A7) be fulfilled. For $x, y, v \in K$ it holds*

$$\langle (\mathcal{F} - \mathcal{L}_y)(y) - (\mathcal{F} - \mathcal{L}_y)(v), x - v \rangle \geq -\frac{1}{4\gamma} \| y - x \|^2,$$

where $\gamma > 0$ is the modulus of weakened co-coercivity of $\mathcal{F} - \mathcal{L}_y$.

Proof. In view of Assumption (A7), we get

$$
\begin{aligned}
&\langle(\mathcal{F}-\mathcal{L}_y)(y)-(\mathcal{F}-\mathcal{L}_y)(v), x-v\rangle\\
&=\langle(\mathcal{F}-\mathcal{L}_y)(y)-(\mathcal{F}-\mathcal{L}_y)(v), x-y\rangle+\langle(\mathcal{F}-\mathcal{L}_y)(y)-(\mathcal{F}-\mathcal{L}_y)(v), y-v\rangle\\
&\geq-\langle(\mathcal{F}-\mathcal{L}_y)(y)-(\mathcal{F}-\mathcal{L}_y)(v), y-x\rangle+\gamma\parallel(\mathcal{F}-\mathcal{L}_y)(y)-(\mathcal{F}-\mathcal{L}_y)(v)\parallel^2\\
&\geq-\gamma\parallel(\mathcal{F}-\mathcal{L}_y)(y)-(\mathcal{F}-\mathcal{L}_y)(v)\parallel^2-\frac{1}{4\gamma}\parallel y-x\parallel^2\\
&\quad+\gamma\parallel(\mathcal{F}-\mathcal{L}_y)(y)-(\mathcal{F}-\mathcal{L}_y)(v)\parallel^2\\
&=-\frac{1}{4\gamma}\parallel y-x\parallel^2,
\end{aligned}
$$

where for the last inequality estimate (A.2) from Appendix A.4 is used with $\xi:=\frac{1}{2\gamma}$. □

We proceed with the convergence analysis and prove boundedness of the sequence $\{x^k\}$ of iterates in the next theorem.

Theorem 3.4.3. *Let $\{x^k\}$ be a sequence generated by Algorithm 3.1. Suppose that the Assumptions (A1), (A2), (A3), (A5), (A6), (A7), relation (3.15) for the choice of $\mathcal{Q}^k$, and the conditions (3.20)–(3.23) on the controlling parameters are fulfilled. Then,*

(i) $\{x^k\}$ is bounded,

(ii) $\lim_{k\to\infty}\parallel x^{k+1}-x^k\parallel=0$.

Proof. According to Theorem 3.3.1, Algorithm 3.1 is well-defined and $\{x^k\}$ belongs to $\mathrm{dom}(\mathcal{Q})\cap\mathrm{int}(K)$. Let $\{q^k(x^{k+1})\}$ and $\{e^{k+1}\}$ be the corresponding sequences of iteration scheme (P_e^k). Because of Assumption (A3) and Theorem 2.1.1, the operator

$$\tilde{\mathcal{Q}}:=\mathcal{Q}+\mathcal{N}_K$$

is maximal monotone with $\mathrm{dom}(\tilde{\mathcal{Q}})=\mathrm{dom}(\mathcal{Q})\cap K$. Relation (3.15) and Theorem 2.4.1(b) imply

$$\mathcal{Q}+\mathcal{N}_K\subset\mathcal{Q}^k+\mathcal{N}_K\subset\mathcal{Q}_{\epsilon_k}+\mathcal{N}_K\subset(\mathcal{Q}+\mathcal{N}_K)_{\epsilon_k},$$

which in terms of the operator $\tilde{\mathcal{Q}}$ means that

$$\tilde{\mathcal{Q}}\subset\mathcal{Q}^k+\mathcal{N}_K\subset\tilde{\mathcal{Q}}_{\epsilon_k}.$$

Recalling that $\mathcal{N}_K(x^{k+1})=\{0\}$ for $x^{k+1}\in\mathrm{int}(K)$ provides

$$q^k(x^{k+1})\in\mathcal{Q}^k(x^{k+1})=(\mathcal{Q}^k+\mathcal{N}_K)(x^{k+1}),$$

and hence

$$q^k(x^{k+1}) \in \tilde{\mathcal{Q}}_{\epsilon_k}(x^{k+1}).$$

The definition of the ϵ-enlargement yields

$$\left\langle x - x^{k+1}, q - q^k(x^{k+1}) \right\rangle \geq -\epsilon_k \quad \forall x \in \mathrm{dom}(\tilde{\mathcal{Q}}),\ \forall q \in \tilde{\mathcal{Q}}(x).$$

We divide this inequality by $\chi_k > 0$, insert $-e^{k+1} + e^{k+1}$ and get for an arbitrary $x \in \mathrm{dom}(\tilde{\mathcal{Q}})$ and $q \in \tilde{\mathcal{Q}}(x)$

$$\frac{1}{\chi_k} \left\langle x - x^{k+1}, q - e^{k+1} + e^{k+1} - q^k(x^{k+1}) \right\rangle \geq -\frac{\epsilon_k}{\chi_k},$$

which can be rearranged to

$$\frac{1}{\chi_k} \left\langle x - x^{k+1}, q - e^{k+1} \right\rangle \geq \frac{1}{\chi_k} \left\langle x - x^{k+1}, q^k(x^{k+1}) - e^{k+1} \right\rangle - \frac{\epsilon_k}{\chi_k}. \tag{3.25}$$

From iteration scheme (P_e^k) we have

$$q^k(x^{k+1}) - e^{k+1} = -\mathcal{F}(x^k) - \mathcal{L}^k(x^{k+1}) + \mathcal{L}^k(x^k) - \chi_k \nabla_I D(x^{k+1}, x^k). \tag{3.26}$$

Inserting (3.26) into (3.25) results in

$$\begin{aligned}
&\frac{1}{\chi_k} \left\langle x - x^{k+1}, q - e^{k+1} \right\rangle \\
&\geq \frac{1}{\chi_k} \left\langle x - x^{k+1}, -\mathcal{F}(x^k) - \mathcal{L}^k(x^{k+1}) + \mathcal{L}^k(x^k) - \chi_k \nabla_I D(x^{k+1}, x^k) \right\rangle - \frac{\epsilon_k}{\chi_k} \\
&= \left\langle x - x^{k+1}, -\nabla_I D(x^{k+1}, x^k) \right\rangle + \\
&\quad \frac{1}{\chi_k} \left\langle x - x^{k+1}, -\mathcal{F}(x^k) - \mathcal{L}^k(x^{k+1}) + \mathcal{L}^k(x^k) \right\rangle - \frac{\epsilon_k}{\chi_k}.
\end{aligned} \tag{3.27}$$

Let x^* be an element of $\mathrm{SOL}(\mathcal{F}, \mathcal{Q}, K)$. Then, clearly, $x^* \in \mathrm{dom}(\mathcal{Q}) \cap K = \mathrm{dom}(\tilde{\mathcal{Q}})$. Further, recalling the equivalence of $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ and $\mathrm{IP}(\mathcal{F}, \mathcal{Q}, K)$, it holds that $-\mathcal{F}(x^*) \in \tilde{\mathcal{Q}}(x^*)$. Thus, $x = x^*$ and $q = -\mathcal{F}(x^*)$ can be inserted into (3.27) which gives

$$
\begin{aligned}
&\frac{1}{\chi_k}\left\langle x^* - x^{k+1}, -e^{k+1}\right\rangle \\
&\geq \left\langle x^* - x^{k+1}, -\nabla_I D(x^{k+1}, x^k)\right\rangle \\
&\quad + \frac{1}{\chi_k}\left\langle x^* - x^{k+1}, \mathcal{F}(x^*) - \mathcal{F}(x^k) - \mathcal{L}^k(x^{k+1}) + \mathcal{L}^k(x^k)\right\rangle - \frac{\epsilon_k}{\chi_k} \\
&= \left\langle x^* - x^{k+1}, -\nabla_I D(x^{k+1}, x^k)\right\rangle + \frac{1}{\chi_k}\left\langle x^* - x^{k+1}, \mathcal{L}^k(x^*) - \mathcal{L}^k(x^{k+1})\right\rangle \\
&\quad + \frac{1}{\chi_k}\left\langle x^* - x^{k+1}, (\mathcal{F} - \mathcal{L}^k)(x^*) - (\mathcal{F} - \mathcal{L}^k)(x^k)\right\rangle - \frac{\epsilon_k}{\chi_k} \\
&\geq \left\langle x^* - x^{k+1}, -\nabla_I D(x^{k+1}, x^k)\right\rangle \\
&\quad + \frac{1}{\chi_k}\left\langle x^* - x^{k+1}, (\mathcal{F} - \mathcal{L}^k)(x^*) - (\mathcal{F} - \mathcal{L}^k)(x^k)\right\rangle - \frac{\epsilon_k}{\chi_k}, \qquad (3.28)
\end{aligned}
$$

where for the last inequality the monotonicity of $\mathcal{L}^k$ (see (A6)) was used. Consider now the term $\left\langle x^* - x^{k+1}, -\nabla_I D(x^{k+1}, x^k)\right\rangle$ and write $\nabla_I D(x^{k+1}, x^k)$ explicitly as

$$
\nabla_I D(x^{k+1}, x^k) = -\sum_{i=1}^{p} a_i \left(2l_i(x^{k+1}) - l_i(x^k) - \frac{l_i(x^k)^2}{l_i(x^{k+1})}\right) \qquad (3.29)
$$

in order to get

$$
\begin{aligned}
&\left\langle x^* - x^{k+1}, -\nabla_I D(x^{k+1}, x^k)\right\rangle \\
&= \left\langle x^* - x^{k+1}, \sum_{i=1}^{p} a_i \left(2l_i(x^{k+1}) - l_i(x^k) - \frac{l_i(x^k)^2}{l_i(x^{k+1})}\right)\right\rangle \\
&= \sum_{i=1}^{p}\left(2l_i(x^{k+1}) - l_i(x^k) - \frac{l_i(x^k)^2}{l_i(x^{k+1})}\right)\left\langle x^* - x^{k+1}, a_i\right\rangle \\
&= \sum_{i=1}^{p}\left(2l_i(x^{k+1}) - l_i(x^k) - \frac{l_i(x^k)^2}{l_i(x^{k+1})}\right)(l_i(x^{k+1}) - l_i(x^*)). \qquad (3.30)
\end{aligned}
$$

Applying relation (3.11) with $s = l_i(x^k), t = l_i(x^{k+1})$, and $u = l_i(x^*)$ and recalling the definition of l_i, it follows that

$$
\begin{aligned}
&\left\langle x^* - x^{k+1}, -\nabla_I D(x^{k+1}, x^k)\right\rangle \\
&\geq \sum_{i=1}^{p} \frac{3}{2}\left[(l_i(x^*) - l_i(x^{k+1}))^2 - (l_i(x^*) - l_i(x^k))^2\right] + \frac{1}{2}(l_i(x^{k+1}) - l_i(x^k))^2 \\
&= \sum_{i=1}^{p} \frac{3}{2}\left[(b_i - \langle a_i, x^*\rangle - b_i + \left\langle a_i, x^{k+1}\right\rangle)^2 - (b_i - \langle a_i, x^*\rangle - b_i + \left\langle a_i, x^k\right\rangle)^2\right] \\
&\quad + \frac{1}{2}(b_i - \left\langle a_i, x^{k+1}\right\rangle - b_i + \left\langle a_i, x^k\right\rangle)^2 \\
&= \sum_{i=1}^{p} \frac{3}{2}\left[\left\langle a_i, x^{k+1} - x^*\right\rangle^2 - \left\langle a_i, x^k - x^*\right\rangle^2\right] + \frac{1}{2}\left\langle a_i, x^k - x^{k+1}\right\rangle^2 \\
&= \frac{3}{2}(\parallel A(x^* - x^{k+1}) \parallel^2 - \parallel A(x^* - x^k) \parallel^2) + \frac{1}{2} \parallel A(x^{k+1} - x^k) \parallel^2 . \qquad (3.31)
\end{aligned}
$$

Combining (3.28) and (3.31) and applying Lemma 3.4.2 with $x = x^{k+1}$, $y = x^k$ and $v = x^*$, one gets

$$
\begin{aligned}
&\frac{1}{\chi_k}\left\langle x^* - x^{k+1}, -e^{k+1}\right\rangle \\
&\geq \frac{3}{2}(\parallel A(x^* - x^{k+1}) \parallel^2 - \parallel A(x^* - x^k) \parallel^2) + \frac{1}{2} \parallel A(x^{k+1} - x^k) \parallel^2 \\
&\quad - \frac{1}{\chi_k}\frac{1}{4\gamma} \parallel x^{k+1} - x^k \parallel^2 - \frac{\epsilon_k}{\chi_k}. \qquad (3.32)
\end{aligned}
$$

In view of the norm equivalence (3.3) with constant $a > 0$ and condition (3.20) for the regularization parameter χ_k, it can be concluded that

$$
\begin{aligned}
&\frac{1}{\chi_k}\left\langle x^* - x^{k+1}, -e^{k+1}\right\rangle \\
&\geq \frac{3}{2} \parallel A(x^* - x^{k+1}) \parallel^2 - \frac{3}{2} \parallel A(x^* - x^k) \parallel^2 + \frac{a^2}{2} \parallel x^{k+1} - x^k \parallel^2 \\
&\quad - \frac{1}{\chi_k}\frac{1}{4\gamma} \parallel x^{k+1} - x^k \parallel^2 - \frac{\epsilon_k}{\chi_k} \\
&\geq \frac{3}{2} \parallel A(x^* - x^{k+1}) \parallel^2 - \frac{3}{2} \parallel A(x^* - x^k) \parallel^2 \\
&\quad + \left(\frac{a^2}{2} - \frac{1}{\underline{\chi}}\frac{1}{4\gamma}\right) \parallel x^{k+1} - x^k \parallel^2 - \frac{\epsilon_k}{\underline{\chi}}. \qquad (3.33)
\end{aligned}
$$

The idea for the following transformations is taken from [54, Section 2.3].

To estimate the term $\parallel x^* - x^{k+1} \parallel\parallel e^{k+1} \parallel$ in the case $e^{k+1} \neq 0$, we apply the one-dimensional form of relation (A.2) (see Appendix A.4) with $x = \parallel e^{k+1} \parallel$, $y = \parallel x^* - x^{k+1} \parallel$ and $\xi = \parallel e^{k+1} \parallel$ and obtain

$$\begin{aligned}
&\frac{1}{\chi_k}\left\langle x^* - x^{k+1}, -e^{k+1}\right\rangle \\
&\leq \frac{1}{\chi_k} \parallel x^* - x^{k+1} \parallel \parallel e^{k+1} \parallel \\
&\leq \frac{1}{\chi_k}\left(\frac{1}{2 \parallel e^{k+1} \parallel} \parallel e^{k+1} \parallel^2 + \frac{\parallel e^{k+1} \parallel}{2} \parallel x^* - x^{k+1} \parallel^2\right) \\
&\leq \frac{1}{\underline{\chi}}\left(\frac{1}{2} \parallel e^{k+1} \parallel + \frac{1}{2} \parallel x^* - x^{k+1} \parallel^2 \parallel e^{k+1} \parallel\right) \\
&\leq \frac{1}{\underline{\chi}}\left(\frac{1}{2} \parallel e^{k+1} \parallel + \frac{1}{2a^2} \parallel x^* - x^{k+1} \parallel_A^2 \parallel e^{k+1} \parallel\right), \qquad (3.34)
\end{aligned}$$

where (3.3) and (3.20) are used. If $e^{k+1} = 0$, relation (3.34) is obvious.

Estimates (3.33) and (3.34) now yield

$$\begin{aligned}
&\frac{1}{\underline{\chi}}\left(\frac{1}{2} \parallel e^{k+1} \parallel + \frac{1}{2a^2} \parallel x^* - x^{k+1} \parallel_A^2 \parallel e^{k+1} \parallel\right) \\
&\geq \frac{3}{2} \parallel A(x^* - x^{k+1}) \parallel^2 - \frac{3}{2} \parallel A(x^* - x^k) \parallel^2 + \left(\frac{a^2}{2} - \frac{1}{\underline{\chi}}\frac{1}{4\gamma}\right) \parallel x^{k+1} - x^k \parallel^2 - \frac{\epsilon_k}{\underline{\chi}},
\end{aligned}$$

which can be rearranged to

$$\begin{aligned}
&\left(\frac{3}{2} - \frac{1}{\underline{\chi}}\frac{1}{2a^2} \parallel e^{k+1} \parallel\right) \parallel x^* - x^{k+1} \parallel_A^2 \\
&\quad \leq \frac{3}{2} \parallel x^* - x^k \parallel_A^2 - \left(\frac{a^2}{2} - \frac{1}{\underline{\chi}}\frac{1}{4\gamma}\right) \parallel x^{k+1} - x^k \parallel^2 + \frac{1}{\underline{\chi}}\frac{1}{2} \parallel e^{k+1} \parallel + \frac{\epsilon_k}{\underline{\chi}}
\end{aligned}$$

and

$$\begin{aligned}
&\left(1 - \frac{1}{3\underline{\chi}a^2} \parallel e^{k+1} \parallel\right) \parallel x^* - x^{k+1} \parallel_A^2 \\
&\quad \leq \parallel x^* - x^k \parallel_A^2 - \left(\frac{a^2}{3} - \frac{1}{6\underline{\chi}\gamma}\right) \parallel x^{k+1} - x^k \parallel^2 + \frac{1}{3\underline{\chi}} \parallel e^{k+1} \parallel + \frac{2}{3}\frac{\epsilon_k}{\underline{\chi}}. \qquad (3.35)
\end{aligned}$$

Because of (3.24), $\lim_{k\to\infty} \parallel e^{k+1} \parallel = 0$. Due to $\underline{\chi} > 0$ and $a > 0$, there exists $k_0 \in \mathbb{N}$ such that $\frac{\|e^{k+1}\|}{3\underline{\chi}a^2} \leq \frac{1}{2}$ holds for all $k \geq k_0$. Then, simple calculus (see (A.3) in Appendix A.4) yields

$$1 \leq \left(1 - \frac{1}{3\underline{\chi}a^2} \parallel e^{k+1} \parallel\right)^{-1} \leq 1 + \frac{2}{3\underline{\chi}a^2} \parallel e^{k+1} \parallel \leq 2 \quad \forall k \geq k_0.$$

For (3.35) this implies

$$
\begin{aligned}
&\| x^* - x^{k+1} \|_A^2 \\
&\quad \leq \left(1 - \frac{1}{3\underline{\chi}a^2} \| e^{k+1} \|\right)^{-1} \| x^* - x^k \|_A^2 \\
&\qquad - \left(1 - \frac{1}{3\underline{\chi}a^2} \| e^{k+1} \|\right)^{-1} \left(\frac{a^2}{3} - \frac{1}{6\underline{\chi}\gamma}\right) \| x^{k+1} - x^k \|^2 \\
&\qquad + \left(1 - \frac{1}{3\underline{\chi}a^2} \| e^{k+1} \|\right)^{-1} \frac{1}{3\underline{\chi}} \| e^{k+1} \| \\
&\qquad + \left(1 - \frac{1}{3\underline{\chi}a^2} \| e^{k+1} \|\right)^{-1} \frac{2}{3}\frac{\epsilon_k}{\underline{\chi}} \\
&\quad \leq \left(1 + \frac{2}{3\underline{\chi}a^2} \| e^{k+1} \|\right) \| x^* - x^k \|_A^2 - \left(\frac{a^2}{3} - \frac{1}{6\underline{\chi}\gamma}\right) \| x^{k+1} - x^k \|^2 \\
&\qquad + \frac{2}{3\underline{\chi}} \| e^{k+1} \| + \frac{4}{3}\frac{\epsilon_k}{\underline{\chi}} \qquad (3.36) \\
&\quad \leq \left(1 + \frac{2}{3\underline{\chi}a^2} \| e^{k+1} \|\right) \| x^* - x^k \|_A^2 + \frac{2}{3\underline{\chi}} \| e^{k+1} \| + \frac{4}{3}\frac{\epsilon_k}{\underline{\chi}} \quad \forall k \geq k_0, \qquad (3.37)
\end{aligned}
$$

where for the last inequality condition (3.21) was used, which guarantees that $\left(\frac{a^2}{3} - \frac{1}{6\underline{\chi}\gamma}\right) > 0$. Now, in view of (3.23) and (3.24), Polyak's lemma (see Appendix, Lemma A.4.2) provides that

$$\{\| x^* - x^k \|_A\} \text{ is convergent.} \qquad (3.38)$$

Owing to the norm equivalence (3.3), it follows that

$$\{\| x^* - x^k \|\} \text{ is bounded,} \qquad (3.39)$$

which gives us the desired result that the sequence

$$\{x^k\} \text{ is bounded.}$$

Finally, returning to (3.36) we have

$$
\begin{aligned}
0 &\leq \left(\frac{a^2}{3} - \frac{1}{6\underline{\chi}\gamma}\right) \| x^{k+1} - x^k \|^2 \\
&\leq \left(1 + \frac{2}{3\underline{\chi}a^2} \| e^{k+1} \|\right) \| x^* - x^k \|_A^2 - \| x^* - x^{k+1} \|_A^2 + \frac{2}{3\underline{\chi}} \| e^{k+1} \| + \frac{4}{3}\frac{\epsilon_k}{\underline{\chi}}.
\end{aligned}
$$

Remembering (3.23), (3.24), (3.38), and $\left(\frac{a^2}{3} - \frac{1}{6\underline{\chi}\gamma}\right) > 0$ we obtain

$$\lim_{k\to\infty} \| x^{k+1} - x^k \| = 0.$$

□

Remark 3.4.4. *As a side product of Theorem 3.4.3 the following result can be proved, which appears, e.g., in the analysis of Bregman function based proximal methods (see [54, Proposition 1]):*

$$\lim_{k\to\infty} \left\langle v - x^{k+1}, e^{k+1} \right\rangle = 0 \quad \forall v \in \mathbb{R}^n.$$

Indeed, $\{x^k\}$ is bounded due to Theorem 3.4.3(i), and $\lim_{k\to\infty} \| e^k \| = 0$ in view of (3.24). With

$$0 \le |\left\langle v - x^{k+1}, e^{k+1} \right\rangle| \le \| v - x^{k+1} \| \| e^{k+1} \| \quad \forall v \in \mathbb{R}^n$$

the stated result is proved.

We also like to remark that the stronger result

$$\sum_{k=0}^{\infty} \| x^{k+1} - x^k \| < \infty$$

can be obtained from (3.36) and a generalization of Polyak's lemma as given in the Appendix, Lemma A.4.3.

We are ready to present the main convergence result.

Theorem 3.4.5. *Let the assumptions of Theorem 3.4.3 be valid. Suppose further that Assumptions (A4) and (A8) hold. Then the sequence $\{x^k\}$, generated by Algorithm 3.1, converges to a solution of* $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$.

Proof. Combining relations (3.27) and (3.30) from the proof of Theorem 3.4.3, we get for $\tilde{\mathcal{Q}} := \mathcal{Q} + \mathcal{N}_K$ and arbitrary $x \in \mathrm{dom}(\tilde{\mathcal{Q}})$ and $q \in \tilde{\mathcal{Q}}(x)$

$$\begin{aligned}
&\left\langle x - x^{k+1}, q - e^{k+1} \right\rangle \\
&\ge \chi_k \left\langle x - x^{k+1}, -\nabla_I D(x^{k+1}, x^k) \right\rangle \\
&\quad + \left\langle x - x^{k+1}, -\mathcal{F}(x^k) - \mathcal{L}^k(x^{k+1}) + \mathcal{L}^k(x^k) \right\rangle - \epsilon_k \\
&= \chi_k \sum_{i=1}^{p} (l_i(x^{k+1}) - l_i(x)) \left(2l_i(x^{k+1}) - l_i(x^k) - \frac{l_i(x^k)^2}{l_i(x^{k+1})} \right) \\
&\quad + \left\langle x - x^{k+1}, -\mathcal{F}(x^k) - \mathcal{L}^k(x^{k+1}) + \mathcal{L}^k(x^k) \right\rangle - \epsilon_k. \qquad (3.40)
\end{aligned}$$

Note that (3.30) is not only valid for $x = x^*$ but for all $x \in \mathrm{dom}(\tilde{\mathcal{Q}})$. Now, let us estimate the first summand on the right hand side of (3.40). Applying (3.13) with $t = l_i(x^{k+1}), u = l_i(x), s = l_i(x^k)$ and incorporating the boundedness of $\{\chi_k\}$ as in (3.20), we get the relation

$$\begin{aligned}
&\chi_k \sum_{i=1}^{p} (l_i(x^{k+1}) - l_i(x)) \left(2l_i(x^{k+1}) - l_i(x^k) - \frac{l_i(x^k)^2}{l_i(x^{k+1})} \right) \\
&\geq \bar{\chi} \min\{0, \sum_{i=1}^{p} (l_i(x^k) - l_i(x^{k+1}))(3l_i(x) - (l_i(x^k) + 2l_i(x^{k+1})))\} \\
&=: \bar{\chi} c_k(x). \qquad (3.41)
\end{aligned}$$

Theorem 3.4.3 provides that $\lim_{k\to\infty} \parallel x^{k+1} - x^k \parallel = 0$. Therefore, it follows for all $i = 1, \ldots, p$

$$0 \leq \lim_{k\to\infty} |l_i(x^k) - l_i(x^{k+1})| = \lim_{k\to\infty} |\left\langle a_i, x^{k+1} - x^k \right\rangle| \leq \lim_{k\to\infty} \parallel a_i \parallel \parallel x^{k+1} - x^k \parallel = 0$$

and thus

$$\lim_{k\to\infty} l_i(x^k) - l_i(x^{k+1}) = 0.$$

Further, Theorem 3.4.3 establishes that $\{x^k\}$ is a bounded sequence, which implies that

$$\{l_i(x^k) + 2l_i(x^{k+1})\} = \{3b_i - \left\langle a_i, x^k \right\rangle - 2\left\langle a_i, x^{k+1} \right\rangle\} \quad \text{is bounded.}$$

As a consequence, for all $x \in \mathrm{dom}(Q) \cap K$,

$$\lim_{k\to\infty} \bar{\chi} c_k(x) = 0. \qquad (3.42)$$

Because of the boundedness of $\{x^k\}$, there exists a subsequence $\{x^{k_j}\}$ such that

$$\lim_{j\to\infty} x^{k_j} = x^\infty. \qquad (3.43)$$

With the relation

$$0 \leq \parallel x^{k_j+1} - x^\infty \parallel = \parallel x^{k_j+1} - x^{k_j} + x^{k_j} - x^\infty \parallel \leq \parallel x^{k_j+1} - x^{k_j} \parallel + \parallel x^{k_j} - x^\infty \parallel$$

and Theorem 3.4.3(ii) it follows that

$$\lim_{j\to\infty} x^{k_j+1} = x^\infty. \qquad (3.44)$$

Now, we pass to the subsequence $\{x^{k_j}\}$ in (3.40) and (3.41) and obtain

$$\begin{aligned}&\left\langle x - x^{k_j+1}, q - e^{k_j+1}\right\rangle \\ &\geq \bar{\chi} c_{k_j}(x) + \left\langle x - x^{k_j+1}, -\mathcal{F}(x^{k_j}) - \mathcal{L}^{k_j}(x^{k_j+1}) + \mathcal{L}^{k_j}(x^{k_j})\right\rangle - \epsilon_{k_j}. \end{aligned} \tag{3.45}$$

Consider the limit for $j \to \infty$ in (3.45). Recall that $\mathcal{F}$ is continuous as assumed in (A4) and that $\mathcal{L}^{k_j}$ fulfills the convergence condition (A8). Further, (3.23) and (3.24) ensure that $\lim_{j\to\infty} e^{k_j+1} = 0$ and $\lim_{j\to\infty} \epsilon_{k_j} = 0$. Together with (3.42), (3.43), and (3.44) this results in

$$\langle x - x^\infty, q - (-\mathcal{F}(x^\infty))\rangle \geq 0. \tag{3.46}$$

Since $\tilde{\mathcal{Q}}$ is maximal monotone and $x \in \mathrm{dom}(Q) \cap K$ and $q \in \tilde{\mathcal{Q}}(x)$ are arbitrary, we get

$$-\mathcal{F}(x^\infty) \in \tilde{\mathcal{Q}}(x^\infty). \tag{3.47}$$

Hence, $x^\infty \in \mathrm{dom}(\mathcal{Q}) \cap K$ and

$$x^\infty \in \mathrm{SOL}(\mathcal{F}, \mathcal{Q}, K). \tag{3.48}$$

Now, repeating the argumentation in the proof of Theorem 3.4.3 for x^∞ instead of x^*, we have (see (3.38)) that

$$\{\parallel x^\infty - x^k \parallel_A\} \text{ is convergent.}$$

Since $\lim_{j\to\infty} x^{k_j} = x^\infty$, it follows that $\lim_{j\to\infty} \parallel x^\infty - x^{k_j} \parallel_A = 0$ and therefore

$$\lim_{k\to\infty} \parallel x^\infty - x^k \parallel_A = 0.$$

In view of the norm equivalence (3.3), relation

$$0 \leq \parallel x^\infty - x^k \parallel \leq \frac{1}{a} \parallel x^\infty - x^k \parallel_A$$

leads to the conclusion that the entire sequence $\{x^k\}$ converges to the solution x^∞. □

4. Self-concordance of the Logarithmic-quadratic Distance

In the papers of Auslender/Teboulle/Ben-Tiba [4, 5, 6] it is mentioned without proof that the logarithmic-quadratic distance function satisfies a self-concordance property, which allows to solve the auxiliary problems by an efficient Newton method. We will have a closer look at that relation because in Chapter 6 the Newton method will be used to solve the LQPAP auxiliary problems. We recall the basic definition and properties of (strongly) self-concordant functions and then give a proof that the logarithmic-quadratic distance function $D(\cdot, y)$ is a strongly self-concordant function on $\operatorname{int}(K)$. Moreover, we explain why $D(\cdot, y)$ is not a self-concordant barrier.

The notation used in this chapter is adopted from Nesterov/Nemirovskii [73]. Let $F : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a three times continuously differentiable, proper, convex function with $\operatorname{dom}(F)$ open. The first, second, and third derivative of F at $x \in \operatorname{dom}(F)$ are denoted by $F'(x)$, $F''(x)$, and $F'''(x)$, respectively. Further, denote

$$F'''(x)[h] = \lim_{t \to 0} \frac{1}{t}[F''(x + th) - F''(x)].$$

Note that on the right hand side we have $(n \times n)$-matrices. We define for a point $x \in \operatorname{dom}(F)$ and a vector $h \in \mathbb{R}^n$

$$\begin{aligned} \mathcal{D}F(x)[h] &= \langle F'(x), h \rangle , \\ \mathcal{D}^2F(x)[h, h] &= \langle F''(x)h, h \rangle , \\ \mathcal{D}^3F(x)[h, h, h] &= \langle F'''(x)[h]h, h \rangle . \end{aligned}$$

In general, $\mathcal{D}^kF(x)[h_1, \ldots, h_k]$ denotes the value of the k-th differential of F taken at x along the collection of directions $h_1, \ldots, h_k$.

4.1 Self-concordant functions and self-concordant barriers

Motivation of self-concordant functions. Nesterov/Nemirovskii [73] introduced the notion of self-concordance to develop a general theory of interior point polynomial-time methods for convex programming. The motivation for this notion comes from a closer study of the Newton method for minimizing F.

The Newton scheme

$$x^{k+1} = x^k - (F''(x^k))^{-1}F'(x^k)$$

locally converges quadratically if F is strongly convex with constant κ and F'' is Lipschitz continuous with constant L, i.e.,

$$\| (F''(x) - F''(y))v \| \leq L \| x - y \| \| v \| \quad \forall\, x, y, v \in \mathbb{R}^n$$

(see [76, Theorem 1]). Locally quadratic convergence means that if a start point x^0 fulfills

$$q := \frac{L}{2\kappa^2} \| F'(x^0) \| < 1,$$

it holds

$$\| x^k - x^* \| \leq \frac{2\kappa}{L} q^{2^k}.$$

The above Lipschitz condition implies for a point $x \in \mathbb{R}^n$ that

$$\| F'''(x)[h]v \| \leq L \| h \| \| v \| \quad \forall\, h, v \in \mathbb{R}^n.$$

This means that at any point $x \in \mathbb{R}^n$ we have

$$\langle F'''(x)[h]v, v\rangle \leq L \| h \| \| v \|^2 \quad \forall\, h, v \in \mathbb{R}^n.$$

Nesterov/Nemirovskii replace the Euclidean norm in the definition of Lipschitz continuity by a local seminorm induced by the second-order differential of F, i.e.,

$$\| h \|_{F''(x)} = \langle F''(x)h, h\rangle^{1/2}.$$

Then the property

$$\langle F'''(x)[h]h, h\rangle \leq \vartheta \| h \|^3_{F''(x)}$$

with $\vartheta \geq 0$ leads to the class of *self-concordant* functions. Nesterov/Nemirovskii show that this property implies interesting results on the behavior of the Newton method as applied to F (see Section 4.3).

Definition of self-concordant functions. Now we give a precise definition of a self-concordant function.

Definition 4.1.1 ([73], Definition 2.1.1, [72], Definition 4.1.1). *Let $S \subset \mathbb{R}^n$ be an open, nonempty, convex set, $F : S \to \mathbb{R} \cup \{+\infty\}$ a three times continuously differentiable function, $\vartheta \geq 0$. F is called self-concordant on S with parameter ϑ (ϑ-self-concordant) if F is a convex function on S and*

$$|\mathcal{D}^3 F(x)[h, h, h]| \leq \vartheta(\mathcal{D}^2 F(x)[h, h])^{3/2} \quad \forall x \in S,\ \forall h \in \mathbb{R}^n. \tag{4.1}$$

A function F that is ϑ-self-concordant on S is called strongly ϑ-self-concordant if the sets

$$\{x \in \mathbb{R}^n : F(x) \leq t\} \cap S$$

are closed in $\mathbb{R}^n$ for each $t \in \mathbb{R}$.

Note that this definition does not exactly match the definition of a ϑ-self-concordant function as given in [73]. The above definition is adopted from [72], and a ϑ-self-concordant function in our definition is in fact a $\frac{4}{\vartheta^2}$-self-concordant function in [73].

It is easy to see that condition (4.1) is equivalent to

$$|\mathcal{D}^3 F(x)[h,h,h]| \leq \vartheta \parallel h \parallel^3_{F''(x)} \quad \forall x \in S,\ \forall h \in \mathbb{R}^n,$$

and that in the case $n = 1$ condition (4.1) reduces to

$$|F'''(x)| \leq \vartheta (F''(x))^{3/2} \quad \forall x \in S.$$

Closedness of the level sets $\{x \in \mathbb{R}^n : F(x) \leq t\}$ of a function $F : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is equivalent to F being lower semicontinuous on $\mathbb{R}^n$. Since $F \in C^3(\mathbb{R}^n)$ is required in Definition 4.1.1, F is continuous on $\mathbb{R}^n$. It follows that every function F that is ϑ-self-concordant on $\mathbb{R}^n$ is strongly ϑ-self-concordant. This is no longer true if F is self-concordant on a proper subset $S \subset \mathbb{R}^n$. In the case $\{x \in \mathbb{R}^n : F(x) \leq t\} \supset S$ for some $t \in \mathbb{R}$ the set $\{x \in S : F(x) \leq t\}$ is not closed. We have the following characterization of a strongly self-concordant function.

Lemma 4.1.2 ([73], Remark 2.1.1). *A function F that is self-concordant on S is strongly self-concordant if and only if S is the "natural domain", i.e., if and only if*

$$F(x^i) \to +\infty \quad \text{if} \quad S \ni x^i \to \mathrm{bd}(S).$$

Examples and properties of self-concordant functions. Some examples of self-concordant functions are:

1. Constant functions, linear functions and convex quadratic functions are (strongly) 0-self-concordant on $\mathbb{R}^n$.
2. The logarithmic barrier function for $\mathbb{R}_{++}$, i.e., $F : \mathbb{R}_{++} \to \mathbb{R}$, $F(x) = -\log(x)$, is 2-self-concordant on $\mathbb{R}_{++}$.
3. The logarithmic barrier function for $S := \{x \in \mathbb{R}^n : \langle a, x\rangle < \beta\}$, defined by $F : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$,

$$F(x) = \begin{cases} -\log(\beta - \langle a, x\rangle) & \text{if } \langle a, x\rangle < \beta \\ +\infty & \text{otherwise,} \end{cases}$$

   is 2-self-concordant on S.

On the other hand, it is easy to verify that the following functions of one variable are *not* self-concordant:

$$F(x) = e^x, \quad F(x) = \frac{1}{x^p},\ x > 0,\ p > 0, \quad F(x) = |x|^p,\ p > 2.$$

Self-concordance is an affine-invariant property and stable under scaling, summation, and with respect to direct products.

Lemma 4.1.3 ([72], Theorem 4.1.2). *Let $F : S \to \mathbb{R} \cup \{+\infty\}$ be (strongly) ϑ-self-concordant on S. Let further $\mathcal{A} : \mathbb{R}^n \to \mathbb{R}^m$, $\mathcal{A}(x) = Ax + b$ be given such that $S' := \{x \in \mathbb{R}^n : \mathcal{A}(x) \in S\} \neq \emptyset$. Then the function $F' : S' \to \mathbb{R} \cup \{+\infty\}$, $F'(x) = F(\mathcal{A}(x))$ is also (strongly) ϑ-self-concordant.*

Lemma 4.1.4 ([72], Theorem 4.1.1). *Let $F_i : S_i \to \mathbb{R} \cup \{+\infty\}$ be ϑ_i-self-concordant on S_i, $p_i > 0$, $i = 1, 2$, and $S_1 \cap S_2 \neq \emptyset$. Consider the function*

$$F : S_1 \cap S_2 \to \mathbb{R} \cup \{+\infty\}, \quad F(x) = p_1 F_1(x) + p_2 F_2(x).$$

Then F is ϑ-self-concordant on $S_1 \cap S_2$ with

$$\vartheta = \max\left\{p_1^{-1/2}\vartheta_1, p_2^{-1/2}\vartheta_2\right\}.$$

If under the above assumptions either F_i is strongly ϑ_i-self-concordant on S_i, $i = 1, 2$, or F_1 is strongly ϑ_1-self-concordant on S_1 and $S_1 \subseteq S_2$, then F is strongly ϑ-self-concordant on $S_1 \cap S_2$.

Corollary 4.1.5 ([72], Corollary 4.1.2). *Let $F : S \to \mathbb{R} \cup \{+\infty\}$ be ϑ-self-concordant on S and $p > 0$. Then*

$$\tilde{F} : S \to \mathbb{R} \cup \{+\infty\}, \quad \tilde{F}(x) = pF(x)$$

is self-concordant on S with parameter $p^{-1/2}\vartheta$.

In view of the above corollary it is possible to scale every ϑ-self-concordant function F by $p = \vartheta^2/4$ to get a 2-self-concordant function.

Lemma 4.1.6 ([73], Proposition 2.1.1 (iii)). *Let $F_1 : S_1 \to \mathbb{R} \cup \{+\infty\}$ be ϑ-self-concordant on S_1, and $F_2 : S_2 \to \mathbb{R} \cup \{+\infty\}$ be ϑ-self-concordant on S_2. Then $F : S_1 \times S_2 \to \mathbb{R} \cup \{+\infty\}$, $F(x, y) = F_1(x) + F_2(y)$ is ϑ-self-concordant.*

Self-concordant barriers. We now consider the definition of self-concordant barriers. These functions play a central role in the interior point algorithms investigated by Nesterov/Nemirovskii [73]. As demonstrated above, a self-concordant function can be described as a smooth convex function with the second-order differential being Lipschitz continuous with respect to the local seminorm induced by this second-order differential. Self-concordant barriers are functions that, in addition, are themselves Lipschitz continuous with respect to the above local seminorm.

Definition 4.1.7 ([71], Definition 2.1). *Let S be an open, nonempty, convex subset of $\mathbb{R}^n$, $F : S \to \mathbb{R} \cup \{+\infty\}$ a three times continuously differentiable function. F is called a self-concordant barrier for* $\mathrm{cl}(S)$ *if F is a convex function on S and there exist constants $c_1, c_2 \geq 0$ such that*

$$|\mathcal{D}^3 F(x)[h,h,h]| \leq c_1 (\mathcal{D}^2 F(x)[h,h])^{3/2}, \tag{4.2}$$

$$|\mathcal{D} F(x)[h]| \leq c_2 (\mathcal{D}^2 F(x)[h,h])^{1/2} \tag{4.3}$$

hold for all $x \in S$ and $h \in \mathbb{R}^n$.

Constant functions are self-concordant barriers for $\mathbb{R}^n$ with $c_1 = c_2 = 0$. A self-concordant barrier for $\mathbb{R}_+$ is, for example, $F(x) = -\log(x)$ with $c_1 = 2$ and $c_2 = 1$.

It is shown in [73, Proposition 2.3.1] that analogous statements as in Lemmata 4.1.3, 4.1.4, and 4.1.6 hold for self-concordant barriers, i.e., this property is stable under affine substitutions, with respect to summation, and with respect to direct products.

4.2 Strongly self-concordance of the logarithmic-quadratic distance function

We are now ready to prove that the logarithmic-quadratic distance function (see (3.4)) with fixed second argument is a strongly self-concordant function on its domain. Let $y \in \mathrm{int}(K)$ be arbitrary, but fixed. We recall the first and second differential of $D(\cdot, y)$ using the notation within this chapter and give the values of $\mathcal{D}^2 D(x,y)[h,h]$ and $\mathcal{D}^3 D(x,y)[h,h,h]$. For $x \in \mathrm{int}(K)$ and $h \in \mathbb{R}^n$ it holds

$$\begin{aligned}
D'(x,y) &= -\sum_{i=1}^{p} a_i \left(2l_i(x) - l_i(y) - \frac{l_i(y)^2}{l_i(x)} \right), \\
D''(x,y) &= \sum_{i=1}^{p} \left(2 + \frac{l_i(y)^2}{l_i(x)^2} \right) a_i a_i^T, \\
\mathcal{D}^2 D(x,y)[h,h] &= \langle D''(x,y)h, h \rangle \\
&= \left\langle \sum_{i=1}^{p} \left(2 + \frac{l_i(y)^2}{l_i(x)^2} \right) a_i a_i^T \cdot h, h \right\rangle \\
&= \sum_{k=1}^{n} \sum_{j=1}^{n} h_k h_j \sum_{i=1}^{p} \left(2 + \frac{l_i(y)^2}{l_i(x)^2} \right) a_{ik} a_{ij}, \\
\mathcal{D}^3 D(x,y)[h,h,h] &= \sum_{k=1}^{n} \sum_{j=1}^{n} \sum_{r=1}^{n} h_k h_j h_r \sum_{i=1}^{p} \frac{2 l_i(y)^2}{l_i(x)^3} a_{ik} a_{ij} a_{ir}.
\end{aligned}$$

We first show that $d(\cdot, v)$ (see (3.5)) is ϑ-self-concordant on $\mathbb{R}^p_{++}$ for all $v \in \mathbb{R}^p_{++}$. For that purpose, we define

$$\delta : \mathbb{R} \times \mathbb{R}_{++} \to \mathbb{R}, \quad \delta(\mu, \nu) = \begin{cases} \mu^2 - \mu\nu - \nu^2 \log \frac{\mu}{\nu} & \text{if } \mu \in \mathbb{R}_{++} \\ +\infty & \text{otherwise} \end{cases} \tag{4.4}$$

to get for $u = (u_1, \ldots, u_p)^T \in \mathbb{R}^p_+$ and $v = (v_1, \ldots, v_p)^T \in \mathbb{R}^p_{++}$ that

$$d(u, v) = \sum_{i=1}^{p} \delta(u_i, v_i).$$

Lemma 4.2.1. *For all fixed $\nu > 0$, function $\delta(\cdot, \nu)$ is self-concordant on $\mathbb{R}_{++}$ with parameter $2\nu^{-1}$.*

Proof. Function $\delta(\cdot, \nu)$ is a convex function on the open, convex set $\mathbb{R}_{++}$. We analyze each summand of $\delta(\mu, \nu)$ $(\mu, \nu > 0)$ separately. $\delta_1(\mu, \nu) = \mu^2$ is a convex-quadratic function and thus 0-self-concordant on $\mathbb{R}_{++}$. $\delta_2(\mu, \nu) = -\mu\nu$ is linear in μ and therefore 0-self-concordant on $\mathbb{R}_{++}$. Now, consider $\delta_3(\mu, \nu) = -\nu^2 \log \frac{\mu}{\nu}$. By Example 2 (page 69) and Lemma 4.1.3, we conclude that $\mu \mapsto -\log \frac{\mu}{\nu}$ is 2-self-concordant on $\mathbb{R}_{++}$. Corollary 4.1.5 implies that $\delta_3(\cdot, \nu)$ is self-concordant on $\mathbb{R}_{++}$ with parameter $2\nu^{-1}$. With Lemma 4.1.4 we can conclude that $\delta(\cdot, v)$ is self-concordant on $\mathbb{R}_{++}$ with parameter $2\nu^{-1}$. □

If a function is self-concordant with parameter ϑ then it is also self-concordant with any parameter $\vartheta' \geq \vartheta$. We use this property and Lemma 4.1.6 to show that $d(\cdot, v)$ is strongly self-concordant for all fixed $v \in \mathbb{R}^p_{++}$.

Lemma 4.2.2. *Let $v \in \mathbb{R}^p_{++}$. Then function $d(\cdot, v)$ is strongly self-concordant on $\mathbb{R}^p_{++}$ with parameter $\vartheta = \max\{2v_i^{-1} : i = 1, \ldots, p\}$.*

Proof. Let $v = (v_1, \ldots, v_p)^T \in \mathbb{R}^p_{++}$ be fixed. For all $i = 1, \ldots, p$, Lemma 4.2.1 states that $\delta(\cdot, v_i)$ is self-concordant with parameter $2v_i^{-1}$. Therefore, the collection of functions $\{\delta(\cdot, v_i)\}_{i=1}^p$ is self-concordant with parameter $\vartheta = \max\{2v_i^{-1} : i = 1, \ldots, p\}$. Lemma 4.1.6 leads to the conclusion that $d(\cdot, v)$ is ϑ-self-concordant. To prove strong self-concordance, let $\{u^j\}$ be a sequence in $\mathbb{R}^p_{++}$ that converges to the boundary of $\mathbb{R}^p_{++}$, i.e.,

$$J_1 := \{l \in \{1, \ldots, p\} : u_l^j \to 0 \text{ for } j \to \infty\} \neq \emptyset.$$

Define further

$$J_2 := \{l \in \{1, \ldots, p\} : u_l^j \to \bar{u}_l \in \mathbb{R}_{++} \text{ for } j \to \infty\},$$
$$J_3 := \{l \in \{1, \ldots, p\} : u_l^j \to +\infty \text{ for } j \to \infty\}.$$

$J_2 = \emptyset$ and/or $J_3 = \emptyset$ is possible. For $j \to \infty$ we have

$$(u_l^j)^2 - u_l^j v_l - v_l^2 \log \frac{u_l^j}{v_l} \to +\infty \quad \text{for } l \in J_1,$$
$$(u_l^j)^2 - u_l^j v_l - v_l^2 \log \frac{u_l^j}{v_l} \to (\bar{u}_l)^2 - \bar{u}_l v_l - v_l^2 \log \frac{\bar{u}_l}{v_l} \quad \text{for } l \in J_2.$$

For $l \in J_3$ it holds

$$\begin{aligned}(u_l^j)^2 - u_l^j v_l - v_l^2 \log \frac{u_l^j}{v_l} &\geq (u_l^j)^2 - u_l^j v_l + v_l^2 (1 - \frac{u_l^j}{v_l}) \\ &= (u_l^j)^2 - 2u_l^j v_l + v_l^2 \\ &= (u_l^j - v_l)^2 \to +\infty \quad \text{for } j \to \infty.\end{aligned}$$

So,

$$(u_l^j)^2 - u_l^j v_l - v_l^2 \log \frac{u_l^j}{v_l} \to +\infty \quad \text{for } l \in J_3.$$

Since $J_1 \neq \emptyset$ it follows that

$$d(u^j, v) = \sum_{l=1}^{p} (u_l^j)^2 - u_l^j v_l - v_l^2 \log \frac{u_l^j}{v_l} \to +\infty \quad \text{for } j \to \infty.$$

Now, Lemma 4.1.2 completes the proof. □

Now, we are ready to present the main result.

Theorem 4.2.3. *Let $y \in \operatorname{int}(K)$. Then function $D(\cdot, y)$ is strongly self-concordant on $\operatorname{int}(K)$ with parameter*

$$\vartheta_y = \max \left\{ \frac{2}{l_i(y)} : i = 1, \ldots, p \right\}. \tag{4.5}$$

Proof. Let $y \in \operatorname{int}(K)$. Having $D(\cdot, y) = d(\cdot, l(y)) \circ l$ with $l(x) = b - Ax$, it follows from Lemma 4.1.3 and Lemma 4.2.2 that $D(\cdot, y)$ is ϑ_y-self-concordant on $\operatorname{int}(K)$. Let $\{x^j\}$ be a sequence in $\operatorname{int}(K)$ converging to the boundary of K. Then $l(x^j)$ converges to the boundary of $\mathbb{R}^p_{++}$. Hence, $D(x^j, y) = d(l(x^i), l(y)) \to +\infty$ for $j \to \infty$, and with Lemma 4.1.2 strong self-concordance is established. □

Remark 4.2.4. *It is common to call a continuous function $F : K \to \mathbb{R}$ a* barrier function *for K if $F(x) \to +\infty$ when x approaches the boundary of K (see, e.g., [72, Definition 1.3.2]). Thus, we have just proved that for all fixed $y \in \operatorname{int}(K)$, $D(\cdot, y)$ is a barrier function for K. Note that this notion is different to that of a self-concordant barrier.*

In the following lemma we finally show that $\delta(\cdot,\nu)$ is not a self-concordant barrier for $\mathbb{R}_+$, which implies that $D(\cdot,y)$ is not a self-concordant barrier for K. We can state in view of (4.3) :

Lemma 4.2.5. *For the function $\delta(\cdot,\nu)$, $\nu\in\mathbb{R}_{++}$, there is no constant $c\geq 0$ such that*

$$|\delta'_\mu(\mu,\nu)|\leq c(\delta''_\mu(\mu,\nu))^{1/2}\quad\forall\mu>0.$$

Proof. Suppose that a constant c with the desired property exists. Fix $\nu>0$. For $\mu>0$ it holds

$$\begin{aligned}
&|\delta'_\mu(\mu,\nu)|\leq c(\delta''_\mu(\mu,\nu))^{1/2}\\
&\Leftrightarrow |2\mu-\nu-\frac{\nu^2}{\mu}|\leq c(2+\frac{\nu^2}{\mu^2})^{1/2}\\
&\Leftrightarrow (2\mu-\nu-\frac{\nu^2}{\mu})^2\leq c^2(2+\frac{\nu^2}{\mu^2})\\
&\Leftrightarrow \frac{(2\mu-\nu-\frac{\nu^2}{\mu})^2}{(2+\frac{\nu^2}{\mu^2})}\leq c^2\\
&\Leftrightarrow \frac{4\mu^2-4\mu\nu+2\nu^3\mu^{-1}+\nu^4\mu^{-2}-3\nu^2}{2+\frac{\nu^2}{\mu^2}}\leq c^2.
\end{aligned}$$

However, for $\mu\to+\infty$ the left hand side tends to infinity. This is a contradiction. □

4.3 Effect on the Newton method

On the use of self-concordant barriers. The aim of Nesterov/Nemirovskii [73] is to present a general approach to the design of polynomial-time interior point methods for nonlinear convex problems. Their approach originates in the following observation about interior point methods for linear programs: It is shown by Gonzaga [37] that the logarithmic barrier method for a linear program results in a polynomial-time algorithm if a Newton method is used to solve the auxiliary problems. A closer look at the properties of the logarithmic barrier shows that only two of them are responsible for this efficiency. These are exactly the properties described by the notion of a self-concordant barrier. Thus, Nesterov/Nemirovskii investigate in the extension to use some self-concordant barrier for a general closed, convex feasible set to get a polynomial-time barrier method for a linear, convex constrained program. They show that the accuracy of a given approximate solution can be improved by a constant factor if a certain amount of Newton steps is performed, where this amount only depends on

the parameters c_1 and c_2 of the self-concordant barrier. This gives a theoretical reason to use the Newton method for the solution of the auxiliary problems occurring in such a barrier method.

Consequences of the strong self-concordance of $D(\cdot, y)$. Now, return to the logarithmic-quadratic distance function. Lemma 4.2.5 shows that $D(\cdot, y)$ is not a self-concordant barrier for K. Thus, $D(\cdot, y)$ cannot be used within the above described approach to construct an efficient barrier method. But the fact that $D(\cdot, y)$ is a strongly ϑ_y-self-concordant function, with ϑ_y as in (4.5), has some interesting consequences.

To explain these consequences, we first describe the properties of the (damped) Newton method as applied to a function $F : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ that is strongly ϑ-self-concordant on S (see [73], Chapter 2.2). For that purpose, the notion of the *Newton decrement* will be needed which is defined as follows. Let $F : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be ϑ-self-concordant on S. Let further F be *nondegenerate* on S, i.e., $F''(x)$ is nonsingular for every $x \in S$. Then the quantity

$$\lambda(F, x) = \frac{\vartheta}{2} \sqrt{(F'(x))^T [F''(x)]^{-1} F'(x)} \tag{4.6}$$

is called the Newton decrement of F at $x \in S$. In other words, the Newton decrement $\lambda(F, x)$ is, up to a constant factor, the (local) norm of the gradient $F'(x)$ measured by $\| \cdot \|_{F''(x)^{-1}}$. Another interpretation of the Newton decrement is as follows. Consider the quadratic approximation of F in x:

$$\Phi(y) = F(x) + \langle F'(x), y - x \rangle + \frac{1}{2} \langle F''(x)(y - x), y - x \rangle .$$

Its minimum is attained at $y = x - F''(x)^{-1} F'(x)$. The corresponding minimal value is equal to $F(x) - \frac{1}{2} \langle F'(x), F''(x)^{-1} F'(x) \rangle$. Thus, $\lambda(F, x)$ is an accuracy measure in the following sense:

$$F(x) - \min\{\Phi(y) : y \in \mathbb{R}^n\} = \frac{1}{2} \left\langle F'(x), F''(x)^{-1} F'(x) \right\rangle = \frac{2}{\vartheta^2} (\lambda(F, x))^2.$$

One important property of the Newton decrement is that it provides information about the existence of a unique minimizer of F.

Theorem 4.3.1 ([73], Theorem 2.2.2). *Let $F : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a function that is strongly ϑ-self-concordant on S and nondegenerate on S. Suppose that $\lambda(F, x) < 1$ for some $x \in S$. Then F attains its unique minimum over S.*

Now, consider the (damped) Newton iteration applied on F starting at $x^0 \in S$ and given by

$$x^{k+1} = x^k - s(\lambda(F, x^k))[F''(x^k)]^{-1}F'(x^k). \tag{4.7}$$

The step size s is chosen in a special way depending on the Newton decrement $\lambda_k := \lambda(F, x^k)$. Let $\lambda_* = 2 - \sqrt{3} \approx 0.2679$ and $\lambda' \in [\lambda_*, 1)$. Then

$$s(\lambda_k) = \begin{cases} \frac{1}{1+\lambda_k} & \text{if } \lambda_k > \lambda' \\ \frac{1-\lambda_k}{\lambda_k(3-\lambda_k)} & \text{if } \lambda' \geq \lambda_k \geq \lambda_* \\ 1 & \text{if } \lambda_k < \lambda_*. \end{cases} \tag{4.8}$$

The following theorem contains the main result concerning the method (4.7)–(4.8):

Theorem 4.3.2 ([73], Theorem 2.2.3). *Let $F : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a function that is strongly ϑ-self-concordant on S and nondegenerate on S. Then*

(i) F is bounded from below on S if and only if it attains its minimum over S.

(ii) The following relations hold for the method (4.7)–(4.8):

(a) $\{\lambda_k > \lambda'\} \Rightarrow$
$\{F(x^{k+1}) \leq F(x^k) - \frac{4}{\vartheta^2}(\lambda_k - \log(1+\lambda_k)) \leq F(x^k) - \frac{4}{\vartheta^2}(\lambda' - \log(1+\lambda'))\}$,

(b) $\{\lambda' \geq \lambda_k \geq \lambda_*\} \Rightarrow$
$\left\{\lambda_{k+1} \leq \frac{6\lambda_k - \lambda_k^2 - 1}{4} < \lambda_k\right\}$ *and* $\left\{1 - \lambda_{k+1} \geq \frac{5-\lambda_k}{4}(1-\lambda_k) \geq \frac{5-\lambda'}{4}(1-\lambda_k)\right\}$,

(c) $\{\lambda_k < \lambda_*\} \Rightarrow$
$\left\{\lambda_{k+1} \leq \left(\frac{\lambda_k}{1-\lambda_k}\right)^2 < \frac{\lambda_k}{2}\right\}$.

Moreover, if $\lambda_k < \frac{1}{3}$ then

$$F(x^k) - \min_{x \in S} F(x) \leq \frac{2}{\vartheta^2} \frac{(\omega(\lambda_k))^2(1+\omega(\lambda_k))}{1-\omega(\lambda_k)},$$

where $\omega(\lambda_k) = 1 - (1-3\lambda_k)^{1/3}$.

In other words, if F is a function that is strongly ϑ-self-concordant on S then the objective values of the Newton iterates converge to the minimal value of F over S. Further, $\lambda_k \to 0$ as $k \to \infty$, and the Newton process can be divided into three sequential stages depending on the value of λ_k. At the first stage, the Newton method decreases the function values in each iteration at least by a constant that is not smaller than $\frac{4}{\vartheta^2}(\lambda' - \log(1+\lambda')) > 0$. The number N_1 of steps at this stage is bounded by

$$N_1 \leq \frac{\vartheta^2}{4}(\lambda' - \log(1+\lambda'))^{-1}(F(x^0) - \min_{x \in S} F(x)).$$

In the second stage, the values λ_k decrease and the values $(1 - \lambda_k)$ increase with geometric progression. The number N_2 of iterations at this stage is bounded by

$$N_2 \leq 1 + (\log((5 - \lambda')/4))^{-1} \log \left(\frac{1 - \lambda_*}{1 - \lambda'} \right).$$

In the third stage, the standard Newton method with step size one is applied. Here, the efficiency of the method becomes obvious because the Newton decrement converges quadratically from any point where it is less than the constant $\lambda_* = 2 - \sqrt{3}$.

Consider now the problem of minimizing a convex function $f : \mathbb{R}^n \to \mathbb{R}$ over the polyhedral set $K = \{x \in \mathbb{R}^n : Ax \leq b\}$. If f is ϑ_f-self-concordant then the function

$$f + \chi D(\cdot, y)$$

with $\chi > 0$ and $y \in \operatorname{int}(K)$ is strongly ϑ-self-concordant with $\vartheta = \max\{\vartheta_f, \chi^{-1/2}\vartheta_y\}$ (see Lemma 4.1.4).

This is an interesting information if the LQPAP method is applied to a variational inequality $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ where the auxiliary problems (P_e^k) are equivalent to the inexact solution of

$$\min_{x \in \mathbb{R}^n} \left\{ f(x) + \chi_k D(x, x^k) \right\}. \tag{4.9}$$

If f is ϑ_f-self-concordant, the (damped) Newton method (4.7)–(4.8) applied to (4.9) has the described properties of the Newton decrements and the function values.

5. Categories of Problems and Analysis of the Assumptions on $\mathcal{L}^k$

In the preceding chapters, the LQPAP method and the logarithmic-quadratic distance function were theoretically analyzed. In this chapter, we start to work towards numerical implementations.

We first describe the categories of problems that will be considered for implementation. Then we discuss the possible choices of the operators $\mathcal{Q}^k$ and the auxiliary operators $\mathcal{L}^k$ and the resulting LQPAP auxiliary problems.

Finally, we take a closer look at the assumptions on the auxiliary operator $\mathcal{L}^k$, because for its usage in concrete test examples it is important to know how to verify these assumptions. Our focus will lie on Assumption (A7), which describes the interrelation of $\mathcal{F}$ and $\mathcal{L}^k$. To this end, a more intensive study of the notion of co-coercivity is needed.

In the following, $\{x^k\}$ denotes a generated sequence of LQPAP iterates in $\mathrm{dom}(\mathcal{Q}) \cap \mathrm{int}(K)$.

Recall that for a matrix $C \in \mathbb{R}^{n\times n}$ the Euclidean matrix norm can be calculated as

$$\|C\|_2 = \sqrt{\mu}$$

where μ is the largest eigenvalue of $C^T C$. Positive semidefiniteness (resp. positive definiteness) of a matrix $C \in \mathbb{R}^{n\times n}$ is defined without supposing symmetry of C, i.e., C is said to be positive semidefinite (resp. positive definite) if

$$\langle Cx, x\rangle \geq 0 \quad \forall x \in \mathbb{R}^n \quad (\text{resp. } \langle Cx, x\rangle > 0 \quad \forall x \in \mathbb{R}^n \setminus \{0\}).$$

A nonsymmetric matrix C is positive (semi)definite if and only if the same is valid for its symmetric part

$$\widehat{C} = \frac{1}{2}\left(C + C^T\right).$$

5.1 Categories of problems under consideration

Let $\mathrm{VI}(\mathcal{T}, K)$ be a variational inequality problem with a maximal monotone operator $\mathcal{T}$ and a polyhedral restriction set K. The LQPAP method is based on an appropriate

splitting of $\mathcal{T}$ into $\mathcal{F} + \mathcal{Q}$, where $\mathcal{F}$ is a continuous, monotone, and single-valued operator, and $\mathcal{Q}$ is a maximal monotone, multi-valued operator. We will now consider some possibilities of such splittings.

In general, the splitting of $\mathcal{T}$ into $\mathcal{F} + \mathcal{Q}$ is rather flexible. However, for an implementation we intend to exploit the advantage of the LQPAP scheme that even problems with a nonsymmetric operator $\mathcal{T}$ can be solved by means of optimization problems. The only restriction is that $\mathcal{T}$ must not contain a nonsymmetric multi-valued part. Then the nonsymmetric single-valued parts of $\mathcal{T}$ can be included into $\mathcal{F}$. In the LQPAP scheme, $\mathcal{F}$ is fixed at the current iterate which enables the transformation of the LQPAP auxiliary problems into optimization problems.

Of course, other choices of $\mathcal{F}$ can be considered if there is no nonsymmetric part. Altogether, one has the following possibilities:

- $\mathcal{F}$ single-valued, continuous, monotone, nonsymmetric,
- $\mathcal{F} = \nabla\psi$, with $\psi : \mathbb{R}^n \to \mathbb{R}$ convex, twice continuously differentiable,
- $\mathcal{F} = 0$.

In view of Assumption (A7), $\mathcal{F}$ should be chosen such that it possesses some monotonicity reserve because $\mathcal{F}$ must be co-coercive if $\mathcal{L}^k = 0$.

Components of $\mathcal{T}$ with no monotonicity reserve and which are symmetric and possibly multi-valued should be represented by the operator $\mathcal{Q}$. The following choices can be distinguished:

- $\mathcal{Q} = \partial\varphi$ with $\varphi : \mathbb{R}^n \to \mathbb{R}$ convex, nondifferentiable,
- $\mathcal{Q} = \nabla\psi$ with $\psi : \mathbb{R}^n \to \mathbb{R}$ convex, differentiable,
- $\mathcal{Q} = 0$.

Among all possible types of problems we will focus on the following three categories in the sequel:

- **Category 1:** VI$(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{F} = 0$, $\mathcal{Q} = \nabla\psi$, or with $\mathcal{F} = \nabla\psi$, $\mathcal{Q} = 0$, i.e.,

$$\text{Find } x^* \in K : \ \langle \nabla\psi(x^*), x - x^* \rangle \geq 0 \quad \forall x \in K,$$

  which is equivalent to x^* being a solution of

$$\min \ \psi(x), \quad \text{s.t. } x \in K.$$

- **Category 2:** VI$(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{F}$ nonsymmetric, $\mathcal{Q} = 0$, i.e.,

$$\text{Find } x^* \in K : \ \langle \mathcal{F}(x^*), x - x^* \rangle \geq 0 \quad \forall x \in K.$$

- **Category 3:** VI$(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{F} = \nabla\psi$, $\mathcal{Q} = \partial\varphi$, i.e.,

$$\text{Find } x^* \in K, \ q^*(x^*) \in \partial\varphi(x^*) : \ \langle \nabla\psi(x^*) + q^*(x^*), x - x^* \rangle \geq 0 \quad \forall x \in K,$$

  which is equivalent to x^* being a solution of

$$\min \ \{\psi(x) + \varphi(x)\}, \quad \text{s.t. } x \in K.$$

5.2 Choice of $\mathcal{L}^k$ and $\mathcal{Q}^k$ and types of auxiliary problems

The original idea to introduce auxiliary operators $\mathcal{L}^k$ in the APP scheme was to unify the analysis of different types of descent methods and decomposition methods. A further motivation is to approximate the operator $\mathcal{F}$ by $\mathcal{L}^k$ such that the solution of the auxiliary problems becomes easier. Especially with symmetric auxiliary operators we can write the auxiliary problems as optimization problems. Among others, the following linear approximations of $\mathcal{F}$ can be considered:

$$\mathcal{L}^k(x) = B(x^k)x,$$

where $B(x^k) \in \mathbb{R}^{n \times n}$ is a symmetric matrix like, for example,

- $B(x^k) = \nabla\mathcal{F}(x^k)$ if $\nabla\mathcal{F}(x^k)$ is symmetric,
- $B(x^k) \approx \nabla\mathcal{F}(x^k)$, e.g., like in quasi-Newton schemes,
- $B(x^k) = \frac{1}{2}(\nabla\mathcal{F}(x^k) + \nabla\mathcal{F}(x^k)^T)$ if $\nabla\mathcal{F}(x^k)$ is nonsymmetric,
- $B(x^k) = \text{diag}(\nabla\mathcal{F}(x^k))$, where $\text{diag}(\nabla\mathcal{F}(x^k))$ is the matrix consisting of the diagonal elements of $\nabla\mathcal{F}(x^k)$.

The general symmetric setting can be represented as

- $\mathcal{L}^k(x) = \nabla S^k(x)$ with $S^k : \mathbb{R}^n \to \mathbb{R}$ convex and continuously differentiable.

Although a general nonsymmetric setting for $\mathcal{L}^k$ is theoretically possible, it prohibits a transformation of the LQPAP auxiliary problems into optimization problems and will therefore not be considered in the sequel[1]. Apart from the above choices for $\mathcal{L}^k$, one can omit $\mathcal{L}^k$ completely by setting

[1] Nonsymmetric settings lead to other classes of numerical methods, like merit function based algorithms, gap function based algorithms or equation based methods.

- $\mathcal{L}^k = 0$ for all k,

which is the only reasonable choice if $\mathcal{F} = 0$.

Let us now consider the choice of $\mathcal{Q}^k$. It was discussed in Section 2.4.3 (page 43) that the only known numerically meaningful outer approximation $\mathcal{Q}^k$ of a symmetric operator $\mathcal{Q} = \partial\varphi$ fulfilling

$$\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k}$$

is the ϵ_k-subdifferential of φ. Thus, we restrict ourselves to the two choices

- $\mathcal{Q}^k = \partial_{\epsilon_k}\varphi$, or
- $\mathcal{Q}^k = \mathcal{Q}$ for all k.

Depending on the concrete choices for $\mathcal{F}, \mathcal{Q}, \mathcal{Q}^k$, and $\mathcal{L}^k$, one can differentiate between different types of LQPAP auxiliary problems. Let us first consider the general situation

$$\begin{aligned}&\mathcal{F} \text{ nonsymmetric}, \mathcal{Q} = \partial\varphi, \varphi : \mathbb{R}^n \to \mathbb{R} \text{ convex},\\ &\mathcal{Q}^k = \partial_{\epsilon_k}\varphi, \mathcal{L}^k(x) = \nabla S^k(x), S^k : \mathbb{R}^n \to \mathbb{R} \text{ convex, continuously differentiable.}\end{aligned}$$

Then the corresponding LQPAP auxiliary problem (P_e^k) is of the form

$$\begin{aligned}&\text{Find } x^{k+1} \in K \text{ and } e^{k+1} \in \mathbb{R}^n \text{ with}\\ &e^{k+1} \in \mathcal{F}(x^k) + \partial_{\epsilon_k}\varphi(x^{k+1}) + \nabla S^k(x^{k+1}) - \nabla S^k(x^k) + \chi_k \nabla_1 D(x^{k+1}, x^k) \qquad (5.1)\\ &\text{and } \| e^{k+1} \| \leq \delta_k.\end{aligned}$$

For $\delta_k = \epsilon_k = 0$, (5.1) is equivalent to the optimization problem

$$\min_{x \in \mathbb{R}^n} \left\{ \left\langle \mathcal{F}(x^k) - \nabla S^k(x^k), x - x^k \right\rangle + S^k(x) + \varphi(x) + \chi_k D(x, x^k) \right\} \qquad (5.2)$$

and one can use a suitable minimization method to find an approximate (in the sense of (5.1)) solution x^{k+1}.

Table 5.1 considers the LQPAP auxiliary problems corresponding to the three categories of main problems and presents them as optimization problems. Actually, Category 1a is a reduction of the LQPAP scheme to a PPA-like scheme, whereas Category 1b corresponds to an APP-like scheme. In Category 2 the possibility to solve nonsymmetric variational inequality problems by means of optimization problems is realized. Finally, Category 3 includes a splitting of the given main operator into $\mathcal{F} = \nabla\psi$ and $\mathcal{Q} = \partial\varphi$ and realizes the PAP idea.

Setting of $\mathcal{F}, \mathcal{Q}, \mathcal{Q}^k, \mathcal{L}^k$	**Type of LQPAP auxiliary problem**
Category 1a: $\mathcal{Q} = \nabla\psi$, $\mathcal{F} = 0$, $\mathcal{Q}^k = Q$, $\mathcal{L}^k(x) = 0$	Strongly convex, differentiable optimization problem: $\min_{x\in\mathbb{R}^n} \ \{\psi(x) + \chi_k D(x, x^k)\}$
Category 1b: $\mathcal{Q} = 0$, $\mathcal{F} = \nabla\psi$, $\mathcal{Q}^k = 0$, $\mathcal{L}^k(x) = B(x^k)x$	Strongly convex, differentiable optimization problem: $\min_{x\in\mathbb{R}^n} \ \{\langle \nabla\psi(x^k) - B(x^k)x^k, x - x^k\rangle + \frac{1}{2}\langle B(x^k)x, x\rangle + \chi_k D(x, x^k)\}$
Category 2: $\mathcal{Q} = 0$, $\mathcal{F}$ nonsymmetric, $\mathcal{Q}^k = 0$, $\mathcal{L}^k(x) = 0$	Strongly convex, differentiable optimization problem: $\min_{x\in\mathbb{R}^n} \ \{\langle \mathcal{F}(x^k), x - x^k\rangle + \chi_k D(x, x^k)\}$
Category 3: $\mathcal{Q} = \partial\varphi$, $\mathcal{F} = \nabla\psi$, $\mathcal{Q}^k = \partial_{\epsilon_k}\varphi$, $\mathcal{L}^k(x) = 0$	Strongly convex, *non*differentiable optimization problem: $\min_{x\in\mathbb{R}^n} \ \{\langle \nabla\psi(x^k), x - x^k\rangle + \varphi(x) + \chi_k D(x, x^k)\}$

Table 5.1. Types of LQPAP auxiliary problems

5.3 Monotonicity and continuity assumptions on $\mathcal{L}^k$

Assumptions (A6) and (A8) require that each operator $\mathcal{L}^k$ is monotone and continuous on K and that for any convergent sequence $\{x^k\} \subset \mathrm{dom}(\mathcal{Q}) \cap K$ it holds

$$\mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k) \to 0 \quad \text{for} \quad k \to \infty. \tag{5.3}$$

A sufficient condition for (5.3) is the uniform Lipschitz continuity of $\{\mathcal{L}^k\}$ on K, i.e., there exists $L > 0$ independent of k such that

$$\| \mathcal{L}^k(x) - \mathcal{L}^k(y) \| \leq L \| x - y \| \quad \forall x, y \in K, \ \forall k \in \mathbb{N}.$$

For a linear approximation scheme with $\mathcal{L}^k(x) = B(x^k)x$, conditions (A6) and (A8) are fulfilled if for each $x^k \in K$

$$B(x^k) \in \mathbb{R}^{n\times n} \text{ is symmetric and positive semidefinite} \tag{5.4}$$

$$\text{and } \exists L > 0 \text{ with } \| B(x^k) \|_2 \leq L \text{ for all } k \in \mathbb{N}, \tag{5.5}$$

where (5.5) is surely true if $B(x^k)$ continuously depends on x^k. In the case that $\mathcal{F} = \nabla\psi$ and $B(x^k) = \nabla\mathcal{F}(x^k) = \nabla^2\psi(x^k)$, (A6) and (A8) are fulfilled if $\psi : \mathbb{R}^n \to \mathbb{R}$ is convex and twice continuously differentiable. Clearly, (A6) and (A8) also admit the choice $\mathcal{L}^k = 0$ for all $k \in \mathbb{N}$.

5.4 Analysis of the weakened co-coercivity assumption on $\mathcal{F} - \mathcal{L}^k$

Assumption (A7) on the operators $\mathcal{F} - \mathcal{L}^k$ is surely fulfilled if the operators $\mathcal{F} - \mathcal{L}^k$ are co-coercive on K with a common modulus $\gamma > 0$. We first examine how to verify co-coercivity for a general operator $\mathcal{T}$ and in the case of an affine operator $\mathcal{T}(x) = Cx + d$. In the latter case, easy criteria can be given which are based on positive (semi)definiteness arguments. Then, the question is discussed how to find for a given operator $\mathcal{F}$ a suitable choice of the operators $\mathcal{L}^k$ such that $\mathcal{F} - \mathcal{L}^k$ is co-coercive. Our systematic analysis shows that under the given assumptions an a priori setting for $\mathcal{L}^k$ is hard to find (apart from a very special case). For that reason, we suggest to set $\mathcal{L}^k = 0$ in the end. However, this is not a drawback because the presented numerical solution methods in Chapters 6 and 8 are independent of $\mathcal{L}^k$.

5.4.1 Verification of co-coercivity for a general operator $\mathcal{T}$

Remember that an operator $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$ is called co-coercive on the set $K \subset \mathbb{R}^n$ if there exists $\gamma > 0$ with

$$\langle \mathcal{T}(x) - \mathcal{T}(y), x - y \rangle \geq \gamma \parallel \mathcal{T}(x) - \mathcal{T}(y) \parallel^2 \quad \forall x, y, \in K.$$

Some basic information about co-coercive operators was already given in Section 2.1. In the symmetric, monotone case, i.e., $\mathcal{T} = \nabla\psi$ for a convex function $\psi : \mathbb{R}^n \to \mathbb{R}$, co-coercivity of $\mathcal{T}$ is equivalent to Lipschitz continuity of $\mathcal{T}$:

Lemma 5.4.1 ([92],Proposition 3.5). *Let $\psi : \mathbb{R}^n \to \mathbb{R}$ be a convex and differentiable function. Then $\nabla\psi$ is Lipschitz continuous with constant L if and only if $\nabla\psi$ is co-coercive with modulus L^{-1}.*

The above equivalence is not true in the general nonsymmetric case. Consider for example $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}$, $T(x_1, x_2) = (-x_2, x_1)$. Then $\mathcal{T}$ is Lipschitz continuous and monotone on $\mathbb{R}^2$ but not co-coercive.

The next lemma provides two sufficient conditions for co-coercivity.

Lemma 5.4.2. *For $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$ and $K \subset \mathbb{R}^n$ the following statements hold:*

(1) If $\mathcal{T}$ is strongly monotone on K with modulus β and Lipschitz continuous on K with constant L then $\mathcal{T}$ is co-coercive on K with modulus $\gamma = \frac{\beta}{L^2}$ [92, Proposition 3.1].

(2) Let $\mathcal{T}$ be twice continuously differentiable and Lipschitz continuous with constant L. If $\nabla\mathcal{T}(x)$ and $\nabla\mathcal{T}(x)^2$ are positive semidefinite for all $x \in K$, then $\mathcal{T}$ is co-coercive on K with modulus $\frac{1}{4L}$ [69, Proposition 2.1].

We now present a necessary and sufficient condition for a differentiable operator $\mathcal{T}$ to be co-coercive. For that purpose, the concept of a psd-plus (positive semidefinite-plus) matrix is needed.

Definition 5.4.3. *A matrix $C \in \mathbb{R}^{n\times n}$ is psd-plus if it is positive semidefinite and for all $x \in \mathbb{R}^n$ the inclusion*

$$\langle Cx, x\rangle = 0 \quad \Rightarrow \quad Cx = 0$$

holds.

It is clear that every positive definite matrix is a psd-plus matrix. We have the following characterization of a psd-plus matrix.

Lemma 5.4.4 ([68], Proposition 1). *A matrix $C \in \mathbb{R}^{n\times n}$ is psd-plus if and only if C can be written as*

$$C = E^T M E$$

for some matrix $E \in \mathbb{R}^{r\times n}$ and some positive definite matrix $M \in \mathbb{R}^{r\times r}$, where r is the rank of C. Especially, M can be chosen as $M = I + B$ with $B^T = -B$.

In the following theorem, a matrix C is called psd-plus with modulus γ if the operator $x \mapsto Cx$ is co-coercive with the same modulus γ.

Theorem 5.4.5 ([92], Theorem 3.2). *Let $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable on $K \subset \mathbb{R}^n$. Then $\mathcal{T}$ is co-coercive on K if and only if, for every $x \in K$, $\nabla\mathcal{T}(x)$ is psd-plus with uniform modulus.*

Remark 5.4.6. *The modulus of co-coercivity in Theorem 5.4.5 is determined as follows. Let $\nabla\mathcal{T}(x)$ be psd-plus for every $x \in K$ with uniform constant $\gamma > 0$. This means that for all $x \in K$*

$$\langle \nabla\mathcal{T}(x)(y-z), y-z\rangle \geq \gamma \parallel \nabla\mathcal{T}(x)(y-z) \parallel^2 \quad \forall y, z \in \mathbb{R}^n.$$

Then $\mathcal{T}$ is co-coercive with modulus γ.

5.4.2 Co-coercivity in the affine case and calculation of the modulus γ

For our purpose, it is not only important to verify co-coercivity of an operator, but also to know the particular value of the modulus γ of co-coercivity. For a general operator $\mathcal{T}$ this value can be hard to determine. Thus, for simplicity, we concentrate on affine operators

$$\mathcal{T}(x) = Cx + d,$$

where $C \in \mathbb{R}^{n\times n}$ and $d \in \mathbb{R}^n$.

If C is symmetric the modulus of co-coercivity can be calculated using Lemma 5.4.1.

Lemma 5.4.7. *Let $C \in \mathbb{R}^{n\times n} \setminus \{0\}$ be symmetric, positive semidefinite and $d \in \mathbb{R}^n$. Then the operator $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$, $\mathcal{T}(x) = Cx + d$ is co-coercive with modulus*

$$\gamma = \frac{1}{\| C \|_2}.$$

The operator $\mathcal{T}' : \mathbb{R}^n \to \mathbb{R}^n$, $\mathcal{T}'(x) = d$ is co-coercive with arbitrary $\gamma > 0$.

For the case that C is not symmetric, the following lemmata describe situations in which the modulus of co-coercivity can be calculated.

With Lemma 5.4.2(1) the following statement can be proved.

Lemma 5.4.8. *Let $C \in \mathbb{R}^{n\times n}$ be positive definite and $d \in \mathbb{R}^n$. Then the operator $\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^n$, $\mathcal{T}(x) = Cx + d$ is co-coercive with modulus*

$$\gamma = \frac{\lambda_{min}(\widehat{C})}{\| C \|_2^2},$$

where $\lambda_{min}(\widehat{C})$ is the smallest eigenvalue of $\widehat{C} = \frac{1}{2}(C + C^T)$.

Proof. Because $\langle \widehat{C}x, x\rangle = \langle Cx, x\rangle$ and C is positive definite, also $\widehat{C}$ is positive definite. Further, $\widehat{C}$ is symmetric per definition. Thus, $\lambda_{min}(\widehat{C})$ is positive. With the well-known Rayleigh-principle it follows

$$\langle Cx, x\rangle = \langle \widehat{C}x, x\rangle \geq \lambda_{min}(\widehat{C}) \| x \|^2 \quad \forall x \in \mathbb{R}^n.$$

This establishes the strong monotonicity of $\mathcal{T}$ with modulus $\lambda_{min}(\widehat{C})$. It is further clear that $\mathcal{T}$ is Lipschitz continuous with $L = \| C \|_2$. Lemma 5.4.2(1) completes the proof. □

If C is a psd-plus matrix, the modulus of co-coercivity can also be specified. In the affine case, Theorem 5.4.5 reduces to:

Lemma 5.4.9 ([92], Proposition 3.4). *Let $C \in \mathbb{R}^{n\times n}$, $d \in \mathbb{R}^n$. Then the operator $\mathcal{T}(x) = Cx + d$ is co-coercive if and only if the matrix C is psd-plus. The modulus of co-coercivity is*

$$\gamma = \frac{\lambda_{\min}(\widehat{M})}{\| E^T M \|_2^2},$$

where $C = E^T M E$ is a decomposition according to Lemma 5.4.4.

We will now focus on Lemma 5.4.2(2) in the special case of an affine operator.

Lemma 5.4.10. *Let $C \in \mathbb{R}^{n\times n} \setminus \{0\}$, $d \in \mathbb{R}^n$. If C and C^2 are positive semidefinite then $\mathcal{T}(x) = Cx + d$ is co-coercive with modulus*

$$\gamma = \frac{1}{4 \| C \|_2}.$$

Proof. Since $\mathcal{T}$ is Lipschitz continuous with constant $L = \| C \|_2$, the statement follows from Lemma 5.4.2(2). □

Let us give some interesting remarks on the condition that C and C^2 be positive semidefinite. If C is symmetric then C^2 is positive semidefinite since $C^2 = C^T C$. If C is not symmetric, this is not necessarily the case (see Remark 5.4.13 further down).

A necessary and sufficient condition for C^2 to be positive semidefinite is

Lemma 5.4.11 ([39], Proposition 1). *Let $C \in \mathbb{R}^{n\times n}$ be a matrix. Then C^2 is positive semidefinite if and only if*

$$\left\|(C - C^T)x\right\| \leq \left\|(C + C^T)x\right\| \quad \forall x \in \mathbb{R}^n.$$

In other words, the condition of Lemma 5.4.10 is fulfilled if C is positive semidefinite and not too asymmetric.

A necessary but not sufficient condition for C^2 to be positive semidefinite is

Lemma 5.4.12 ([39], page 685). *Let $C \in \mathbb{R}^{n\times n}$. If C^2 is positive semidefinite then*

$$\| C - C^T \|_2 \leq \| C + C^T \|_2 .$$

Remark 5.4.13. *The converse of the preceding lemma is not true. As a counterexample take* $C = \begin{pmatrix} 4 & -9 \\ 7 & 8 \end{pmatrix}$. *Then* $\| C - C^T \|_2 = 16 < 16.4721 \approx \| C + C^T \|_2$. *But for* $x = (-1.5, 0.5)^T$ *we get* $\| (C - C^T)x \|_2 \approx 25.2982 > 17.0294 \approx \| (C + C^T)x \|_2$. *Thus, using Lemma 5.4.11,* C^2 *is not positive semidefinite.*

5.4.3 Co-coercivity of $\mathcal{F} - \mathcal{L}^k$ and the choice $\mathcal{L}^k = 0$

The affine case. To explain the difficulties concerning the choice of $\mathcal{L}^k$ we exemplarily examine the case

$$\mathcal{F}(x) = Cx + d, \quad \mathcal{L}^k(x) = Bx.$$

The minimal requirements on the matrices $B, C \in \mathbb{R}^{n \times n}$ are

- C positive semidefinite $\quad (\Rightarrow \mathcal{F}$ monotone),
- B symmetric, positive semidefinite $\quad (\Rightarrow \mathcal{L}^k$ symmetric, monotone)

Table 5.2 specifies different criteria for $x \mapsto (\mathcal{F} - \mathcal{L}^k)(x) = (C-B)x+d$ to be co-coercive. The case that C is symmetric is separated from the case that C is nonsymmetric.

Case 1: C symmetric, positive semidefinite, B symmetric, positive semidefinite.	If $\mathbf{C - B}$ **is positive semidefinite** then $x \mapsto (C - B)x + d$ is monotone and Lipschitz continuous with $L = \| C - B \|_2$ (if $C \neq B$) or $L > 0$ arbitrary (if $C = B$). Thus, $x \mapsto (C-B)x+d$ is co-coercive with $\gamma = \frac{1}{L}$ (see Lemma 5.4.7).
Case 2: C nonsymmetric, positive semidefinite, B symmetric, positive semidefinite.	• If $\mathbf{C - B}$ **is positive definite** then $x \mapsto (C - B)x + d$ is co-coercive with $\gamma = \frac{\lambda_{\min}(\frac{C-B}{2})}{\|C-B\|_2^2}$ (see Lemma 5.4.8). • If $\mathbf{C - B}$ **and** $\mathbf{(C - B)^2}$ **are positive semidefinite** then $x \mapsto (C - B)x + d$ is co-coercive with $\gamma = \frac{1}{4\|C-B\|_2}$ (see Lemma 5.4.10).

Table 5.2. Sufficient conditions for co-coercivity of $x \mapsto (\mathcal{F} - \mathcal{L}^k)(x) = (C - B)x + d$.

Settings for B in $\mathcal{L}^k(x) = Bx$ in the case of diagonal dominance. In general, the difference of two positive (semi)definite matrices does not have to be positive (semi)definite. Thus, without more information about C it is difficult to choose B appropriately. A sufficient information about C that allows us to choose B as a special diagonal matrix is related to the notion of *diagonal dominance* [43, Definition 6.1.9].

A matrix $C = (c_{ij}) \in \mathbb{R}^{n \times n}$ is called diagonally dominant if

$$|c_{ii}| \geq \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ij}| \quad \forall i = 1, \ldots, n.$$

It is said to be strictly diagonally dominant if

$$|c_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ij}| \quad \forall i = 1, \ldots, n.$$

The following statement describes the relation between positive (semi)definiteness and (strictly) diagonal dominance of a symmetric matrix.

Lemma 5.4.14 ([43], Theorem 6.1.10, Theorem 7.2.1). *Let $C \in \mathbb{R}^{n \times n}$ be a symmetric matrix. If C is diagonally dominant (resp. strictly diagonally dominant) and $c_{ii} \geq 0$ (resp. $c_{ii} > 0$) for all $i = 1, \ldots, n$, then C is positive semidefinite (resp. positive definite).*

In the nonsymmetric case, Lemma 5.4.14 is no longer valid. As a counterexample regard, e.g., $C = \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}$. Nevertheless, since positive (semi)definiteness of a nonsymmetric matrix C is equivalent to positive (semi)definiteness of its symmetric part $\widehat{C} = \frac{1}{2}\left(C + C^T\right)$, we have the following characterization.

Lemma 5.4.15. *Let $C \in \mathbb{R}^{n \times n}$ be a nonsymmetric matrix. If $\widehat{C} = \frac{1}{2}\left(C + C^T\right)$ is strictly diagonally dominant, i.e.,*

$$|c_{ii}| > \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ij} + c_{ji}| \quad \forall i = 1, \ldots, n$$

and $c_{ii} > 0$ for all $i = 1, \ldots, n$, then C is positive definite.

An analogous statement holds for diagonal dominance and positive semidefiniteness.

Note that double-diagonal dominance of C, i.e.

$$|c_{ii}| \geq \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ij}| \quad \forall i = 1, \ldots, n, \quad \text{and} \quad |c_{ii}| \geq \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ji}| \quad \forall i = 1, \ldots, n,$$

is a sufficient criterion for $\widehat{C}$ to be diagonally dominant.

Now, return to co-coercivity of $x \mapsto (C-B)x+d$. For a (strictly) diagonally dominant matrix C the following two lemmata present how the choice of B as a special diagonal matrix ensures co-coercivity of $x \mapsto (C-B)x+d$, while B itself is symmetric and positive semidefinite.

Lemma 5.4.16. *Let $C \in \mathbb{R}^{n\times n}$ be a symmetric matrix. Let further C be diagonally dominant and $c_{ii} \geq 0$ for all $i = 1, \ldots, n$. Define $B \in \mathbb{R}^{n\times n}$ as a diagonal matrix with diagonal entries*

$$b_{ii} = c_{ii} - \sum_{\substack{j=1 \\ j\neq i}}^{n} |c_{ij}|, \quad i = 1, \ldots, n.$$

Then B is symmetric and positive semidefinite, and $x \mapsto (C-B)x+d$ is co-coercive.

Proof. According to Lemma 5.4.14, C is positive semidefinite. From the definition of B it is clear that B is diagonally dominant with nonnegative diagonal entries. Thus, B is positive semidefinite. For all $i = 1, \ldots, n$ it holds

$$|(C-B)_{ii}| = \sum_{\substack{j=1 \\ j\neq i}}^{n} |c_{ij}| = \sum_{\substack{j=1 \\ j\neq i}}^{n} |(C-B)_{ij}|$$

and $(C-B)_{ii} \geq 0$. Hence, in view of Lemma 5.4.14, $C-B$ is positive semidefinite. Now, co-coercivity of $x \mapsto (C-B)x+d$ follows from Lemma 5.4.7. □

Lemma 5.4.17. *Let $C \in \mathbb{R}^{n\times n}$ be a nonsymmetric matrix. Let further $\widehat{C} = \frac{1}{2}\left(C + C^T\right)$ be strictly diagonally dominant and $c_{ii} > 0$ for all $i = 1, \ldots, n$. Choose values $\tau_i > 0$, $i = 1, \ldots, n$ such that*

$$c_{ii} \geq \frac{1}{2} \sum_{\substack{j=1 \\ j\neq i}}^{n} |c_{ij} + c_{ji}| + \tau_i, \quad i = 1, \ldots, n.$$

Define $B \in \mathbb{R}^{n\times n}$ as a diagonal matrix with diagonal entries

$$b_{ii} = c_{ii} - \frac{1}{2} \sum_{\substack{j=1 \\ j\neq i}}^{n} |c_{ij} + c_{ji}| - \tau_i, \quad i = 1, \ldots, n.$$

Then B is symmetric and positive semidefinite, and $x \mapsto (C-B)x+d$ is co-coercive.

Proof. In view of Lemma 5.4.15, C is positive definite. From the definition of B it is clear that B is diagonally dominant with $b_{ii} \geq 0$ for all $i = 1, \ldots, n$. Thus, according to

Lemma 5.4.14, B is positive semidefinite. Consider now $\widehat{C} - B$, which is the symmetric part of $C - B$. For all $i = 1, \ldots, n$ it holds

$$(\widehat{C} - B)_{ii} = c_{ii} - b_{ii} = \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ij} + c_{ji}| + \tau_i.$$

This implies that $(\widehat{C} - B)_{ii} > 0$. Further, for $j \neq i$ it holds

$$(\widehat{C} - B)_{ij} + (\widehat{C} - B)_{ji} = c_{ij} + c_{ji}.$$

Now,

$$(\widehat{C} - B)_{ii} = \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ij} + c_{ji}| + \tau_i > \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{n} |c_{ij} + c_{ji}| = \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{n} |(\widehat{C} - B)_{ij} + (\widehat{C} - B)_{ji}|,$$

which shows strictly diagonal dominance of $\widehat{C} - B$. Thus, in view of Lemma 5.4.15, $C - B$ is positive definite and, therefore, $x \mapsto (C - B)x + d$ is co-coercive according to Lemma 5.4.8. □

Consider now the k-th LQPAP auxiliary problem for the setting $\mathcal{F}(x) = Cx + d$, $\mathcal{L}^k(x) = Bx$, $\mathcal{Q}(x) = \partial\varphi(x)$, $\mathcal{Q}^k = \mathcal{Q}$. The equivalent formulation of this auxiliary problem as an optimization problem is

$$\min_{x \in \mathbb{R}^n} \left\{ \left\langle (C - B)x^k + d, x - x^k \right\rangle + \frac{1}{2} \langle Bx, x \rangle + \varphi(x) + \chi_k D(x, x^k) \right\}.$$

Setting $\mathcal{L}^k(x) = Bx$ (with B as a diagonal matrix as described in Lemma 5.4.16 or Lemma 5.4.17) has the effect that a convex quadratic term, which includes some diagonal information of C, appears in the objective function. If B additionally is positive definite then a regularizing effect is given. It will be examined in Chapter 6 if this is numerically advantageous compared to the choice $B = 0$.

Other settings for B in $\mathcal{L}^k(x) = Bx$. Let us now discuss other settings for B that correspond to the suggestions for $\mathcal{L}^k$ on page 81, i.e.,

$$B = C, \quad B = \frac{1}{2}\left(C + C^T\right), \quad B = \operatorname{diag}(C). \tag{5.6}$$

The following three examples demonstrate that all these settings are not interesting in our context.

Example 5.4.18 ($B = C$). *Take $\mathcal{Q}(x) = \partial\varphi(x)$ and $\mathcal{Q}^k = \mathcal{Q}$. Let $C \in \mathbb{R}^{n\times n}$ be symmetric, positive semidefinite and $d \in \mathbb{R}^n$. Define $\mathcal{F}(x) = Cx + d$ and $\mathcal{L}^k(x) = Cx$. Then*

$$x \mapsto (\mathcal{F} - \mathcal{L}^k)(x) = d$$

is co-coercive with arbitrary $\gamma > 0$. The corresponding k-th LQPAP auxiliary problem can be transformed into the following optimization problem

$$\min_{x\in\mathbb{R}^n} \left\{ \frac{1}{2} \langle Cx, x\rangle + \langle d, x\rangle + \varphi(x) + \chi_k D(x, x^k) \right\}.$$

However, this scheme is covered by the choice $\mathcal{Q} = \nabla\psi + \partial\varphi$, where $\psi = \frac{1}{2}\langle Cx, x\rangle + \langle d, x\rangle$. Thus, the above setting of $\mathcal{F}$ and $\mathcal{L}^k$ is not an interesting case.

Example 5.4.19 ($B = \frac{1}{2}\left(C + C^T\right)$). *Let $C \in \mathbb{R}^{n\times n}$ be nonsymmetric and positive semidefinite and $d \in \mathbb{R}^n$. Define $\mathcal{F}(x) = Cx + d$ and $\mathcal{L}^k(x) = \frac{1}{2}\left(C + C^T\right)x$. We demonstrate that*

$$x \mapsto (\mathcal{F} - \mathcal{L}^k)(x) = \frac{1}{2}\left(C - C^T\right) + d$$

is co-coercive if and only if $C = C^T$.

If $C = C^T$ then $(\mathcal{F} - \mathcal{L}^k)(x) = d$, which is co-coercive with arbitrary $\gamma > 0$. Now, suppose that $(\mathcal{F} - \mathcal{L}^k)(x) = \frac{1}{2}\left(C - C^T\right) + d$ is co-coercive. With Lemma 5.4.9 it follows that $E := \frac{1}{2}\left(C - C^T\right)$ is psd-plus. Since E is the skew-symmetric part of C it holds that $E = -E^T$. Therefore, it is clear that $\langle Ex, x\rangle = 0$ for all $x \in \mathbb{R}^n$. Now, the definition of a psd-plus matrix requires that $Ex = 0$ must hold for all $x \in \mathbb{R}^n$. This is only true if $E = 0$ and, therefore, $C = C^T$. Hence, we are back to the symmetric case of Example 5.4.18.

Example 5.4.20 ($B = \operatorname{diag}(C)$). *Let $C \in \mathbb{R}^{n\times n}$ be positive semidefinite and $d \in \mathbb{R}^n$. Define $\mathcal{F}(x) = Cx + d$ and $\mathcal{L}^k(x) = diag(C)x$.*

We will show that

$$x \mapsto (\mathcal{F} - \mathcal{L}^k)(x) = (C - diag(C))x + d$$

is co-coercive if and only if C is a diagonal matrix. So, the choice $B = diag(C)$ is covered by Example 5.4.18 and thus not interesting.

The if-case is clear. Thus, suppose that $(\mathcal{F} - \mathcal{L}^k)(x) = (C - diag(C))x + d$ is co-coercive. It follows from Lemma 5.4.9 that $E := (C - diag(C))$ is psd-plus. For every unit vector $e^i \in \mathbb{R}^n$, $i = 1, \ldots, n$, it holds $\langle Ee^i, e^i\rangle = 0$. In view of the definition of a psd-plus matrix, this implies that $Ee^i = 0$ for all $i = 1, \ldots, n$. Hence, $E = 0$, which is only true if C is a diagonal matrix.

The nonaffine case. The discussion of the affine case shows that apart from the situation of diagonal dominance (Lemmata 5.4.16 and 5.4.17) the standard choices for $\mathcal{L}^k$ (see (5.6)) are not of any interest. Therefore, turning to the general case of nonaffine, monotone operators $\mathcal{F}$, it is clear that an appropriate choice of $\mathcal{L}^k$ becomes even more difficult.

Let $\mathcal{F}$ be a monotone operator and consider a linear approximation scheme with

$$\mathcal{L}^k(x) = B(x^k)x$$

where $B(x^k)$ is a symmetric and positive semidefinite matrix which continuously depends on x^k. In the case that $\mathcal{F}$ is nonsymmetric, some sufficient criteria for co-coercivity of

$$x \mapsto (\mathcal{F} - \mathcal{L}^k)(x) = \mathcal{F}(x) - B(x^k)x$$

are (see Lemma 5.4.2):

- $\mathcal{F} - \mathcal{L}^k$ is strongly monotone and Lipschitz continuous.
- $\mathcal{F} - \mathcal{L}^k$ is Lipschitz continuous, and $\nabla\mathcal{F}(x) - B(x^k)$ and $(\nabla\mathcal{F}(x) - B(x^k))^2$ are positive semidefinite for all x.

In the case that $\mathcal{F}$ is symmetric, i.e., $\mathcal{F} = \nabla\psi$ with $\psi : \mathbb{R}^n \to \mathbb{R}$ convex and differentiable, co-coercivity of $\mathcal{F} - \mathcal{L}^k$ is equivalent to (see Lemma 5.4.1)

- $\nabla^2\psi(x) - B(x^k)$ is positive semidefinite and $\nabla\psi(x) - B(x^k)x$ is Lipschitz continuous.

In practice these criteria are hard to verify for nonaffine operators $\mathcal{F}$. Note, for example, that the conditions based on positive (semi)definiteness have to hold for all $x \in \mathbb{R}^n$ at an element x^k of the unknown sequence of iterates. Moreover, the difference of a positive (semi)definite and a positive semidefinite matrix does not have to be positive semidefinite.

The following example even shows that the choice $\mathcal{L}^k(x) = \nabla\mathcal{F}(x^k)x$ is not of interest in the symmetric case.

Example 5.4.21. *Let $\mathcal{F}$ be symmetric, i.e., $\mathcal{F} = \nabla\psi$ with $\psi : \mathbb{R}^n \to \mathbb{R}$ convex and twice continuously differentiable. Let $\mathcal{L}^k(x) = \nabla\mathcal{F}(x^k)x = \nabla^2\psi(x^k)x$. Then $\mathcal{F} - \mathcal{L}^k$ is co-coercive if and only if*

(i) $\nabla^2\psi(x) - \nabla^2\psi(x^k)$ is positive semidefinite, and

(ii) $x \mapsto \nabla\psi(x) - \nabla^2\psi(x^k)x$ is Lipschitz continuous.

Positive semidefiniteness has to hold for all $x \in \mathbb{R}^n$ at a fixed x^k. Since the sequence of iterates is a priori unknown, one has to require that $\nabla^2\psi(x) - \nabla^2\psi(y)$ is positive semidefinite for all $x, y \in \mathbb{R}^n$ to ensure monotonicity of $\mathcal{F} - \mathcal{L}^k$ for all k. Thus, $\nabla^2\psi(x)$ has to be independent of x. This restricts the choice of ψ to the class of convex, quadratic functions. However, this class, i.e., $\mathcal{F}(x) = Cx + d$, $\mathcal{L}^k(x) = Cx$, was already discussed in Example 5.4.18 leading to the conclusion that this case is not interesting in our context.

Summary: Choose $\mathcal{L}^k = 0$. The initial aim of introducing auxiliary operators in the APP scheme was to cover different descent methods like gradient or Newton methods (see page 22). Thus, the APP scheme itself includes the method with which the auxiliary problems are solved. In order to keep this idea alive in the extensions of the APP scheme it is often mentioned in the corresponding papers that "the choice of $\mathcal{L}^k$ depends on the method under consideration". However, the preceding discussion shows that this idea is hardly realizable in our context of the LQPAP scheme since, in general, a suitable choice of $\mathcal{L}^k$ is impossible. Apart from the possibility to use $\mathcal{L}^k$ as an approximation of $\mathcal{F}$ to facilitate the solution of the auxiliary problems (see the case of diagonal dominance) we, therefore, propose to set $\mathcal{L}^k = 0$. Thus, the LQPAP scheme does not suggest (via $\mathcal{L}^k$) a solution method for the auxiliary problems. Special methods to solve the LQPAP auxiliary problems will be described in the next chapters: the damped Newton method for differentiable auxiliary problems and a bundle method for nondifferentiable auxiliary problems.

6. LQPAP Method and Differentiable Convex Optimization Problems

This chapter is devoted to the numerical realization of the LQPAP method for main problems of Category 1. Given is a variational inequality $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{Q} = \nabla\psi$, $\mathcal{F} = 0$, or with $\mathcal{Q} = 0$, $\mathcal{F} = \nabla\psi$, where $\psi : \mathbb{R}^n \to \mathbb{R}$ is a convex and twice continuously differentiable function (which is additionally co-coercive in the second case). The feasible set is given as $K = \{x \in \mathbb{R}^n : Ax \leq b\}$ with a matrix $A \in \mathbb{R}^{p\times n}$ of full column rank and a vector $b \in \mathbb{R}^p$, and it is further supposed that $\mathrm{int}(K) \neq \emptyset$. This type of variational inequality problem can equivalently be formulated as a differentiable convex optimization problem with linear constraints:

$$\begin{aligned} &\min\ \psi(x) \\ &\text{s.t. } Ax \leq b. \end{aligned} \tag{6.1}$$

Depending on the modeling with $\mathcal{Q}$ and $\mathcal{F}$ we focus on two types of auxiliary problems.

Category 1a: $\mathcal{Q} = \nabla\psi$, $\mathcal{F} = 0$, $\mathcal{Q}^k = \mathcal{Q}$, $\mathcal{L}^k = 0$.
At step $(k+1)$ we have a current iterate x^k and calculate the iterate x^{k+1} by solving the problem

$$\begin{aligned} &\text{Find } x^{k+1} \in K \text{ and } e^{k+1} \in \mathbb{R}^n\text{:} \\ &e^{k+1} = \nabla\psi(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k) \\ &\text{with } \parallel e^{k+1} \parallel \leq \delta_k. \end{aligned} \tag{6.2}$$

Due to the interior point effect, this auxiliary problem can be considered as unconstrained, and x^{k+1} can be calculated as an inexact solution (i.e., with $\parallel e^{k+1} \parallel \leq \delta_k$) of the strongly convex, differentiable optimization problem

$$\min_{x\in\mathbb{R}^n} \left\{\psi(x) + \chi_k D(x, x^k)\right\}. \tag{6.3}$$

Category 1b: $\mathcal{Q} = 0$, $\mathcal{F} = \nabla\psi$, $\mathcal{Q}^k = 0$, $\mathcal{L}^k(x) = B(x^k)x$.
At step $(k+1)$ we have a current iterate x^k and calculate the iterate x^{k+1} by solving the problem

$$\begin{aligned}&\text{Find } x^{k+1} \in K \text{ and } e^{k+1} \in \mathbb{R}^n\text{:}\\ &e^{k+1} = \nabla\psi(x^k) + B(x^k)x^{k+1} - B(x^k)x^k + \chi_k \nabla_I D(x^{k+1}, x^k)\\ &\text{with } \parallel e^{k+1} \parallel \leq \delta_k.\end{aligned} \tag{6.4}$$

Thus, x^{k+1} is an inexact solution (with $\parallel e^{k+1} \parallel \leq \delta_k$) of the unconstrained, strongly convex, differentiable optimization problem

$$\min_{x\in\mathbb{R}^n} \left\{ \left\langle \nabla\psi(x^k) - B(x^k)x^k, x - x^k \right\rangle + \frac{1}{2}\left\langle B(x^k)x, x\right\rangle + \chi_k D(x, x^k) \right\}. \tag{6.5}$$

For the solution of (6.3) and (6.5) we apply the damped Newton method and describe two rules for the calculation of the step size: an Armijo rule and a rule based on the self-concordance property. Furthermore, we describe how the sequence $\{\chi_k\}$ of regularization parameters is determined. Moreover, it is interesting to compare the LQPAP method and the BrPAP method. For problems where both methods are applicable we intend to answer the question which method is preferable. For that purpose, we describe how to adapt the implementation of the LQPAP method to Bregman-distances.

Afterwards, a set of test examples is described with which the behavior of the methods is analyzed. A summary is given for different numerical experiments concerning different step size rules, different ways of modeling, and an adaptive initialization of χ_0. Finally, based on the gained experience, the idea of under-relaxation is described as a possibility to improve the numerical performance of the LQPAP algorithm.

The algorithm is implemented in MATLAB® R2008b.

6.1 Numerical realization of the LQPAP method

6.1.1 Newton method for solving the auxiliary problems

The conceptual algorithmic formulation of the damped Newton method for solving the convex, differentiable auxiliary problems (6.3) and (6.5) is presented in Algorithm 6.1. To unify the description for Category 1a and 1b let f^k denote the objective function of (6.3) respectively (6.5) without the term $\chi_k D(x, x^k)$, i.e., for Category 1a we have

$$f^k = \psi, \tag{6.6}$$

and for Category 1b we have

$$f^k : x \mapsto \left\langle \nabla\psi(x^k) - B(x^k)x^k, x - x^k \right\rangle + \frac{1}{2}\left\langle B(x^k)x, x\right\rangle. \tag{6.7}$$

Thus, for given x^k and χ_k we consider the problem

$$\min_{x\in\mathbb{R}^n} \left\{ f^k(x) + \chi_k D(x, x^k) \right\}. \tag{6.8}$$

With y^j we denote the iterates of the Newton method. For a current iterate y^j a Newton step for the solution of (6.8) consists in the calculation of the Newton direction

$$p^j = -(\nabla^2 f^k(y^j) + \chi_k \nabla_I^2 D(y^j, x^k))^{-1}(\nabla f^k(y^j) + \chi_k \nabla_I D(y^j, x^k)) \tag{6.9}$$

and a step size α_j to set

$$y^{j+1} = y^j + \alpha_j p^j.$$

The computation of the inverse in formula (6.9) is done with an intern MATLAB® routine which solves the corresponding system of linear equations. Although the exactness of the solution depends on the condition of the involved matrix, the occurring errors will not be included in our consideration.

Algorithm 6.1: Newton method for solving $\min\{f^k(x) + \chi_k D(x, x^k)\}$

Input: x^k, δ_k, and χ_k.

1. (*Initialization*) Set $y^0 = x^k$, $j := 0$.

2. (*Stopping criterion*) If $\| \nabla f^k(y^j) + \chi_k \nabla_I D(y^j, x^k) \| \leq \delta_k$ then stop and set $x^{k+1} := y^j$.

3. (*Calculate Newton direction*)
$p^j = -(\nabla^2 f^k(y^j) + \chi_k \nabla_I^2 D(y^j, x^k))^{-1}(\nabla f^k(y^j) + \chi_k \nabla_I D(y^j, x^k))$.

4. (*Calculate step size*)
Find $\alpha_j \geq 0$ according to the Armijo rule. (If f^k is self-concordant, α_j can be determined with the self-concordance rule.)

5. (*Update*) Set $y^{j+1} = y^j + \alpha_j p^j$, $j := j + 1$ and go to step 2.

We present two rules for the calculation of the step size α_j.

Armijo step size. Let y^j be the current iterate of the Newton method and p^j the calculated Newton direction. We use an Armijo rule for the determination of a step size α_j that works as follows. For an initial step size $\alpha > 0$ and factors $\zeta, \rho \in (0, 1)$ let m be the smallest natural number with

$$\begin{aligned} f^k(y^j + \alpha\zeta^m p^j) + \chi_k D(y^j + \alpha\zeta^m p^j, x^k) - (f^k(y^j) + \chi_k D(y^j, x^k)) \\ \leq \alpha\zeta^m \rho (\nabla f^k(y^j) + \chi_k \nabla_I D(y^j, x^k))^T p^j. \end{aligned} \tag{6.10}$$

Then set $\alpha_j = \alpha\zeta^m$. In our implementation we choose $\alpha = 1$, $\zeta = 0.5$, and $\rho = 0.1$.

Self-concordance step size. In Theorem 4.2.3 it is shown that $D(\cdot, x^k)$ is strongly self-concordant with parameter $\vartheta(x^k) = \max\left\{\frac{2}{l_i(x^k)} : i = 1, \ldots, p\right\}$. If f^k is ϑ_f^k self-concordant then $f^k + \chi_k D(\cdot, x^k)$ is ϑ_k self-concordant with

$$\vartheta_k = \max\{\vartheta_f^k, \chi_k^{-1/2}\vartheta(x^k)\}.$$

As presented in Section 4.3, the following step size rule leads to an efficient Newton method.

Let $\lambda_* = 2 - \sqrt{3} \approx 0.2679$ and $\lambda' \in [\lambda_*, 1)$. The Newton decrement is calculated by

$$\lambda_j = \frac{\vartheta_k}{2}\sqrt{-(\nabla f^k(y^j) + \chi_k \nabla_I D(y^j, x^k))^T p^j},$$

where y^j is the current Newton iterate and p^j the calculated Newton direction. Then the step size is set to

$$\alpha_j = \begin{cases} \frac{1}{1+\lambda_j} & \text{if } \lambda_j > \lambda' \\ \frac{1-\lambda_j}{\lambda_j(3-\lambda_j)} & \text{if } \lambda' \geq \lambda_j \geq \lambda_* \\ 1 & \text{if } \lambda_j < \lambda_*. \end{cases}$$

In our implementation we set $\lambda' = 0.9$.

Distance value outside int(K). At the beginning of the determination of an Armijo step size it is possible that the test points $y^j + \alpha\zeta^m p^j$ lie outside $\text{int}(K)$. In this case the value of the logarithmic-quadratic distance function is $+\infty$ per definition. In the implementation we set $D(x, y) = 10^{12}$ if $x \notin \text{int}(K)$.

Stopping criterion. The Newton iteration has to be stopped if

$$\| \nabla f^k(y^j) + \chi_k \nabla_I D(y^j, x^k) \| \leq \delta_k.$$

Then $x^{k+1} := y^j$ is a solution of schemes (6.2) respectively (6.4) with $e^{k+1} = \nabla f^k(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k)$. However, we observed that this stopping rule may not take effect near the boundary of the feasible set since the admitted step sizes are too small. For that reason, we additionally stop the Newton method if $\min\{(b - Ay^j)_i : i = 1, \ldots, p\} \leq 10^{-16}$. Furthermore, to avoid a step size that is beyond machine precision, the calculation is terminated if a value smaller than 10^{-10} is reached. Such a value is interpreted as being zero and therefore the Newton iteration is stopped with $x^{k+1} := y^j$.

6.1.2 Initialization and update of the regularization parameter χ_k

According to conditions (3.20) and (3.21), the sequence $\{\chi_k\}$ of regularization parameters has to be bounded with a lower bound being strictly greater than a special constant $\underline{\chi}$:

$$0 \leq \underline{\chi} \leq \chi_k \leq \overline{\chi} < \infty \quad \forall k \in \mathbb{N}_0, \tag{6.11}$$

$$\underline{\chi} > \frac{1}{2a^2\gamma}. \tag{6.12}$$

Determination of $\underline{\chi}$ and $\overline{\chi}$. Possibilities to calculate the modulus γ of the (weakened) co-coercivity condition (A7) were mentioned in Section 5.4. In order to determine a lower bound $\underline{\chi}$, it remains to investigate the calculation of a constant $a > 0$ that fulfills

$$\| Au \| \geq a \| u \| \quad \forall u \in \mathbb{R}^n.$$

To this end, we make use of the Rayleigh-principle for a symmetric matrix $B \in \mathbb{R}^{n\times n}$, which states that the smallest eigenvalue of B can be determined as

$$\lambda_{\min}(B) = \min_{u\neq 0} \frac{\langle Bu, u\rangle}{\| u \|^2}$$

(see [43, Theorem 4.2.2]). An immediate consequence is

Lemma 6.1.1. *Let $A \in \mathbb{R}^{p\times n}$ be a matrix with rank$(A) = n$. Define*

$$a = \sqrt{\lambda_{\min}(A^T A)}.$$

Then $a > 0$ and $\| Au \| \geq a \| u \|$ for all $u \in \mathbb{R}^n$.

Having calculated γ and a we set, according to (6.12),

$$\underline{\chi} = \frac{1}{2a^2\gamma} + 10^{-3}. \tag{6.13}$$

However, if $\mathcal{F} = 0$ and $\mathcal{L}^k = 0$ for all k (as in Category 1a), condition (A7) is fulfilled with an arbitrary $\gamma > 0$. This allows to choose any lower bound $\underline{\chi} > 0$. In this case it is empirically reasonable to set $\underline{\chi} = 10^{-3}$. The value of $\overline{\chi}$ is chosen sufficiently large, for example, $\overline{\chi} = \chi_0 \cdot 10^3$.

Initialization and update of χ_k. The parameter χ_k controls the regularizing effect of the distance function. A large value of χ_k implies a strong regularizing effect and keeps the next iterate x^{k+1} close to the current iterate x^k. On the other hand, the smaller the value of χ_k, the less influence has the distance function. This results in a larger step from x^k to x^{k+1}.

Conditions (6.11)–(6.12) are rather general and allow multiple possibilities for the sequence $\{\chi_k\}$. However, for an implementation of the method we are interested in an

explicit and hopefully "efficient" specification. Efficient means that the method will find a good approximation of the solution within a number of iterations that will be small compared to other settings. It is an open question how to find such an appropriate choice for the sequence $\{\chi_k\}$. In literature, helpful information is scarcely available. Mostly, the settings are based on heuristics or experienced data. Theoretically, it is allowed to take a constant sequence

$$\chi_k = \chi_0 \quad \forall k \in \mathbb{N}.$$

But it is known from implementations of the PPA and the BrPAP (see [47], [63]) that an iteratively decrease in the sense of $\chi_{k+1} = \chi_0 r^{k+1}$ with $r \in (0,1)$ leads to an acceleration of the method. To respect the lower bound $\underline{\chi}$ the precise choice should be

$$\chi_{k+1} = \max\{\chi_0 r^{k+1}, \underline{\chi}\}, \quad r \in (0,1). \tag{6.14}$$

6.1.3 Choice of the tolerance parameter δ_k and the stopping criterion

The nonnegative sequence of error tolerance parameters $\{\delta_k\}$ must be chosen a priori such that it is summable according to condition (3.22). This is realized in our implementation by setting

$$\delta_{k+1} = c\delta_k, \quad \delta_0 \geq 0, \quad c \in (0,1).$$

Then we have $\sum_{k=0}^{\infty} \delta_k = \delta_0 \sum_{k=0}^{\infty} c^k$ and summability of the error tolerance parameters is established since $c \in (0,1)$. The concrete values taken in the implementation are $\delta_0 = 10^{-3}$, $c = 0.999$.

A commonly used stopping criterion for numerical methods is to test if

$$\| x^k - x^{k+1} \| < \theta.$$

Because the resulting optimization problems (6.3) respectively (6.5) are at least strictly convex, this indicates that the iterates are close to an optimum since the algorithm does not make any substantial progress. In our implementation we set $\theta = 10^{-5}$. Nevertheless, we have to pay attention if the iterates reach the boundary of the feasible set before being close to an optimal solution. The resulting small step sizes may lead to a stop of the algorithm. This situation will further be discussed within the coming sections.

6.1.4 The overall LQPAP algorithm

The preceding considerations about the implementation of the LQPAP method for convex optimization problems are summarized in Algorithm 6.2.

Algorithm 6.2: LQPAP algorithm for convex, differentiable optimization problems

1. *(Initialization)* Choose a start iterate $x^0 \in \text{int}(K)$, an initial tolerance parameter δ_0, a changing factor $c \in (0,1)$ for δ_k, a stopping parameter $\theta > 0$, a lower and upper bound $\underline{\chi}$ resp. $\overline{\chi}$, an initial regularization parameter χ_0, and a changing factor $r \in (0,1)$ for χ_k. Define f^k according to (6.6) resp. (6.7). Set $k := 0$.

2. *(Solution of the auxiliary problem with the Newton method)* Calculate x^{k+1} with Algorithm 6.1.

3. *(Stopping criterion)* If $\| x^k - x^{k+1} \| < \theta$ then stop: x^{k+1} is an approximate solution of (6.1).

4. *(Update of parameters)* $\chi_{k+1} = \max\{\underline{\chi}, r\chi_k\}$, $\delta_{k+1} = c\delta_k$.

5. Set $k := k+1$ and go to step 2.

6.1.5 Adaptations for the BrPAP method

To adapt our implementation of the LQPAP method to the BrPAP method introduced in Section 2.4.1, we only need to exchange the logarithmic-quadratic distance with a Bregman-distance and to appropriately choose the lower bound $\underline{\chi}$ for the regularization parameters.

Category 1a. In the context of Category 1a the BrPAP scheme is reduced to a proximal-like scheme. In this case, a *strictly* convex and zone coercive Bregman-function with zone $\text{int}(K)$ is sufficient, e.g.,

$$h(x) = \sum_{i=1}^{p} l_i(x) \log(l_i(x)) \quad (0 \log(0) := 0) \tag{6.15}$$

with Bregman-distance

$$D_h(x,y) = \sum_{i=1}^{p} l_i(x) \log \frac{l_i(x)}{l_i(y)} - l_i(x) + l_i(y).$$

For fixed $y \in \text{int}(K)$ the gradient and Hesse matrix of $D_h(\cdot, y)$ at $x \in \text{int}(K)$ are

$$\nabla_I D_h(x,y) = -\sum_{i=1}^{p} a_i \left(\log \frac{l_i(x)}{l_i(y)} \right),$$

$$\nabla_I^2 D_h(x,y) = \sum_{i=i}^{p} \left(\frac{1}{l_i(x)} \right) a_i a_i^T.$$

Furthermore, the lower bound is set to $\underline{\chi} = 10^{-3}$.

Category 1b. For Category 1b the Bregman-distance has to be based on a *strongly* convex and zone coercive Bregman function with zone $\mathrm{int}(K)$. With a simple modification of h a strongly convex Bregman function (with modulus κ) is obtained as

$$\tilde{h}(x) = h(x) + \frac{\kappa}{2} \parallel x \parallel^2, \quad \kappa > 0. \tag{6.16}$$

The corresponding Bregman distance is

$$D_{\tilde{h}}(x, y) = D_h(x, y) + \frac{\kappa}{2} \parallel x - y \parallel^2 .$$

$D_{\tilde{h}}(x, y)$ can be seen as a double regularization by $D_h(x, y)$ and the standard quadratic distance function. To avoid too much influence of the latter, it is reasonable to set $\kappa = 1$. According to the Condition (BrPAP)(3)(b) (see page 32), the lower bound $\underline{\chi}$ is set to

$$\underline{\chi} = \frac{1}{4\gamma} + 10^{-3}. \tag{6.17}$$

A final remark is devoted to the value of the Bregman-distance for arguments outside $\mathrm{int}(K)$. In contrast to the logarithmic-quadratic distance function, the Bregman distance is finite for arguments x belonging to $\mathrm{bd}(K)$. This is due to the convention $0 \log(0) = 0$. For points $x \notin K$ we set $D_h(x, y)$ respectively $D_{\tilde{h}}(x, y)$ to 10^{12}.

6.2 Academic test examples

This section presents some academic test problems which can be found in literature or which are randomly generated. The problems are of the type

$$\begin{aligned} &\min \ \psi(x) \\ &\text{s.t. } Ax \leq b, \end{aligned}$$

where $\psi : \mathbb{R}^n \to \mathbb{R}$ is a convex, twice continuously differentiable function. For each example we give the data ψ, A, and b, the dimension n, the number of constraints p, the solution set X^* or the (exact or approximate) unique solution x^*, the optimal value ψ^*, and one or more considered initial points x^0.

6.2.1 Two-dimensional examples

With the following two-dimensional ill-posed examples we intend to analyze the geometric behavior of the LQPAP and the BrPAP method by plotting graphics with the sequences of iterates.

The first example consists of a quadratic objective function that is convex but not strictly convex. More precisely, the objective function is convex with respect to the first variable and linear with respect to the second variable. Furthermore, the solution set is not a singleton.

The second example represents an ill-conditioned convex-quadratic problem, i.e., the contour lines are flat ellipses. Here, the solution is unique. With $\mathrm{cond}(C)$ we denote the condition number of the matrix C.

Example 6.2.1 (First 2-dim example).

$$\psi(x) = (x_1 - 2)^2,$$

$$A = \begin{pmatrix} 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \\ -1 & 1 \\ 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1.25 \\ 1.25 \\ 1.25 \end{pmatrix},$$

$n = 2$, $p = 7$, $x_1^0 = (-0.25, 0.9)^T$, $\psi(x_1^0) = 5.0625$, $x_2^0 = (-0.75, 0.4)^T$, $\psi(x_2^0) = 7.5625$, $x_3^0 = (-0.9, 0)^T$, $\psi(x_3^0) = 8.41$, $x_4^0 = (-0.9, -0.9)^T$, $\psi(x_4^0) = 8.41$,
$X^* = \left\{x = (x_1, x_2)^T : x_1 = 1, x_2 \in [-0.25, 0.25]\right\}$, $\psi^* = -1$.

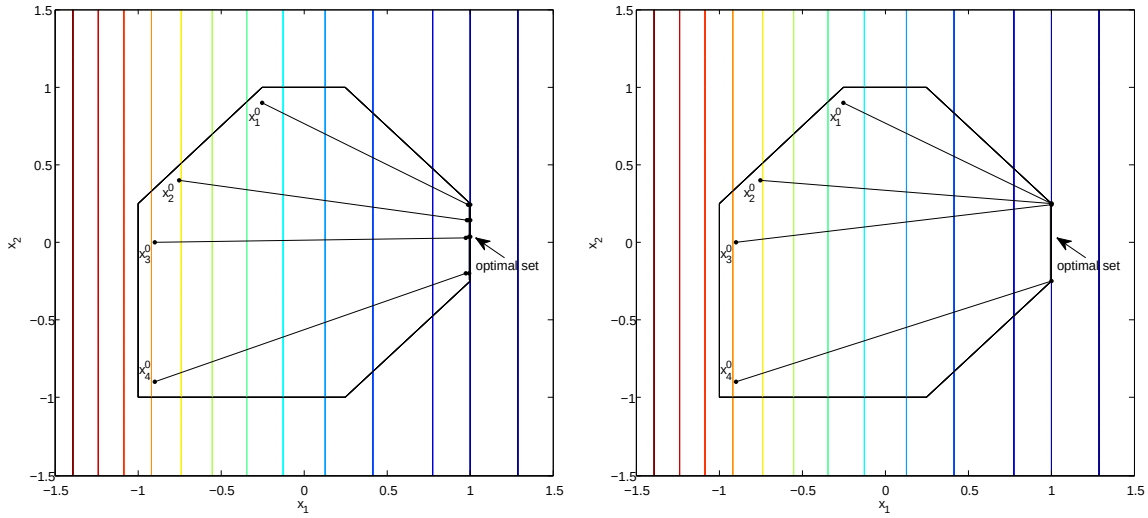
Example 6.2.2 (Second 2-dim example).

$$\psi(x) = \frac{1}{2} \langle Cx, x \rangle + \langle d, x \rangle ,$$

$$C = \begin{pmatrix} 0.4 & 0.01 \\ 0.01 & 10000 \end{pmatrix}, \quad d = \begin{pmatrix} 0.03 \\ 5 \end{pmatrix},$$

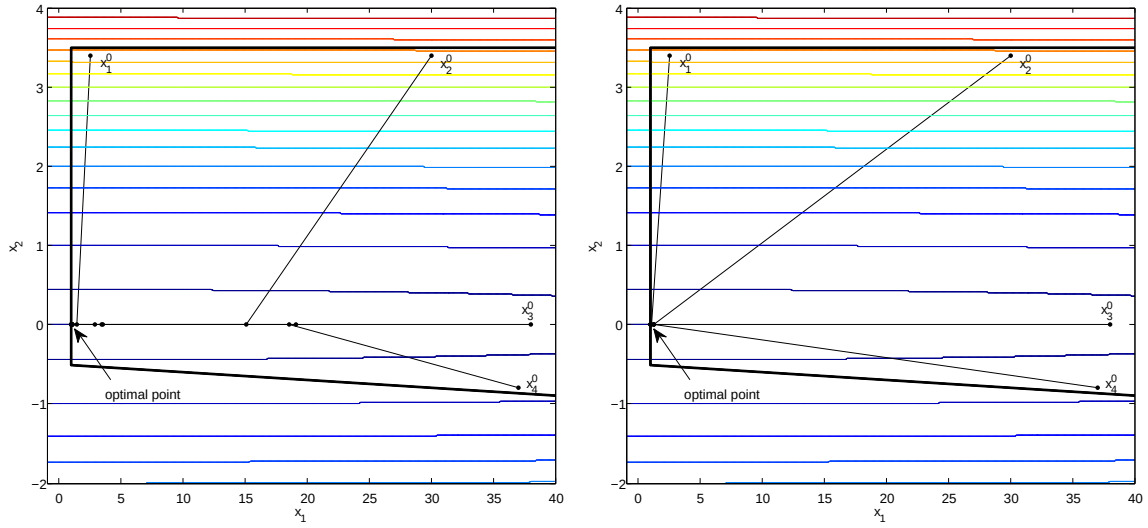
$$A = \begin{pmatrix} -1 & 0 \\ 0 & 1 \\ 0.2 & -1 \end{pmatrix}, \quad b = \begin{pmatrix} -1 \\ 3.5 \\ 0.5 \end{pmatrix},$$

$n = 2$, $p = 3$, $x_1^0 = (2.5, 3.4)^T$, $\psi(x_1^0) = 57818.41$, $x_2^0 = (30, 3.4)^T$, $\psi(x_2^0) = 57998.92$, $x_3^0 = (38, 0)^T$, $\psi(x_3^0) = 289.94$, $x_4^0 = (37, -0.8)^T$, $\psi(x_4^0) = 3470.614$, $x^* = (1, -0.0501)^T$, $\psi^* = 0.228744995$, $cond(C) \approx 2.5 \cdot 10^4$.



(a) LQPAP method (b) BrPAP method

Figure 6.1. Path of the iterates for different initial points in Example 6.2.1.



(a) LQPAP method (b) BrPAP method

Figure 6.2. Path of the iterates for different initial points in Example 6.2.2.

To get a first impression of how the methods work we model the above examples according to Category 1a, adjust the choice of $\{\chi_k\}$ towards a good performance and plot some sequences of iterates for different initial points using the Newton method with Armijo step sizes for the solution of the auxiliary problems.

Figures 6.1–6.2 present the results. The iterates in the graphics are marked by a point and connected by lines. In both examples, only 3–5 iterations are needed to reach an

optimal solution. Often, the first iterate is close to a solution, such that subsequent iterates can hardly be seen in the graphics. In the case of multiple solutions it can be observed for both methods that the calculated solutions can be different for different initial points. Furthermore, Example 6.2.2 shows the different behavior of the two methods in the case of a unique solution. The iterates follow different paths to the optimal solution: Whereas the paths of the iterates of the LQPAP method meet at a horizontal line before reaching the optimal point, the iterates of the BrPAP method are already close to the optimal point after one iteration.

6.2.2 Higher-dimensional examples

The first two higher-dimensional examples are taken from [85] and [42]. Examples 6.2.5 and 6.2.6 represent a class of linear constrained, convex quadratic problems that are randomly generated. In view of Lemma 5.4.16, the examples are generated such that the matrix C in the objective function is symmetric and diagonally dominant. In Example 6.2.5 the feasible set K is an arbitrary polyhedron defined by a matrix A of full column rank and a vector b whose components are greater than zero. Thus, $x = 0$ belongs to $\text{int}(K)$ and can be taken as an initial point. In Example 6.2.6 we consider the special case $K = \mathbb{R}^n_+$. All matrices and vectors of the test examples are given in the Appendix A.5 (except for the problems of dimension 100).

Example 6.2.3 (Schittkowski no. 268, [85]).

$$\psi(x) = \left\langle D^T D x, x \right\rangle - 2 \left\langle Dx, d \right\rangle + \| d \|^2,$$

see Appendix A.5.1 for the setting of D, d, A, and b,
$n = 5$, $p = 5$, $x^0 = (-1.5, 3.5, 0.5, 4.0, -2.0)^T$, $\psi(x^0) = 182799.25$, $x^* = (1, 2, -1, 3, -4)^T$,
$\psi^* = 0$, $cond(D^T D) = 1.1769 \cdot 10^6$.

Example 6.2.4 (Modified Colville, [42]).

$$\psi(x) = x^T C x + d^T x + e^T x,$$

see Appendix A.5.2 for the setting of C, d, e, A, and b,
$n = 5$, $p = 15$, $x^0 = (0.1, 0.1, 0.1, 0.1, 1)^T$, $\psi(x^0) = 11.96$,
$x^* \approx (0.3, 0.322547, 0.4, 0.4017501, 0.2495811)^T$, $\psi^* = -23.0448869$, $\lambda_{\min}(C) = 0$.

Example 6.2.5 (Random convex quadratic example with polyhedral K).

$$\psi(x) = \frac{1}{2}\langle Cx, x\rangle + \langle d, x\rangle, \quad x \in \mathbb{R}^n,$$

$n \in \mathbb{N}$, $p \geq n$, $C \in \mathbb{R}^{n\times n}$ randomly generated, symmetric, diagonally dominant matrix with integer entries $c_{ij} \in [-100, 100]$ (for $i \neq j$) and c_{ii} such that diagonal dominance holds, $d \in \mathbb{R}^n$ randomly generated vector with integer entries $d_i \in [-100, 100]$, $A \in \mathbb{R}^{p\times n}$ randomly generated matrix with full column rank and integer entries $a_{ij} \in [-100, 100]$, $b \in \mathbb{R}^p$ randomly generated vector with integer entries $b_j \in [1, 100]$, $x^0 = (0, \ldots, 0)^T \in \mathbb{R}^n$, ψ^* calculated with the MATLAB® routine fmincon. For our tests we generated

- *Example 6.2.5.a: $n = 10$, $p = 20$, $\psi(x^0) = 0$, $\psi^* \approx -43.14856$, C strictly diagonally dominant, cond$(C) = 4.6428$, see Appendix A.5.3 for the specific data,*
- *Example 6.2.5.b: $n = 100$, $p = 150$, $\psi(x^0) = 0$, $\psi^* \approx -37.02374$, C diagonally dominant, cond$(C) = 1.6465$.*

Example 6.2.6 (Random convex quadratic example with $K = \mathbb{R}^n_+$).

$$\psi(x) = \frac{1}{2}\langle Cx, x\rangle + \langle d, x\rangle, \quad x \in \mathbb{R}^n,$$

$n \in \mathbb{N}$, $p \geq n$, $C \in \mathbb{R}^{n\times n}$ randomly generated, symmetric, diagonally dominant matrix with integer entries $c_{ij} \in [-100, 100]$ (for $i \neq j$) and c_{ii} such that diagonal dominance holds, $d \in \mathbb{R}^n$ randomly generated vector with integer entries $d_i \in [-100, 100]$, $A = -I \in \mathbb{R}^{n\times n}$, $b = 0 \in \mathbb{R}^n$, $x^0 = (10, \ldots, 10)^T \in \mathbb{R}^n$, ψ^* calculated with the MATLAB® routine fmincon. For our tests we generated

- *Example 6.2.6.a: $n = 10$, $\psi(x^0) = 263110$, $\psi^* \approx -19.78359$, C strictly diagonally dominant, cond$(C) = 6.4193$, see Appendix A.5.4 for the specific data,*
- *Example 6.2.6.b: $n = 100$, $\psi(x^0) = 24123620$, $\psi^* \approx -19.68023$, C diagonally dominant, cond$(C) = 1.7686$.*

6.2.3 Numerical results for differentiable examples

The numerical results for the two- and higher-dimensional examples are collected in Table 6.1 for the LQPAP method and Table 6.2 for the BrPAP method. All problems are modeled according to Category 1a, and the Newton method with Armijo step sizes is used for the solution of the auxiliary problems. In Examples 6.2.1 and 6.2.2 the last listed initial point is chosen. The following information is given in the tables:

χ_0:	initial value of the regularization parameter,
r:	decreasing factor to update $\chi_{k+1} = \chi_0 r^{k+1}$,
#iter:	number of iterations,
#New:	total number of Newton iterations,
$\#\psi$:	number of objective function evaluations,
ψ_{calc}:	calculated optimal value,
$\lvert\psi_{calc} - \psi^*\rvert$:	distance between calculated and known optimal value.

The number $\#\psi$ of objective function evaluations depends on the frequency of decreasing steps to find an Armijo step size fulfilling (6.10). The number of gradient evaluations of ψ coincides with the total number of Newton iterations because in each Newton iteration the gradient of ψ is evaluated once in the stopping criterion.

Example		$\{\chi_k\}$		LQPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.01	0.1	3	34	383	1.00000	0.00e+00
6.2.2	Second 2-dim example	0.01	0.7	5	51	490	0.22874	1.39e-16
6.2.3	Schittkowski no. 268	0.01	0.1	40	83	86	0.00000	2.40e-06
6.2.4	Modified Colville	0.01	0.1	3	51	567	-23.04489	6.81e-07
6.2.5.a	Random $n = 10, p = 20$	0.01	0.3	6	55	363	-43.12260	2.60e-02
6.2.5.b	Random $n = 100, p = 150$	0.01	0.1	5	49	355	-36.98940	3.43e-02
6.2.6.a	Random $n = 10$	0.10	0.5	4	67	728	-19.78359	3.95e-11
6.2.6.b	Random $n = 100$	10.00	0.5	5	203	2385	-19.68023	5.56e-08

Table 6.1. Results for the LQPAP method applied to differentiable convex problems.

Example		$\{\chi_k\}$		BrPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.01	0.1	2	36	315	1.00000	0.00e+00
6.2.2	Second 2-dim example	0.10	0.5	4	38	162	0.22874	2.78e-16
6.2.3	Schittkowski no. 268	0.01	0.1	12	29	34	0.00000	3.21e-06
6.2.4	Modified Colville	100.00	0.9	36	178	448	-22.98871	5.62e-02
6.2.5.a	Random $n = 10, p = 20$	1.00	0.7	14	79	218	-43.14853	3.15e-05
6.2.5.b	Random $n = 100, p = 150$	10.00	0.3	9	57	208	-37.02426	5.26e-04
6.2.6.a	Random $n = 10$	100.00	0.9	14	82	180	-19.73598	4.76e-02
6.2.6.b	Random $n = 100$	100.00	0.9	17	93	189	-19.67130	8.93e-03

Table 6.2. Results for the BrPAP method applied to differentiable convex problems.

For a suitable comparison of the LQPAP and the BrPAP method the values for $\chi_0 \in \{0.01, 0.1, 1, 10, 100\}$ and $r \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$ are adapted towards a best performance. The performance is measured by the reached accuracy of the calculated optimal value. This can result in different sequences $\{\chi_k\}$ for the LQPAP and the BrPAP method because the type of distance function is different and, therefore, a different type of parameter choice is possibly needed. In most cases the LQPAP method

is used with a small initial regularization of $\chi_0 = 0.01$ with a fast reduction by $r = 0.1$ or $r = 0.3$. For the BrPAP method such a general statement cannot be given since all ranges of initial values χ_0 and different reduction factors r occur.

For a comparison of the iteration numbers of the LQPAP and the BrPAP method it is important to know that the setting of $\{\chi_k\}$ has an influence on the iteration numbers. A large initial value χ_0 together with a slow reduction implies a strong regularizing effect of the used distance function and results in a larger number of iterations than a small initial value with a fast reduction. This can be seen in Examples 6.2.4–6.2.6.b where the BrPAP method is used with larger initial values χ_0 and larger decreasing factors r than the LQPAP method. Consequently, the BrPAP method needs more iterations. However, in Examples 6.2.5.a and 6.2.5.b the accuracy of the calculated solution has to be taken into account, which is higher in the BrPAP method than in the LQPAP method. In the other examples the LQPAP method calculates optimal values whose accuracy is similar or better than that reached by the BrPAP method.

The number of total inner (Newton) iterations is correlated to the number of outer (LQPAP/BrPAP) iterations. Thus, in the cases where the LQPAP method needs fewer outer iterations than the BrPAP method, the number of total inner iterations in the LQPAP method is similar as or less than that of the BrPAP method (with an exception in Example 6.2.6.b).

In all examples the number $\#\psi$ of function evaluations performed by the LQPAP method is higher than in the BrPAP method. Thus, in the BrPAP method the number of decreasing steps to find an appropriate Armijo step size is less than in the LQPAP method. This indicates that the Newton directions determined in the BrPAP method are "qualitatively better". A more detailed analysis of this situation is given in Section 6.3, where we describe a general observation on the Hesse matrices of the logarithmic-quadratic distance and the Bregman distance.

Let us finally comment on the effectiveness of the methods. In 6 of 8 (LQPAP) respectively 4 of 8 (BrPAP) examples the methods reach an accuracy of 10^{-5} or better in the calculated optimal value. In the examples where the methods have problems to find an accurate solution it can be observed that the iterates reach the boundary of the feasible set before being close to an optimal solution. In this situation, the calculated directions mostly point outside the feasible set. This leads to small step sizes and finally to the termination of the algorithm. It cannot be excluded that a different choice of the regularization parameters (apart from the tested choices) would lead to better results.

In view of the above observations it is difficult to say which method is preferable. To achieve a high accuracy, a "good" choice of the regularization parameters is crucial in both methods. Since the best performance of the LQPAP method is often achieved with smaller values of the regularization parameters than in the BrPAP method, the

iteration numbers in the LQPAP method are less than in the BrPAP method. On the other hand, the BrPAP method should be favored to get small numbers of function evaluations. To obtain more information about the characteristics of the two methods, more experiments and observations are given in the next section.

6.3 Observations and summary of numerical tests

6.3.1 Comparison of the Hesse matrices

The different behavior of the LQPAP algorithm and the BrPAP algorithm can partly be explained with the characteristics of the Hesse matrices of the distance functions.

First, consider the Hesse matrix of the logarithmic-quadratic distance function with respect to x:

$$\nabla_I^2 D(x,y) = \sum_{i=1}^{p} \left(2 + \frac{l_i(y)^2}{l_i(x)^2}\right) a_i a_i^T.$$

The factors $r_i(x,y) := \left(2 + \frac{l_i(y)^2}{l_i(x)^2}\right)$ in front of the dyadic products $a_i a_i^T$ depend on the distance of the points x and y to the boundary of K. If x lies close to the boundary of K then $l_i(x) \approx 0$ for some $i \in \{1,\dots,p\}$. Thus, for fixed y, if x tends to the boundary of K then $r_i(x,y)$ tends to infinity for some i. This situation implies a bad condition of the Hesse matrix and simultaneously constitutes the barrier effect of D.

However, in Algorithm 6.1 the distance function is evaluated at $x = y^j$ and $y = x^k$ where y^j are the iterates of the Newton method (with $y^0 = x^k$). So, in the first Newton iteration we have $r_i(y^0, x^k) = 3$ for all i. Moreover, if the Armijo step sizes are small, which often occurs near the boundary of K, then y^j and x^k lie close to each other. Consequently, $l(y^j) \approx l(x^k)$ and therefore $r_i(y^j, x^k) \approx 3$ for all i. Thus, a bad condition of the Hesse matrix near the boundary of K cannot be observed and a barrier effect of D is hardly given, so that the calculated Newton directions may be insufficiently influenced by the distance function. An inappropriate Newton direction results in step sizes that are almost zero, which leads to a termination of the Newton iteration. To improve the barrier effect of D, an appropriate choice of the regularization parameters is needed, but is eventually hard to find. The experiments show that a fast reduction of χ_k by $r = 0.1$ often leads to the best performance of the algorithm. This is against the classical rules of regularization, which recommend to work with a slow reduction like $r = 0.9$ to allow that the auxiliary problems get well adapted during the first iterations. In view of the above described background the following explanation is possible: With a fast reduction of the influence of D, two consecutive iterates can have a greater distance

to each other than with a slow reduction. So, the effect of having $r_i(y^j, x^k) \approx 3$ for all i is avoided.

Now, recall the Hesse matrix of the Bregman distance function D_h:

$$\nabla_I^2 D_h(x, y) = \sum_{i=1}^{p} \frac{1}{l_i(x)} a_i a_i^T.$$

Here, the factors $r_i^h(x) := \frac{1}{l_i(x)}$ in front of the dyadic products $a_i a_i^T$ only depend on the distance of x to the boundary of K. If x approaches the boundary of K then $r_i^h(x)$ tends to infinity for some i. This results in a bad condition of the Hesse matrix. So, in contrast to the logarithmic-quadratic distance function, the barrier effect of the Bregman distance near the boundary is better indicated in its Hesse matrix.

6.3.2 Armijo versus self-concordance rule

In all test examples the objective function is linear or convex-quadratic. Such functions are 0-self-concordant. Thus, in the LQPAP method it is possible to use the self-concordance rule instead of the Armijo rule to determine the step sizes.

Table 6.3 presents the corresponding results when using the self-concordance step size. For the sequence $\{\chi_k\}$ the best performance choice as in Table 6.1 is used.

Example		$\{\chi_k\}$		LQPAP method				
No.	name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.01	0.1	3	42	0	1.00000	5.33e-15
6.2.2	Second 2-dim example	0.01	0.7	5	76	0	0.22874	2.14e-15
6.2.3	Schittkowski no. 268	0.01	0.1	40	303	0	0.00000	2.40e-06
6.2.4	Modified Colville	0.01	0.1	3	57	0	-23.04489	6.80e-07
6.2.5.a	Random $n = 10, p = 20$	0.01	0.3	6	52	0	-43.07208	7.65e-02
6.2.5.b	Random $n = 100, p = 150$	0.01	0.1	5	53	0	-36.98940	3.43e-02
6.2.6.a	Random $n = 10$	0.10	0.5	4	371	0	-19.78344	1.52e-04
6.2.6.b	Random $n = 100$	10.00	0.5	5	809	0	-19.68023	5.56e-08

Table 6.3. Results for the LQPAP method using the self-concordance step size in the Newton method.

The promised efficiency of the Newton method is not reflected in the number of Newton iterations since in most cases this number is higher than with the Armijo rule. However, since the calculation of the self-concordance step size can be done without any function evaluation of ψ, this advantage compared to the Armijo step size is obvious.

In Examples 6.2.3, 6.2.6.a, and 6.2.6.b we observed that the Newton decrements λ_j can have values in the range of 200–700, especially in the first (about 100) Newton

iterations. As a result, the step sizes are in the range of 10^{-3}. This is the reason why in those examples the number of total Newton iterations is high.

The efficiency of the self-concordance rule (i.e., the quadratic convergence of the Newton decrements) is not given until the Newton decrements have a value smaller than $\lambda^* \approx 0.2679$. Thus, it might be interesting to use the Armijo rule at the beginning and to switch to the self-concordance rule if $\lambda_j < \lambda^*$ holds true. The corresponding results for this strategy are given in Appendix A.6.1. It can be seen that the combination of the step size rules helps to reduce the number of (possibly expensive) function evaluations, while the number of outer and inner iterations (roughly) stays the same as in Table 6.1.

The properties of the sequence $\{\lambda_j\}$ of Newton decrements as presented in Theorem 4.3.2(ii) are exemplarily examined in Appendix A.6.2. The presented results verify the fulfillment of these properties in all cases.

6.3.3 Modeling according to Category 1b

The preceding experiments are all based on a modeling of the given problems as in Category 1a. If $\nabla\psi$ is co-coercive, which is the case in all given test examples, it is also possible to model the problem according to Category 1b. Appendix A.6.3 presents the corresponding results. Due to the only linear approximation of ψ in Category 1b and often high values for $\underline{\chi}$, both methods do not perform well in most test examples. Furthermore, an advantage of using a nonzero auxiliary operator $\mathcal{L}^k$ (in examples where Lemma 5.4.16 is applicable) cannot be observed. Therefore, we do not continue to analyze Category 1b any further.

6.3.4 Adaptive choice of χ_0

A possibility for an adaptive determination of the initial value χ_0 is described in [44, Section 6.2.4.]. We intend to test this strategy and transfer it to our situation. The idea is to calculate at step $k = 0$ an approximation $\tilde{y}^1$ of the solution x^1 of (6.8) and to determine χ_0 such that $\tilde{y}^1$ stays feasible and lies in the unit ball around x^0. For more information we refer to Appendix A.6.4.

Detailed experiments that compare for both methods the adaptive initialization with the best performance choice are also presented in Appendix A.6.4. The result for both methods is: The adaptive initialization procedure for χ_0 leads – under an appropriate choice of the decreasing factor r – to results whose accuracies are comparable to those of a best performance choice (although the iteration numbers are in general higher).

6.4 Idea of under-relaxation

Proximity to the boundary. The best performance values for $\{\chi_k\}$ were found after numerous experiments with different settings for χ_0 and r. Doing so, we observed in many examples that the performance of the LQPAP algorithm is quite sensitive with regard to the choice of the regularization parameter. It may happen that with a given sequence $\{\chi_k\}$ a solution of good accuracy is computed, but that for another choice the optimal solution is not reached. Furthermore, such experiments are of course not realizable with examples where the solution is unknown. The adaptive initialization rule for χ_0 proved to be effective in many examples. But, an appropriate choice of r is crucial because the decreasing factors may not all work well.

The reason for a failure of the methods is that the iterates reach the boundary of the feasible set before being close to an optimal solution.

This is demonstrated in Figure 6.3 for Example 6.2.1. The optimal solution is not reached when starting at $x_1^0 = (-0.9, -0.9)^T$ or $x_2^0 = (-0.24, -0.999)^T$ and using $\chi_0 = 10$, $r = 0.9$.

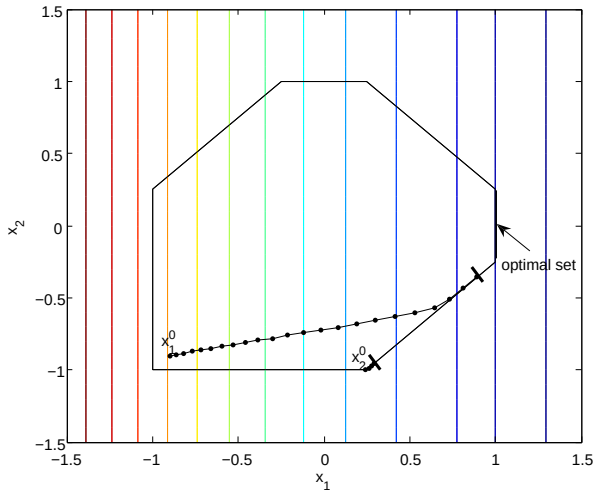


Figure 6.3. Example 6.2.1 with LQPAP method and an inappropriate choice of $\{\chi_k\}$.

Of course, if a situation like with x_2^0 occurs, where the initial point is already close to the boundary and the search direction points outside the feasible set, it can be difficult for the method to proceed.

But also with an initial iterate like $x_1^0 = (-0.9, -0.9)^T$, where the first 18 iterates lie well in the interior of the feasible set, an appropriate shift of the search directions is not realized early enough and the method stops at a suboptimal point.

In some examples we additionally observed that the distance between two consecutive iterates can be quite large in the beginning. For example, iterate x^k lies well in the interior whereas iterate x^{k+1} is already very close to the boundary but not as well close to an optimal solution.

In general, the influence of the distance function D is not important if the iterates lie well in the interior of the feasible set. The barrier effect of D has to start working when the iterates approach the boundary. However, the examples show that an appropriate influence of D may not occur until the iterates are already close to the boundary.

Therefore, we will now propose a strategy that robustifies the LQPAP algorithm with respect to different choices of $\{\chi_k\}$.

Results using under-relaxation. Instead of making full steps in the outer (LQPAP) iteration we suggest to take an iterate lying between the old and the proposed new iterate. This strategy is called *under-relaxation* in literature (see, e.g., [29]).

Let z^{k+1} be the iterate calculated by the Newton-method in step k of the algorithm. Then we set

$$x^{k+1} = x^k + t(z^{k+1} - x^k), \tag{6.18}$$

where $t \in (0, 1)$ is the relaxation parameter. Thus, the iterate x^{k+1} lies on the connecting line between x^k and z^{k+1}. In our implementation we set $t = 0.5$.

The desired effect of using under-relaxation is that the model given by the auxiliary problems can adjust itself earlier to the constraints. As a consequence, the iterates are prevented from tending towards the "wrong" part of the boundary.

Figure 6.4 shows for Example 6.2.1 the path of the iterates when using under-relaxation. For both initial points the results are improved.

In Appendix A.6.5 the effect of under-relaxation is evaluated with detailed graphics for each test example. The reached accuracies over all tested parameter settings for χ_0 and r are almost constant in the range of 10^{-3} or better (with few exceptions), whereas with the standard LQPAP algorithm there are often outliers where the accuracy is in the range of 10^{-2} or worse. Only in Examples 6.2.2 and 6.2.6.b the under-relaxation strategy is constantly worse than the standard LQPAP algorithm. Thus, we can state that under-relaxation robustifies the LQPAP method such that an adequate choice of $\{\chi_k\}$ is not as crucial as without this strategy.

As a drawback of under-relaxation one has to mention that the iteration numbers are higher (about factor 2–3 compared to the best performance choice).

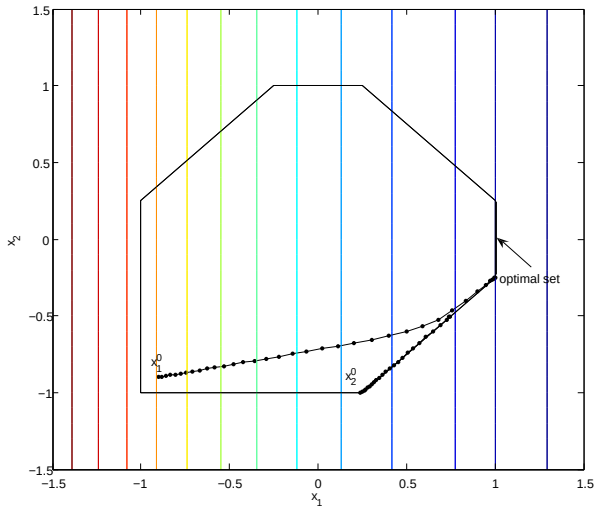


Figure 6.4. Under-relaxation improves the LQPAP method in Example 6.2.1.

The strategy was also tested with the BrPAP method, but similar improvements as with the LQPAP algorithm could not be observed. This is possibly due to the different behavior of the Bregman distance near the boundary as described in Section 6.3.1.

An interesting aspect for further research is to adaptively choose the relaxation parameter t. Some promising results are presented as an outlook in Appendix A.6.5.

6.5 Summary

We considered variational inequalities arising from convex optimization problems with a differentiable objective function ψ. They were solved with the LQPAP method using the operator setting $\mathcal{Q} = \mathcal{Q}^k = \nabla\psi$, $\mathcal{F} = \mathcal{L}^k = 0$. The Newton algorithm with Armijo step sizes turned out to be a suitable method for the solution of the LQPAP auxiliary problems. A combination of the Armijo step size rule with the self-concordance rule can improve the results with respect to the number of function evaluations. We also solved the test examples with the BrPAP method, but a comparison with the LQPAP method is difficult because the performance of both algorithms can essentially depend on the choice of the regularization parameters $\{\chi_k\}$. Nevertheless, with an appropriate choice of $\{\chi_k\}$, most tested examples could be solved satisfactorily with both methods. A failure of the method can occur if the iterates tend quicker towards the boundary than towards optimality. In this context, we could present the under-relaxation strategy as a means to robustify the LQPAP method, such that the problems can be constantly solved well with nearly every (tested) choice of $\{\chi_k\}$.

7. Application to Nonsymmetric Variational Inequalities

An advantage of the LQPAP method is that even variational inequalities $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ with a nonsymmetric operator $\mathcal{F}$ can be solved with the help of optimization problems. In this chapter we concentrate on such types of problems. More precisely, we consider problems of Category 2, i.e.,

$$\text{Find } x^* \in K: \ \langle \mathcal{F}(x^*), x - x^* \rangle \geq 0 \quad \forall x \in K,$$

where $\mathcal{F}$ is nonsymmetric and co-coercive, $\mathcal{Q} = 0$, and $K = \{x \in \mathbb{R}^n : Ax \leq b\}$ with the usual structure. The corresponding LQPAP auxiliary problems are unconstrained, strongly convex, differentiable optimization problems of the form

$$\min_{x \in \mathbb{R}^n} \ \left\{ \left\langle \mathcal{F}(x^k), x - x^k \right\rangle + \chi_k D(x, x^k) \right\}, \tag{7.1}$$

i.e., they follow essentially the auxiliary problem principle idea. The Newton method as given in Algorithm 6.1 can be applied to solve (7.1) (with $f^k(x) = \left\langle \mathcal{F}(x^k), x - x^k \right\rangle$).

To our knowledge, appropriate benchmark examples with nonsymmetric variational inequalities are not available in the literature. Therefore, our motivation in this chapter is

1. to construct operators $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ which are nonsymmetric and co-coercive with a known modulus γ,
2. to, additionally, construct $\mathcal{F}$ and the restriction set K such that the solution of $\mathrm{VI}(\mathcal{F}, K)$ is known, and
3. to test the LQPAP algorithm on some constructed examples and compare the calculated solutions with the known solutions.

In this chapter I_n denotes the $n \times n$ identity matrix. Remember further that $\widehat{A}$ denotes the symmetric part of a quadratic matrix A.

7.1 Construction of nonsymmetric, co-coercive operators

As before, we restrict our considerations to affine operators

$$\mathcal{F}(x) = Cx + d, \quad C \in \mathbb{R}^{n\times n} \text{ nonsymmetric}, \quad d \in \mathbb{R}^n, \tag{7.2}$$

such that the modulus of co-coercivity can be calculated as described in Section 5.4.2. In view of Lemma 5.4.8, we begin with a collection of ideas to generate positive definite, nonsymmetric matrices. We will make use of two estimates which hold for every matrix $C \in \mathbb{R}^{n\times n}$ and every vector $x \in \mathbb{R}^n$:

$$\lambda_{\min}(\widehat{C}) \parallel x \parallel^2 \leq \langle Cx, x\rangle\,, \tag{7.3}$$

$$-\parallel C \parallel_2 \parallel x \parallel^2 \leq \langle Cx, x\rangle\,. \tag{7.4}$$

The first one is a result of the Rayleigh-principle, and the second one is proved with the Cauchy-Schwarz inequality and the compatibility property of the matrix norm.

Lemma 7.1.1. *Let $D = diag(d_1, \ldots, d_n) \in \mathbb{R}^{n\times n}$ be a diagonal matrix with $d_i \geq 0$ for all $i = 1, \ldots, n$, and $B \in \mathbb{R}^{n\times n}$ be a nonsymmetric matrix with*

$$-\lambda_{\min}(\widehat{B}) < \min\{d_i : i = 1, \ldots, n\}. \tag{7.5}$$

Then $C := B + D$ is a nonsymmetric and positive definite matrix.

Proof. Let $x \in \mathbb{R}^n \setminus \{0\}$. Applying (7.3) and (7.5) yields

$$\begin{aligned}\langle Cx, x\rangle &= \langle Bx, x\rangle + \sum_{i=1}^{n} d_i x_i^2 \\ &\geq \lambda_{\min}(\widehat{B}) \parallel x \parallel^2 + \min\{d_i : i = 1, \ldots, n\} \parallel x \parallel^2 \\ &> 0.\end{aligned}$$

□

Remark 7.1.2. *An analogous proof as in Lemma 7.1.1, which uses (7.4) instead of (7.3), shows that condition (7.5) can be replaced by*

$$\parallel B \parallel_2 < \min\{d_i : i = 1, \ldots, n\}.$$

Corollary 7.1.3. *Let $B \in \mathbb{R}^{n\times n} \setminus \{0\}$ be a skew-symmetric matrix, i.e., $B^T = -B$, and $\epsilon > 0$. Then $C := B + \epsilon I_n$ is a nonsymmetric and positive definite matrix.*

Proof. The assertion follows from Lemma 7.1.1 because $\lambda_{\min}(\widehat{B}) = 0$. □

Another consequence of Lemma 7.1.1 is:

Corollary 7.1.4 (Construction of nonsymmetric, positive definite matrices). *Let $B \in \mathbb{R}^{n\times n}$ be an arbitrary nonsymmetric matrix and $\epsilon > 0$. Set*

$$D := (-\lambda_{\min}(\widehat{B}) + \epsilon)I_n. \tag{7.6}$$

Then $C := B + D$ is nonsymmetric and positive definite.

Remark 7.1.5. *If $\lambda_{\min}(\widehat{B}) > 0$ in Corollary 7.1.4 then $D = 0$ fulfills condition (7.5).*

Remark 7.1.6. *In view of Remark 7.1.2, it is also possible to take $D := (\parallel B \parallel_2 +\epsilon)I_n$ with $\epsilon > 0$ in Corollary 7.1.4. However, since we want to construct a nonsymmetric, positive definite matrix, this causes an unnecessary manipulation of B in the case that $\lambda_{\min}(\widehat{B}) > 0$.*

A further possibility to ensure positive definiteness of a nonsymmetric matrix C is to make $\widehat{C}$ strictly diagonally dominant by manipulating the diagonal entries such that

$$|c_{ii}| > \frac{1}{2}\sum_{\substack{j=1\\ j\neq i}}^{n} |c_{ij} + c_{ji}|, \text{ and } c_{ii} > 0 \quad \forall i = 1, \ldots, n$$

(compare Lemma 5.4.15).

Finally, Lemma 5.4.4 can be exploited to generate a psd-plus matrix.

Lemma 7.1.7 (Construction of psd-plus matrices). *Let $B \in \mathbb{R}^{r\times r}$ be a skew-symmetric matrix and $E \in \mathbb{R}^{r\times n}$. Then $C := E^T(I_r + B)E$ is psd-plus.*

Proof. Let $\langle Cx, x\rangle = 0$ hold for some $x \in \mathbb{R}^n$. This is equivalent to $\langle Ex, (I_r + B)Ex\rangle = 0$, which implies that $Ex = 0$ because $B + I_r$ is positive definite due to Corollary 7.1.3. Hence, $Cx = 0$, which proves that C is psd-plus. □

Remark 7.1.8 (Construction of an affine, nonsymmetric, co-coercive $\mathcal{F}$). *In view of the preceding statements, an affine, nonsymmetric, and co-coercive operator $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ can be constructed by generating a nonsymmetric matrix C with Corollary 7.1.4 or Lemma 7.1.7 and defining $\mathcal{F}(x) = Cx + d$ with an arbitrary $d \in \mathbb{R}^n$. The modulus of co-coercivity can be determined by Lemmata 5.4.8 and 5.4.9, respectively.*

7.2 Construction of VI($\mathcal{F}, K$) with known solution(s)

We present two approaches to construct a nonsymmetric, co-coercive operator $\mathcal{F}$ and a polyhedral restriction set K such that the solution set of VI($\mathcal{F}, K$) is known: a geometric and an analytic approach. The first one only works for small dimensions, whereas the second one is applicable for arbitrary dimensions. The case of multiple solutions is of special interest because it constitutes the situation of an ill-posed problem.

7.2.1 Geometric approach

Unique solution. Let $\mathcal{F}(x) = Cx+d$ be given with $C \in \mathbb{R}^{n\times n}$ nonsymmetric, positive definite and $d \in \mathbb{R}^n$. The idea is to exploit the geometric interpretation of a variational inequality

$$\langle \mathcal{F}(x^*), x - x^* \rangle \geq 0 \quad \forall x \in K$$

to construct a set K such that the solution x^* is known.

For that purpose, we choose an arbitrary $x^* \in \mathbb{R}^n$ such that $c := \mathcal{F}(x^*) \neq 0$. Then, a polyhedron K is constructed such that x^* belongs to a facet of K and c is orthogonal to this facet. In other words, the restriction

$$\langle -c, x \rangle \leq \langle -c, x^* \rangle$$

has to appear in K. Then it is clear that $\langle c, x - x^* \rangle \geq 0$ for all $x \in K$, which implies that x^* is a solution of VI($\mathcal{F}, K$). For the application of the LQPAP method it is further important to ensure that the interior of K is nonempty and that the matrix A that defines K has full column rank.

As a simple two-dimensional example we present:

Example 7.2.1. *It is easy to see that*

$$C = \begin{pmatrix} 4 & -1 \\ 0 & 1 \end{pmatrix}$$

is positive definite. With $d = (0,1)^T$ it follows that $\mathcal{F}(x) = Cx + d$ is a co-coercive and nonsymmetric operator. Take $x^* = (1,1)^T$ with value $c = \mathcal{F}(x^*) = (3,2)^T$. Thus, the equation

$$-3x_1 - 2x_2 = -5$$

defines a straight line which is orthogonal to c and includes x^*. By geometric illustration, we construct the set $K = \{x \in \mathbb{R}^2 : Ax \leq b\}$ with

$$A = \begin{pmatrix} -3 & -2 \\ -2 & 3 \\ 3 & 2 \\ 1 & 0 \\ 0 & -1 \end{pmatrix}, \; b = \begin{pmatrix} -5 \\ 7.5 \\ 18 \\ 4 \\ 0 \end{pmatrix}$$

and $x^0 = (3,4)^T \in \operatorname{int}(K)$. *Figure 7.1 illustrates the situation.*

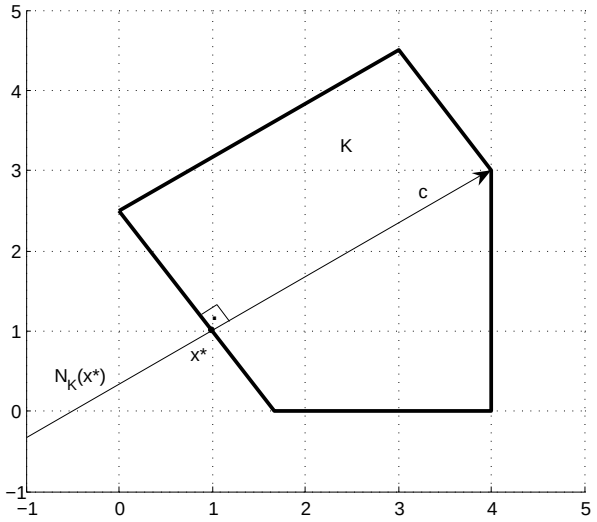


Figure 7.1. Geometric construction of a restriction set K with x^* as a unique solution and $-c = -\mathcal{F}(x^*) \in \mathcal{N}_K(x^*)$.

For higher dimensions it is difficult to find an appropriate randomly generated restriction set K. A deterministic way of constructing K would need a deeper study on analytic geometry, which is beyond the purpose of our work. Only simple higher-dimensional examples with solution $x^* = 0$ are available for the special case $K = \mathbb{R}^n_+$ by choosing $d \geq 0$ and C nonsymmetric, positive definite. Indeed, in such a case it holds $\langle d, x \rangle \geq 0$ for all $x \geq 0$, which implies that $x^* = 0$ is a solution of the variational inequality.

Multiple solutions. Let $\mathcal{F}(x) = Cx + d$ be given with a nonsymmetric, psd-plus matrix $C \in \mathbb{R}^{n \times n}$ such that $\operatorname{rank}(C) = r < n$. Then there exists $\bar{x} \in \mathbb{R}^n \setminus \{0\}$ with

$$C\bar{x} = 0. \tag{7.7}$$

We determine $y, z \in \mathbb{R}^n \setminus \{0\}$ with

$$\mathcal{F}(z) - y = 0, \tag{7.8}$$

$$\langle \bar{x}, y \rangle = 0. \tag{7.9}$$

This is a linear equation system with $n+1$ equations and $2n$ variables. Define for $\bar{\alpha} > 0$ the set

$$S = \{x \in \mathbb{R}^n : x = z + \alpha\bar{x},\ \alpha \in [-\bar{\alpha}, \bar{\alpha}]\}.$$

Now, K has to be constructed such that S is included in a facet of K. Furthermore, y has to be orthogonal to this facet. Thus, the restriction

$$\langle -y, x\rangle \leq \langle -y, z\rangle \tag{7.10}$$

must be included into K. Moreover, $\operatorname{int}(K) \neq \emptyset$ and $\operatorname{rank}(A) = n$ have to hold. Then every $x^* \in S$ solves $\mathrm{VI}(\mathcal{F}, K)$. Indeed, let $x^* = z + \alpha\bar{x}$ hold for some $\alpha \in [-\bar{\alpha}, \bar{\alpha}]$. Feasibility of x^* is given by construction. Moreover, for all $x \in K$,

$$\begin{aligned}\langle \mathcal{F}(x^*), x - x^*\rangle &= \langle Cz + \alpha C\bar{x} + d, x - z - \alpha\bar{x}\rangle \\ &= \langle y, x - z\rangle - \alpha\,\langle y, \bar{x}\rangle \\ &= \langle y, x - z\rangle \\ &\geq 0,\end{aligned}$$

where the last inequality is established by (7.10).

With this construction we are not able to know the entire solution set and, therefore, cannot verify a calculated solution. Furthermore, the idea is not suitable for the construction of high-dimensional examples. Thus, we will not go into more detail here. Instead, we will now focus on an analytic approach that is based on the Lagrange function for a convex optimization problem.

7.2.2 Lagrange function approach

The starting point of this approach is a strongly convex quadratic optimization problem with linear constraints:

$$\begin{aligned}&\min\ \left\{\psi(\tilde{x}) : \tilde{A}\tilde{x} \leq \tilde{b}\right\} \\ &\text{with } \psi(\tilde{x}) = \frac{1}{2}\left\langle \tilde{C}\tilde{x}, \tilde{x}\right\rangle + \left\langle \tilde{d}, \tilde{x}\right\rangle,\end{aligned} \tag{7.11}$$

where $\tilde{C} \in \mathbb{R}^{r\times r}$ is symmetric and positive definite, $\tilde{d} \in \mathbb{R}^r$, $\tilde{A} \in \mathbb{R}^{p\times r}$, $p > r$, $\tilde{b} \in \mathbb{R}^p$. We assume that the feasible set has nonempty interior and that $\tilde{A}$ has full column rank. Let $\tilde{x}^* \in \mathbb{R}^r$ denote the known solution of (7.11) and $\tilde{u}^* \in \mathbb{R}^p$ denote a vector of corresponding Lagrange multipliers.

The idea is to split the constraints of problem (7.11) into two nonempty sets and to include one of them into the Lagrange function. Let

$$\tilde{A} = \begin{pmatrix} A_\kappa \\ A_\lambda \end{pmatrix}, \quad \tilde{b} = \begin{pmatrix} b_\kappa \\ b_\lambda \end{pmatrix}, \quad \tilde{u} = \begin{pmatrix} u_\kappa \\ u_\lambda \end{pmatrix}$$

with $A_\kappa \in \mathbb{R}^{p_\kappa \times r}$, $A_\lambda \in \mathbb{R}^{p_\lambda \times r}$, $b_\kappa, u_\kappa \in \mathbb{R}^{p_\kappa}$, $b_\lambda, u_\lambda \in \mathbb{R}^{p_\lambda}$, $p_\kappa + p_\lambda = p$, $p_\kappa > 0$, $p_\lambda > 0$ be the corresponding splitting of $\tilde{A}$, $\tilde{b}$, and the Lagrange multiplier $\tilde{u}$ (where rows are rearranged if necessary). We further assume that A_κ has full column rank. Thus, necessarily, $r \leq p_\kappa$ has to hold.

We define the Lagrange function $L : \mathbb{R}^r \times \mathbb{R}^{p_\lambda}_+ \to \mathbb{R}$ as

$$L(\tilde{x}, u_\lambda) = \frac{1}{2} \left\langle \tilde{C}\tilde{x}, \tilde{x} \right\rangle + \left\langle \tilde{d}, \tilde{x} \right\rangle + \langle u_\lambda, A_\lambda \tilde{x} - b_\lambda \rangle .$$

Now, the saddle point problem with L is equivalent to VI($\mathcal{F}, K$) with

$$\mathcal{F}(\tilde{x}, u_\lambda) = \begin{pmatrix} \frac{\partial L}{\partial \tilde{x}}(\tilde{x}, u_\lambda) \\ -\frac{\partial L}{\partial u_\lambda}(\tilde{x}, u_\lambda) \end{pmatrix} =: Cx + d,$$
$$K = \{(\tilde{x}, u_\lambda) \in \mathbb{R}^{r+p_\lambda} : A_\kappa \tilde{x} \leq b_\kappa,\ u_\lambda \geq 0\} =: \{x \in \mathbb{R}^n : Ax \leq b\},$$

where

$$C = \begin{pmatrix} \tilde{C} & A_\lambda^T \\ -A_\lambda & 0 \end{pmatrix} \in \mathbb{R}^{n \times n}, \quad d = \begin{pmatrix} \tilde{d} \\ b_\lambda \end{pmatrix} \in \mathbb{R}^n, \quad x = \begin{pmatrix} \tilde{x} \\ u_\lambda \end{pmatrix} \in \mathbb{R}^n,$$
$$A = \begin{pmatrix} A_\kappa & 0 \\ 0 & -I_{p_\lambda} \end{pmatrix} \in \mathbb{R}^{p \times n}, \quad b = \begin{pmatrix} b_\kappa \\ 0 \end{pmatrix} \in \mathbb{R}^p, \quad n = r + p_\lambda.$$

Matrix C is nonsymmetric (since $p_\lambda > 0$), A has full column rank, and $\operatorname{int}(K) \neq \emptyset$. Furthermore, it is clear that $x^* = (\tilde{x}^*, u_\lambda^*)^T$ solves VI($\mathcal{F}, K$).

Unfortunately, C is not psd-plus. Indeed, take $u_\lambda \in \mathbb{R}^{p_\lambda} \setminus \{0\}$ with $A_\lambda^T u_\lambda \neq 0$. For $x = (0, u_\lambda)$ it holds that $\langle Cx, x \rangle = 0$ and $Cx \neq 0$. Therefore, $\mathcal{F}$ is not co-coercive. To obtain a positive definite matrix C, we manipulate the Lagrange function by adding a nonlinear concave function Λ that attains its unconstrained maximum in u_λ^* and in an arbitrary $\tilde{x}$, for example,

$$\Lambda(\tilde{x}, u_\lambda) = -\frac{s}{2} \parallel u_\lambda - u_\lambda^* \parallel^2$$

with $s > 0$. Let

$$\overline{L}(\tilde{x}, u_\lambda) = L(\tilde{x}, u_\lambda) + \Lambda(\tilde{x}, u_\lambda) \tag{7.12}$$

be the modified Lagrange function. This changes C and d to

$$\overline{C} = \begin{pmatrix} \tilde{C} & A_\lambda^T \\ -A_\lambda & sI_{p_\lambda} \end{pmatrix}, \quad \overline{d} = \begin{pmatrix} \tilde{d} \\ b_\lambda - su_\lambda^* \end{pmatrix},$$

while the solution of $\mathrm{VI}(\mathcal{F}, K)$ stays the same. It can easily be verified that $\overline{C}$ is positive definite.

We illustrate the Lagrange function approach by an example:

Example 7.2.2. *Consider problem (7.11) with the data*

$$\tilde{C} = \begin{pmatrix} 3 & 0.2 \\ 0.2 & 8 \end{pmatrix}, \quad \tilde{d} = \begin{pmatrix} 1 \\ 2 \end{pmatrix},$$
$$\tilde{A} = \begin{pmatrix} -1 & 1 \\ -0.2 & 5 \\ -4 & -0.3 \\ 0 & -1 \\ 0.2 & -0.1 \end{pmatrix}, \quad \tilde{b} = \begin{pmatrix} -6 \\ 4 \\ -3 \\ 8 \\ 2 \end{pmatrix}.$$

The unique solution is $\tilde{x}^* = (77/19, -37/19)^T$. *A dual solution* $\tilde{u}^*$ *can be calculated from the KKT system by solving*

$$\begin{aligned} \left\langle \tilde{u}^*, \tilde{A}\tilde{x}^* - \tilde{b} \right\rangle &= 0 \\ \tilde{C}\tilde{x}^* + \tilde{d} + \tilde{A}^T\tilde{u}^* &= 0 \\ \tilde{u}^* &\geq 0. \end{aligned}$$

The result is $\tilde{u}^* = (1213/95, 0, 0, 0, 0)^T$. *Now, we partition as follows:*

$$A_\kappa = \begin{pmatrix} -1 & 1 \\ -0.2 & 5 \\ -4 & -0.3 \\ 0 & -1 \end{pmatrix}, \quad b_\kappa = \begin{pmatrix} -6 \\ 4 \\ -3 \\ 8 \end{pmatrix}, \quad u_\kappa^* = \begin{pmatrix} 1213/95 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$
$$A_\lambda = \begin{pmatrix} 0.2 & -0.1 \end{pmatrix}, \quad b_\lambda = 2, \quad u_\lambda^* = 0.$$

Determining a saddle point of the modified Lagrange function (7.12) (with $s = 5$*) is equivalent to solving the variational inequality* $\mathrm{VI}(\mathcal{F}, K)$ *with*

$$\mathcal{F}(x) = \begin{pmatrix} 3 & 0.2 & 0.2 \\ 0.2 & 8 & -0.1 \\ -0.2 & 0.1 & 5 \end{pmatrix} x + \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix},$$
$$K = \{x \in \mathbb{R}^3 : Ax \leq b\}, \quad \textit{where}$$
$$A = \begin{pmatrix} -1 & 1 & 0 \\ -0.2 & 5 & 0 \\ -4 & -0.3 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad b = \begin{pmatrix} -6 \\ 4 \\ -3 \\ 8 \\ 0 \end{pmatrix}.$$

The unique solution of VI($\mathcal{F}, K$) *is* $x^* = (77/19, -37/19, 0)^T$ *and we have* $x^0 = (10, 0.3, 20)^T \in \operatorname{int}(K)$.

With a higher-dimensional problem of type (7.11) it is easy to generate a higher-dimensional nonsymmetric variational inequality with a co-coercive operator $\mathcal{F}$ and a known solution (see Appendix A.7).

7.2.3 Multiple solutions via linear transformations

Now, we turn to an analytic approach to generate nonsymmetric variational inequalities with known multiple solutions.

In the preceding section we have constructed a nonsymmetric, co-coercive operator $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n,\ \mathcal{F}(x) = Cx + d$ and a suitable restriction set $K = \{x \in \mathbb{R}^n : Ax \leq b\}$ such that the solution x^* of VI($\mathcal{F}, K$) is unique and known. To obtain a variational inequality VI($\widetilde{\mathcal{F}}, \widetilde{K}$) with multiple solutions, we consider a linear transformation of the solution of VI($\mathcal{F}, K$) with the following matrix

$$E = \begin{pmatrix} I_n & -e_1 \end{pmatrix} \in \mathbb{R}^{n \times (n+1)}, \tag{7.13}$$

where $e_1 = (1, 0, \ldots, 0)^T \in \mathbb{R}^n$. When substituting variable x by variable v according to the transformation

$$Ev = x, \quad v \in \mathbb{R}^{n+1},$$

the inequality $\langle Cx^* + d, x - x^* \rangle \geq 0$ gets the form $\langle CEv^* + d, Ev - Ev^* \rangle \geq 0$, which is equivalent to

$$\left\langle E^T CEv^* + E^T d, v - v^* \right\rangle \geq 0.$$

Thus, we obtain the operator

$$\widetilde{\mathcal{F}} : \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}, \quad \widetilde{\mathcal{F}}(v) = E^T CEv + E^T d.$$

The restriction set K is described in the new variable by

$$K' = \{v \in \mathbb{R}^{n+1} : A'v \leq b\}, \quad \text{where } A' = AE \in \mathbb{R}^{p \times (n+1)}.$$

However, since $\operatorname{rank}(A') = n$ holds by construction, A' does not have full column rank. To achieve this, we add the restriction $v_{n+1} \geq 0$ to K' and obtain the set

$$\widetilde{K} = \{v \in \mathbb{R}^{n+1} : \widetilde{A}v \leq \widetilde{b}\}, \quad \text{where } \widetilde{A} = \begin{pmatrix} AE \\ -e_{n+1}^T \end{pmatrix},\ \widetilde{b} = \begin{pmatrix} b \\ 0 \end{pmatrix}$$

and $e_{n+1} = (0, \ldots, 0, 1)^T \in \mathbb{R}^{n+1}$.

As a first result we state that for all $x \in K$ there exist (multiple) $v \in \widetilde{K}$ with $Ev = x$.

Lemma 7.2.3. *Let $x = (x_1, \ldots, x_n)^T \in K$ be given. Define*

$$V(x) = \{(x_1 + t, x_2, \ldots, x_n, t)^T \in \mathbb{R}^{n+1} : t \geq 0\}.$$

Then $V(x) \subset \widetilde{K}$, and $Ev = x$ if and only if $v \in V(x)$.

Proof. The assertion is clear by definition of E and construction of $\widetilde{K}$. □

The following relation between $\mathrm{VI}(\mathcal{F}, K)$ and $\mathrm{VI}(\widetilde{\mathcal{F}}, \widetilde{K})$ is valid.

Lemma 7.2.4. *(a) Let v^* be a solution of $\mathrm{VI}(\widetilde{\mathcal{F}}, \widetilde{K})$. Then $x^* := Ev^*$ is the unique solution of $\mathrm{VI}(\mathcal{F}, K)$.*

(b) Let x^* be the unique solution of $\mathrm{VI}(\mathcal{F}, K)$. Then v^* solves $\mathrm{VI}(\widetilde{\mathcal{F}}, \widetilde{K})$ if and only if $v^* \in V(x^*)$.

Proof. (a) By construction of $\widetilde{K}$ we have $x^* \in K$. Let $x \in K$ be arbitrary. Then, by Lemma 7.2.3, there exists $v \in \widetilde{K}$ with $Ev = x$. It follows that

$$\langle Cx^* + d, x - x^* \rangle = \langle CEv^* + d, Ev - Ev^* \rangle = \left\langle E^T CEv^* + E^T d, v - v^* \right\rangle \geq 0$$

since v^* solves $\mathrm{VI}(\widetilde{\mathcal{F}}, \widetilde{K})$. Thus, x^* solves $\mathrm{VI}(\mathcal{F}, K)$.

(b) Let v^* solve $\mathrm{VI}(\widetilde{\mathcal{F}}, \widetilde{K})$. With (a) it follows that $x^* = Ev^*$, which implies that $v^* \in V(x^*)$ by Lemma 7.2.3. For the reverse implication, let $v^* \in V(x^*)$ respectively $Ev^* = x^*$ hold. Let $v \in \widetilde{K}$ be arbitrary. Then $x := Ev \in K$ per definition of $\widetilde{K}$, and

$$\left\langle E^T CEv^* + E^T d, v - v^* \right\rangle = \langle CEv^* + d, Ev - Ev^* \rangle = \langle Cx^* + d, x - x^* \rangle \geq 0$$

since x^* solves $\mathrm{VI}(\mathcal{F}, K)$. Thus, v^* solves $\mathrm{VI}(\widetilde{\mathcal{F}}, \widetilde{K})$. □

The preceding lemma shows that the solution set of $\mathrm{VI}(\widetilde{\mathcal{F}}, \widetilde{K})$ is equal to $V(x^*)$ if x^* solves $\mathrm{VI}(\mathcal{F}, K)$. Furthermore, it is clear that if K has nonempty interior, this is also the case for $\widetilde{K}$. Indeed, let $x^0 \in \mathrm{int}(K)$. Then each point $v^0 \in V(x^0)$ with $v^0_{n+1} > 0$ is an interior point of $\widetilde{K}$. Note that if v^0 serves as an initial point for the LQPAP algorithm, its last component will determine a representant of the solution set since v^0_{n+1} is already optimal.

It remains to explain that the operator $\widetilde{\mathcal{F}}$ is co-coercive. This follows directly from the next lemma which is based on Lemmata 5.4.4 and 5.4.9.

Lemma 7.2.5. *Let $C \in \mathbb{R}^{n\times n}$ be psd-plus and E as in (7.13). Then E^TCE is psd-plus.*

Proof. Take $v \in \mathbb{R}^{n+1}$ with $\langle E^TCEv, v\rangle = \langle CEv, Ev\rangle = 0$. Since C is psd-plus, we obtain $CEv = 0$, which implies $E^TCEv = 0$ and proves the assertion. □

Corollary 7.2.6. *The operator $\widetilde{\mathcal{F}}(v) = E^TCEv + E^Td$ is co-coercive with modulus $\widetilde{\gamma} = \frac{\lambda_{\min}(\widehat{C})}{\|E^TC\|_2^2}$.*

7.3 Numerical results for nonsymmetric examples

We give a brief characterization of the considered test examples in Table 7.1.

Example	description
7.2.1	2-dimensional, unique solution, $p = 5$, constructed with geometric approach
7.2.2	3-dimensional, unique solution, $p = 5$, constructed with Lagrange approach
D.1.1	15-dimensional, unique solution, $p = 20$, constructed with Lagrange approach
D.1.2	130-dimensional, unique solution, $p = 150$, constructed with Lagrange approach
7.2.1∼	Example 7.2.1 with multiple solutions via linear transformations
7.2.2∼	Example 7.2.2 with multiple solutions via linear transformations
D.1.1∼	Example D.1.1 with multiple solutions via linear transformations
D.1.2∼	Example D.1.2 with multiple solutions via linear transformations

Table 7.1. Description of the nonsymmetric test examples.

In Table 7.2 we present the numerical results for the LQPAP method applied on the test examples. For a comparison we also solve the problems with the BrPAP method and show the results in Table 7.3. As before, we experimentally adapt the choice for χ_0 and r towards a best performance of the methods. Also, under-relaxation is used if the results can be improved. The calculated solutions v_{calc} of the transformed examples with multiple solutions are verified by comparing their transformation $x_{calc} = Ev_{calc}$ with the unique solution of the original example.

The values listed in the table are

$\underline{\chi}$:	lower bound for the regularization parameters,
χ_0:	initial value of the regularization parameter,
r:	decreasing factor to update $\chi_{k+1} = \chi_0 r^{k+1}$,
t:	parameter of under-relaxation,
#iter:	number of iterations,
#New:	total number of Newton iterations,
$\| x^0 - x^* \|$:	distance of the initial point to the solution,
$\| x_{calc} - x^* \|$:	distance of the calculated solution to the known solution.

For the LQPAP method, the reached accuracies are not satisfying and out of the question. The results for the BrPAP method are better but only for the low-dimensional examples. We can explain this bad performance as follows. In the LQPAP auxiliary problems, operator $\mathcal{F}$ is fixed at the current iterate. On the one hand, this allows to formulate the auxiliary problems as optimization problems. On the other hand, this implies a loss of information about $\mathcal{F}$. Thus, when determining the Newton direction as

$$p^j = -(\chi_k \nabla_I^2 D(y^j, x^k))^{-1}(\mathcal{F}(x^k) + \chi_k \nabla_I D(y^j, x^k))$$

operator $\mathcal{F}$ does not occur in the Hesse matrix. Hence, an appropriate search direction may highly depend on a suitable choice of the regularization parameter. Additionally, a flexible choice of the regularization parameters is made difficult in view of the (often large) value of $\underline{\chi}$. This problem was already discussed in Section 6.3.3.

Example	$\{\chi_k\}$			u.relax.	LQPAP method			
No.	$\underline{\chi}$	χ_0	r	t	#iter	#New	$\| x^0 - x^* \|$	$\| x_{calc} - x^* \|$
7.2.1	0.148	10.00	0.3	0.5	49	6093	3.61e+000	1.18e-003
7.2.2	4.005	10.00	0.9	0.5	63	433	2.10e+001	3.14e+000
D.1.1	215.173	215.17	1.0	0.5	193	1542	2.23e+001	2.52e+000
D.1.2	842.801	842.80	1.0	0.5	491	6546	5.46e+001	2.45e+001
7.2.1∼	8.225	8.22	1.0	0.5	889	3893	3.61e+000	3.33e-001
7.2.2∼	8.160	100.00	0.7	0.5	91	536	2.10e+001	3.78e+000
D.1.1∼	623.227	623.23	1.0	0.5	82	1625	2.21e+000	5.91e-001
D.1.2∼	2029.393	2029.39	1.0	0.5	150	1363	5.50e+000	2.94e+000

Table 7.2. Results for the LQPAP method applied to nonsymmetric VIs.

Example	$\{\chi_k\}$			u.relax.	BrPAP method			
No.	$\underline{\chi}$	χ_0	r	t	#iter	#New	$\| x^0 - x^* \|$	$\| x_{calc} - x^* \|$
7.2.1	1.033	10.00	0.7	1.0	21	104	3.61e+000	3.27e-006
7.2.2	2.003	2.00	1.0	0.5	44	365	2.10e+001	3.43e-005
D.1.1	107.587	107.59	1.0	0.5	127	1105	2.23e+001	5.47e-001
D.1.2	421.401	421.40	1.0	1.0	144	853	5.46e+001	1.26e+000
7.2.1∼	2.032	10.00	0.5	1.0	34	152	3.61e+000	1.09e-005
7.2.2∼	2.010	100.00	0.5	1.0	44	5399	2.10e+001	3.04e-006
D.1.1∼	155.806	155.81	1.0	0.5	198	1157	2.21e+000	5.25e-001
D.1.2∼	507.348	507.35	1.0	0.5	377	1719	5.50e+000	1.23e+000

Table 7.3. Results for the BrPAP method applied to nonsymmetric VIs.

We conclude that the auxiliary problem principle idea has the advantage that it allows to solve nonsymmetric variational inequalities by means of optimization problems. However, this theoretical device does not prove to be effective in our tests because we encounter quite inaccurately calculated solutions.

8. LQPAP Method and Nondifferentiable Optimization Problems

In this chapter we are interested in the application of the LQPAP scheme to problems of Category 3, i.e, convex optimization problems of the form

$$\begin{aligned} &\min \ \{\psi(x) + \varphi(x)\} \\ &\text{s.t. } x \in K, \end{aligned} \tag{8.1}$$

where the objective function is splitted into a differentiable, convex function $\psi : \mathbb{R}^n \to \mathbb{R}$ and a nondifferentiable, convex function $\varphi : \mathbb{R}^n \to \mathbb{R}$. The set K is supposed to have the usual polyhedral structure.

The above optimization problem can equivalently be formulated as a variational inequality with

$$\mathcal{F} = \nabla\psi, \ \mathcal{Q} = \partial\varphi.$$

As motivated in Chapter 5 we take $\mathcal{L}^k = 0$ for all k and set

$$\mathcal{Q}^k = \partial_{\epsilon_k}\varphi,$$

where the sequence $\{\epsilon_k\}$ has to fulfill (3.23). The resulting k-th LQPAP auxiliary problem gets the form

$$\begin{aligned} &\text{Find } x^{k+1} \in K \text{ and } e^{k+1} \in \mathbb{R}^n \text{ such that} \\ &e^{k+1} \in \nabla\psi(x^k) + \partial_{\epsilon_k}\varphi(x^{k+1}) + \chi_k \nabla_I D(x^{k+1}, x^k) \\ &\text{and } \ \| \, e^{k+1} \, \| \leq \delta_k. \end{aligned} \tag{8.2}$$

With the choice $\delta_k = \epsilon_k = 0$, (8.2) is equivalent to the nondifferentiable minimization problem

$$\min_{x \in \mathbb{R}^n} \ \left\{ \left\langle \nabla\psi(x^k), x - x^k \right\rangle + \varphi(x) + \chi_k D(x, x^k) \right\}. \tag{8.3}$$

It was shown in Theorem 3.3.1 that the solution of (8.3) is unique and belongs to the interior of K.

We intend to apply the bundle technique (see, e.g., [58, 86]) to approximately solve (8.3) such that its solution fulfills (8.2) with appropriate nonzero values for δ_k and ϵ_k. We call the resulting method the **LQPAP bundle method**.

8.1 Concept of the LQPAP bundle method

8.1.1 The bundle auxiliary problem

Following the concept of bundle methods, the nonsmooth function φ in (8.3) is substituted by a lower, piecewise linear, convex approximation φ^{k+1} that is defined with the help of a bundle described in Section 8.1.2. Then the resulting bundle auxiliary problem is of the form

$$\min_{y\in\mathbb{R}^n} \left\{ \left\langle \nabla\psi(x^k), y - x^k \right\rangle + \varphi^{k+1}(y) + \chi_k D(y, x^k) \right\}. \tag{8.4}$$

Let z^{k+1} denote an inexact solution of (8.4). Thus, it fulfills with an appropriate error vector $\tilde{e}^{k+1} \in \mathbb{R}^n$ the relation

$$\tilde{e}^{k+1} \in \nabla\psi(x^k) + \partial\varphi^{k+1}(z^{k+1}) + \chi_k \nabla_I D(z^{k+1}, x^k). \tag{8.5}$$

Using the definition of the subdifferential and the fact that φ^{k+1} is a lower approximation of φ, (8.5) can be transformed as follows

$$\begin{aligned}
& \tilde{e}^{k+1} - \nabla\psi(x^k) - \chi_k \nabla_I D(z^{k+1}, x^k) \in \partial\varphi^{k+1}(z^{k+1}) \\
\Rightarrow\quad & \varphi^{k+1}(y) \geq \varphi^{k+1}(z^{k+1}) + \left\langle \tilde{e}^{k+1} - \nabla\psi(x^k) - \chi_k \nabla_I D(z^{k+1}, x^k), y - z^{k+1} \right\rangle \\
\Rightarrow\quad & \varphi(y) \geq \varphi(z^{k+1}) + \left\langle \tilde{e}^{k+1} - \nabla\psi(x^k) - \chi_k \nabla_I D(z^{k+1}, x^k), y - z^{k+1} \right\rangle \\
& \qquad - (\varphi(z^{k+1}) - \varphi^{k+1}(z^{k+1})),
\end{aligned}$$

with an arbitrary $y \in \mathbb{R}^n$. Setting

$$\tilde{\epsilon}_{k+1} = \varphi(z^{k+1}) - \varphi^{k+1}(z^{k+1}),$$

we can use the definition of the ϵ-subdifferential to obtain

$$\tilde{e}^{k+1} \in \nabla\psi(x^k) + \partial_{\tilde{\epsilon}_{k+1}}\varphi(z^{k+1}) + \chi_k \nabla_I D(z^{k+1}, x^k). \tag{8.6}$$

Note that $\tilde{\epsilon}_{k+1} \geq 0$ since φ^{k+1} is a lower approximation of φ.

We like to remark that we use a "tilde" for the errors occurring in the LQPAP bundle method to distinguish them from the error terms used in the description of the basic LQPAP method. Moreover, superscripts are used to denote (error) vectors and subscripts to refer to a real number.

In view of the relation $\partial_{\epsilon_1}\varphi \subset \partial_{\epsilon_2}\varphi$ for $\epsilon_1 \leq \epsilon_2$, a comparison of (8.6) and (8.2) shows that a solution z^{k+1} of (8.6) is also a solution of (8.2) if

$$\| \tilde{e}^{k+1} \| \leq \delta_k \quad \text{and} \tag{8.7}$$

$$\tilde{\epsilon}_{k+1} \leq \epsilon_k. \tag{8.8}$$

Condition (8.7) can be achieved by solving problem (8.6) exact enough. To fulfill (8.8), the approximation of φ by φ^{k+1} must be good enough.

8.1.2 Conditions on the lower approximation of φ

In the context of bundle methods there are in general three conditions the lower approximation φ^{k+1} has to fulfill (see (H_1)–(H_3) in [4], (4.7)–(4.9) in [21], and (CP1')–(CP3') in [44]). We adapt the conditions in [44] to our framework and require:

For $k \geq 1$ let φ^k be given. Then φ^{k+1} has to fulfill the conditions

(C1) $\varphi^{k+1}(y) \leq \varphi(y) \quad \forall y \in \mathbb{R}^n$,

(C2) $\varphi^{k+1}(y) \geq \varphi^k(z^k) + \left\langle \tilde{e}^k - \nabla\psi(x^{k-1}) - \chi_{k-1}\nabla_I D(z^k, x^{k-1}), y - z^k \right\rangle \quad \forall y \in \mathbb{R}^n$,

(C3) $\varphi^{k+1}(y) \geq \varphi(z^k) + \left\langle s^k, y - z^k \right\rangle \quad \forall y \in \mathbb{R}^n$,

where $\tilde{e}^k$ is the error vector belonging to z^k, and $s^k \in \partial\varphi(z^k)$. For $k = 0$ we define

$$\varphi^1(y) = \varphi(z^0) + \left\langle s^0, y - z^0 \right\rangle, \tag{8.9}$$

where $z^0 = x^0$, $s^0 \in \partial\varphi(z^0)$.

For example, the following two choices satisfy (C1)–(C3):

- $\varphi^{k+1}(y) = \max\{\varphi(z^j) + \langle s^j, y - z^j\rangle : j = 1, \ldots, k\}$, where $s^j \in \partial\varphi(z^j)$,
- $\varphi^{k+1}(y) = \max\{l^k(y), \varphi(z^k) + \left\langle s^k, y - z^k \right\rangle\}$,

where

$$l^k(y) = \varphi^k(z^k) + \left\langle \tilde{e}^k - \nabla\psi(x^{k-1}) - \chi_{k-1}\nabla_I D(z^k, x^{k-1}), y - z^k \right\rangle \tag{8.10}$$

is the so-called aggregate affine function with

$$\tilde{e}^k - \nabla\psi(x^{k-1}) - \chi_{k-1}\nabla_I D(z^k, x^{k-1}) \in \partial\varphi^k(z^k) \tag{8.11}$$

as the aggregate subgradient (see (8.5)).

We prefer to define φ^{k+1} by

$$\varphi^{k+1}(y) = \max\left\{l^k(y), \varphi(z^j) + \left\langle s^j, y - z^j \right\rangle : j \in J^k\right\} \tag{8.12}$$

where $J^k \subset \{1, \ldots, k\}$ and $k \in J^k$. We call $\{(z^j, s^j) : j \in J^k\}$ the current bundle, where $z^j \in \mathrm{int}(K)$ and $s^j \in \partial\varphi(z^j)$ for all $j \in J^k$. This is a kind of intermediate choice that allows to keep the bundle indexset at a reasonable size and perform an appropriate approximation of φ at the same time. We briefly show that conditions (C1)–(C3) are fulfilled.

With (8.10) and (8.11) we obtain

$$l^k(y) \leq \varphi^k(y) \quad \forall y \in \mathbb{R}^n.$$

For iteration k it holds $\varphi^k(y) \leq \varphi(y)$ for all $y \in \mathbb{R}^n$. It is further clear that for every $j \in J^k$

$$\varphi(z^j) + \left\langle s^j, y - z^j \right\rangle \leq \varphi(y)$$

because φ is a convex function. This establishes (C1). (C2) is clear, and (C3) holds since $k \in J^k$ is required.

The bundle method tries to find an appropriate lower approximation iteratively. It works with so-called *serious steps* and *null steps*: If φ^{k+1} is suitable, which means that $\tilde{\epsilon}_{k+1} = \varphi(z^{k+1}) - \varphi^{k+1}(z^{k+1}) \leq \epsilon_k$, then z^{k+1} is also a solution of (8.2). Then we can take $x^{k+1} = z^{k+1}$ as the next iterate. This is called a serious step. Otherwise, the approximation φ^{k+1} has to be improved. This is done by using (z^{k+1}, s^{k+1}) with $s^{k+1} \in \partial\varphi(z^{k+1})$ as a further bundle element. Then a null step is performed by setting $x^{k+1} = x^k$.

8.1.3 Error conditions and conceptual algorithm

For the well-definedness of the algorithm the following conditions on the error sequence $\{\tilde{e}^k\}$ are needed (see Theorem 8.1.2 below):

$$\lim_{k\to\infty} \left\langle \tilde{e}^k, z^k \right\rangle = 0, \tag{8.13}$$

$$\sum_{k=1}^{\infty} - \left\langle \tilde{e}^k, z^{k+1} - z^k \right\rangle^- < \infty, \tag{8.14}$$

where $\left\langle \tilde{e}^k, z^{k+1} - z^k \right\rangle^- := \min\left\{ \left\langle \tilde{e}^k, z^{k+1} - z^k \right\rangle, 0 \right\}$.

Remark 8.1.1. *(8.14) is implied by the condition* $\sum_{k=1}^{\infty} | \left\langle \tilde{e}^k, z^{k+1} - z^k \right\rangle | < \infty$. *From the convergence analysis of the LQPAP method in Chapter 3 we have the condition* $\sum_{k=0}^{\infty} \delta_k < +\infty$ *on the controlling parameter* δ_k. *Hence, the requirement* $\| \tilde{e}^{k+1} \| \leq \delta_k$ *implies that*

$$\sum_{k=1}^{\infty} \| \tilde{e}^k \| < \infty \tag{8.15}$$

and therefore also

$$\lim_{k\to\infty} \| \tilde{e}^k \| = 0. \tag{8.16}$$

In view of this, (8.13) and (8.14) will be automatically fulfilled if K is compact since then $\{\| z^k \|\}$ and $\{\| z^{k+1} - z^k \|\}$ are bounded. In the case that K is not compact, the error conditions (8.13) and (8.14) have to be ensured during the algorithm. Conditions of this type have already been presented in literature, e.g., in [28].

The conception of the LQPAP bundle method is summarized in Algorithm 8.1.

Algorithm 8.1: Conception of the LQPAP bundle method

1. (*Initialization*) Choose an initial iterate $x^0 \in \mathrm{int}(K)$, the parameters $\chi_0 \geq \underline{\chi}$, $\epsilon_0 > 0$, $\delta_0 \geq 0$, and set $z^0 := x^0$, $k := 0$.

2. (*Convergence test*) If x^k solves problem (8.1) then stop.

3. (*Solve auxiliary problem*) For a lower approximation φ^{k+1} find $z^{k+1} \in \mathrm{int}(K)$ and $\tilde{e}^{k+1} \in \mathbb{R}^n$ with

$$\tilde{e}^{k+1} \in \nabla\psi(x^k) + \partial\varphi^{k+1}(z^{k+1}) + \chi_k \nabla_I D(z^{k+1}, x^k) \tag{8.17}$$

and

$$\| \tilde{e}^{k+1} \| \leq \delta_k \tag{8.18}$$

such that (8.13) and (8.14) hold. Calculate $\tilde{\epsilon}_{k+1} = \varphi(z^{k+1}) - \varphi^{k+1}(z^{k+1})$.
if $\tilde{\epsilon}_{k+1} \leq \epsilon_k$ **then** (*serious step*)
Set $x^{k+1} = z^{k+1}$, build function φ^{k+2} with bundle indexset J^{k+1}, and update $\chi_{k+1}, \epsilon_{k+1}, \delta_{k+1}$.
else (*null step*)
Set $x^{k+1} = x^k$, build function φ^{k+2} with bundle indexset J^{k+1}, set $\chi_{k+1} = \chi_k$, $\epsilon_{k+1} = \epsilon_k$, and update δ_{k+1}.
end

4. (*Update*) Set $k := k + 1$ and go to step 2.

In this context the iteration index k gets a new meaning. Previously, we used index k to denote the k-th auxiliary problem where the current iterate x^k and the regularization parameter χ_k are given and the next iterate x^{k+1} is searched. In the LQPAP bundle method, the nonsmooth function φ is substituted by a lower approximation φ^{k+1} which must be good enough to fulfill the conditions of the LQPAP scheme. Finding such an appropriate lower approximation needs an additional subroutine and, therefore, a different iteration index should be used to symbolize this, and only the final lower approximation should be called φ^{k+1}. However, for better writing we avoid a further index and use the concept of null steps/serious steps. During null steps the lower approximation is improved, the iterate x^k remains the same by setting $x^{k+1} = x^k$, and we stay within the same auxiliary problem. Each serious step leads to a new

auxiliary problem and updates the iteration point by setting $x^{k+1} = z^{k+1}$. Note that the controlling parameter δ_k is updated both in serious and in null steps, such that even in a sequence of null steps the error $\| \tilde{e}^k \|$ is forced to get smaller. This will become important in Theorem 8.1.2. So, actually, only a subsequence of $\{\delta_k\}$ is used in the outer LQPAP scheme.

8.1.4 Well-definedness and convergence theorem

We are going to show that for every iteration point x^k there exists a lower approximation φ^{k+1} which fulfills conditions (C1)–(C3) and ensures that the solution z^{k+1} of the bundle auxiliary problem (8.4) fulfills

$$\tilde{\epsilon}_{k+1} = \varphi(z^{k+1}) - \varphi^{k+1}(z^{k+1}) \leq \epsilon_k.$$

This means, we prove that after finitely many null steps always a serious step will follow.

In the next theorem we work with the following notation: Having x^k as the current iterate, the next iterations are numbered by index $n \geq k$. Then $\{J^n\}_{n\geq k}$ are the corresponding bundle indexsets and $\{\varphi^{n+1}\}_{n\geq k}$ the lower approximations of φ fulfilling (C1)–(C3). For all $n \geq k$ the pairs $(z^l, \tilde{e}^l)$, $l \in J^n$, are chosen such that condition (8.5) is fulfilled. Let $\{z^n\}_{n\geq k}$, $\{s^n\}_{n\geq k}$ (with $s^n \in \partial\varphi(z^n)$), and $\{\tilde{e}^n\}_{n\geq k}$ denote the corresponding sequences.

Theorem 8.1.2. *Suppose that the LQPAP bundle method is used to solve problem (8.1) and let x^k be the current iterate. Assume that a sequence of null steps is carried out, i.e., $\tilde{\epsilon}_{n+1} > \epsilon_n$ for all $n \geq k$. Then, under the error conditions (8.13),(8.14), and (8.16) it holds*

(a) $\lim_{k\leq n\to\infty} \| z^{n+1} - z^n \| = 0$,

(b) $\lim_{k\leq n\to\infty} \tilde{\epsilon}_{n+1} = \lim_{k\leq n\to\infty}(\varphi(z^{n+1}) - \varphi^{n+1}(z^{n+1})) = 0$,

(c) with $d^{n+1} := \tilde{e}^{n+1} - \nabla\psi(x^k) - \chi_k \nabla_I D(z^{n+1}, x^k)$ *it holds* $d^{n+1} \in \partial_{\tilde{\epsilon}_{n+1}}\varphi(z^{n+1})$,

(d) $\{z^{n+1}\}_{n\geq k}$ *converges to the unique solution* $\bar{z}^k$ *of the auxiliary problem (8.3).*

Proof. Within a sequence of null steps we have $x^{n-1} = x^k$ and $\chi_{n-1} = \chi_k$ for all $n \geq k+1$. For all $y \in \text{int}(K)$ we define

$$\begin{aligned}
d^n &:= \tilde{e}^n - \nabla\psi(x^{n-1}) - \chi_{n-1}\nabla_I D(z^n, x^{n-1}) \\
&= \tilde{e}^n - \nabla\psi(x^k) - \chi_k \nabla_I D(z^n, x^k), \\
\hat{l}^n(y) &:= l^n(y) + \left\langle \nabla\psi(x^{n-1}), y - x^{n-1} \right\rangle + \chi_{n-1} D(y, x^{n-1}) \\
&= l^n(y) + \left\langle \nabla\psi(x^k), y - x^k \right\rangle + \chi_k D(y, x^k), \\
\hat{\varphi}^n(y) &:= \varphi^n(y) + \left\langle \nabla\psi(x^{n-1}), y - x^{n-1} \right\rangle + \chi_{n-1} D(y, x^{n-1}) \\
&= \varphi^n(y) + \left\langle \nabla\psi(x^k), y - x^k \right\rangle + \chi_k D(y, x^k).
\end{aligned}$$

Our first aim is to prove convergence of the sequence $\{\hat{l}^n(z^n)\}_{n\geq k}$ by applying an extension of Polyak's lemma as given in Appendix A.4. For that purpose, we establish three estimates.

First, it holds that

$$\varphi(x^k) \geq \varphi^{n+1}(x^k) = \hat{\varphi}^{n+1}(x^k) \geq \hat{\varphi}^{n+1}(z^{n+1}) + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle. \tag{8.19}$$

Indeed, for all $n \geq k$ the pairs $(z^n, \tilde{e}^n)$ are chosen according to (8.5). This means that

$$\tilde{e}^n \in \partial\hat{\varphi}^n(z^n) \quad \forall n \geq k,$$

which by definition of the subdifferential gives

$$\hat{\varphi}^n(z) \geq \hat{\varphi}^n(z^n) + \langle \tilde{e}^n, z - z^n \rangle \quad \forall z \in \mathbb{R}^n.$$

This observation together with (C1) and the fact that $D(x^k, x^k) = 0$ establishes (8.19).

Second, we have

$$\hat{l}^n(z^{n+1}) \leq \hat{\varphi}^{n+1}(z^{n+1}) = \hat{l}^{n+1}(z^{n+1}). \tag{8.20}$$

Indeed, from the definition of l^n and $\hat{l}^n$ we obtain

$$\begin{aligned}
\hat{l}^{n+1}(z^{n+1}) &= l^{n+1}(z^{n+1}) + \left\langle \nabla\psi(x^k), z^{n+1} - x^k \right\rangle + \chi_k D(z^{n+1}, x^k) \\
&= \varphi^{n+1}(z^{n+1}) + \left\langle \tilde{e}^{n+1} - \nabla\psi(x^n) - \chi_n \nabla_I D(z^{n+1}, x^n), z^{n+1} - z^{n+1} \right\rangle \\
&\quad + \left\langle \nabla\psi(x^k), z^{n+1} - x^k \right\rangle + \chi_k D(z^{n+1}, x^k) \\
&= \varphi^{n+1}(z^{n+1}) + \left\langle \nabla\psi(x^k), z^{n+1} - x^k \right\rangle + \chi_k D(z^{n+1}, x^k) \\
&= \hat{\varphi}^{n+1}(z^{n+1}).
\end{aligned}$$

Condition (C2) gives $\varphi^{n+1}(z^{n+1}) \geq l^n(z^{n+1})$ and therefore

$$\hat{\varphi}^{n+1}(z^{n+1}) \geq \hat{l}^n(z^{n+1}).$$

The last two relations result in (8.20).

To obtain the third estimate, namely

$$\hat{l}^n(y) - \hat{l}^n(z^n) \geq \langle \tilde{e}^n, y - z^n \rangle + \chi_k \parallel y - z^n \parallel_A^2, \tag{8.21}$$

some preparations are needed. For all $y \in \text{int}(K)$ the expression $\hat{l}^n(y) - \hat{l}^n(z^n)$ can be transformed to

$$\begin{aligned}
\hat{l}^n(y) - \hat{l}^n(z^n) &= l^n(y) + \left\langle \nabla\psi(x^k), y - x^k \right\rangle + \chi_k D(y, x^k) \\
&\quad - l^n(z^n) - \left\langle \nabla\psi(x^k), z^n - x^k \right\rangle - \chi_k D(z^n, x^k) \\
&= \varphi^n(z^n) + \left\langle \tilde{e}^n - \nabla\psi(x^{n-1}) - \chi_{n-1}\nabla_I D(z^n, x^{n-1}), y - z^n \right\rangle \\
&\quad + \left\langle \nabla\psi(x^k), y - x^k \right\rangle + \chi_k D(y, x^k) \\
&\quad - \varphi^n(z^n) - \left\langle \tilde{e}^n - \nabla\psi(x^{n-1}) - \chi_{n-1}\nabla_I D(z^n, x^{n-1}), z^n - z^n \right\rangle \\
&\quad - \left\langle \nabla\psi(x^k), z^n - x^k \right\rangle - \chi_k D(z^n, x^k) \\
&= \left\langle \tilde{e}^n - \nabla\psi(x^{n-1}) - \chi_{n-1}\nabla_I D(z^n, x^{n-1}), y - z^n \right\rangle \\
&\quad + \left\langle \nabla\psi(x^k), y - z^n \right\rangle + \chi_k (D(y, x^k) - D(z^n, x^k)) \\
&= \langle d^n, y - z^n \rangle + \left\langle \nabla\psi(x^k), y - z^n \right\rangle + \chi_k (D(y, x^k) - D(z^n, x^k)).
\end{aligned} \tag{8.22}$$

By an appropriate splitting of D it is possible to further estimate (8.22). We define for $x, y \in \text{int}(K)$

$$\begin{aligned}
D_1(x, y) &:= \sum_{j=1}^{p} l_j(x) l_j(y) - (l_j(y))^2 \log \frac{l_j(x)}{l_j(y)} - (l_j(y))^2, \\
D_2(x, y) &:= \sum_{j=1}^{p} (l_j(x))^2 - 2 l_j(x) l_j(y) + (l_j(y))^2 \\
&= \parallel l(x) - l(y) \parallel^2 = \parallel A(x - y) \parallel^2 = \parallel x - y \parallel_A^2,
\end{aligned}$$

where l (without superscript) denotes the function $l(x) = (l_1(x), \ldots, l_p(x)) = b - Ax$. It is easy to see that

$$D(x, y) = D_1(x, y) + D_2(x, y)$$

and

$$\nabla_I D_2(x, y) = 2A^T A(x - y),$$

and that

$$D_1(\cdot, y) \text{ is convex}$$

(see Appendix, Lemma A.3.1 for more information). In continuation of (8.22) we get

$$
\begin{aligned}
\hat{l}^n(y) - \hat{l}^n(z^n) &= \chi_k(D(y,x^k) - D(z^n,x^k)) + \langle d^n, y - z^n\rangle + \left\langle \nabla\psi(x^k), y - z^n\right\rangle \\
&= \chi_k(D(y,x^k) - D(z^n,x^k)) \\
&\quad + \left\langle \tilde{e}^n - \nabla\psi(x^k) - \chi_k\nabla_I D(z^n,x^k), y - z^n\right\rangle + \left\langle \nabla\psi(x^k), y - z^n\right\rangle \\
&= \chi_k(D(y,x^k) - D(z^n,x^k)) \\
&\quad + \left\langle \tilde{e}^n - \chi_k(\nabla_I D_1(z^n,x^k) + \nabla_I D_2(z^n,x^k)), y - z^n\right\rangle \\
&= \chi_k(D(y,x^k) - D(z^n,x^k)) \\
&\quad + \left\langle \tilde{e}^n - \chi_k\nabla_I D_1(z^n,x^k), y - z^n\right\rangle + \left\langle -\chi_k\nabla_I D_2(z^n,x^k), y - z^n\right\rangle \\
&= \chi_k(D(y,x^k) - D(z^n,x^k)) \\
&\quad + \left\langle \tilde{e}^n - \chi_k\nabla_I D_1(z^n,x^k), y - z^n\right\rangle + \chi_k(-\left\langle 2A^TA(z^n - x^k), y - z^n\right\rangle) \\
&= \chi_k(D(y,x^k) - D(z^n,x^k)) \\
&\quad + \left\langle \tilde{e}^n - \chi_k\nabla_I D_1(z^n,x^k), y - z^n\right\rangle + \chi_k(\left\langle 2A^TA(x^k - z^n), y - z^n\right\rangle) \\
&= \chi_k(D_1(y,x^k) - D_1(z^n,x^k) + D_2(y,x^k) - D_2(z^n,x^k)) \\
&\quad + \chi_k(\left\langle \tilde{e}^n/\chi_k - \nabla_I D_1(z^n,x^k), y - z^n\right\rangle) + \chi_k(2\left\langle x^k - z^n, y - z^n\right\rangle_A) \\
&= \chi_k(D_1(y,x^k) - D_1(z^n,x^k)) + \chi_k(\parallel y - x^k \parallel_A^2 - \parallel z^n - x^k \parallel_A^2) \\
&\quad + \chi_k(\left\langle \tilde{e}^n/\chi_k - \nabla_I D_1(z^n,x^k), y - z^n\right\rangle) + \chi_k(2\left\langle x^k - z^n, y - z^n\right\rangle_A) \\
&=: a + b
\end{aligned}
$$

with

$$
\begin{aligned}
a &:= \chi_k\left(\left\langle \tilde{e}^n/\chi_k - \nabla_I D_1(z^n,x^k), y - z^n\right\rangle + D_1(y,x^k) - D_1(z^n,x^k)\right), \\
b &:= \chi_k\left(2\left\langle x^k - z^n, y - z^n\right\rangle_A + \parallel y - x^k \parallel_A^2 - \parallel z^n - x^k \parallel_A^2\right).
\end{aligned}
$$

Since $D_1(\cdot, x^k)$ is a convex function, we can deduce for term a that

$$
\begin{aligned}
a &= \chi_k(\left\langle -\nabla_I D_1(z^n,x^k), y - z^n\right\rangle + D_1(y,x^k) - D_1(z^n,x^k)) + \langle \tilde{e}^n, y - z^n\rangle \\
&\geq \langle \tilde{e}^n, y - z^n\rangle .
\end{aligned}
$$

Term b can be transformed to

$$
\begin{aligned}
b &= \chi_k(2\left\langle x^k - z^n, y - z^n\right\rangle_A + \parallel y - x^k \parallel_A^2 - \parallel z^n - x^k \parallel_A^2) \\
&= \chi_k(2\left\langle x^k - z^n, y - x^k + x^k - z^n\right\rangle_A + \parallel y - x^k \parallel_A^2 - \parallel z^n - x^k \parallel_A^2) \\
&= \chi_k(2\left\langle x^k - z^n, y - x^k\right\rangle_A + 2\left\langle x^k - z^n, x^k - z^n\right\rangle_A + \parallel y - x^k \parallel_A^2 - \parallel z^n - x^k \parallel_A^2) \\
&= \chi_k(2\left\langle x^k - z^n, y - x^k\right\rangle_A + \parallel y - x^k \parallel_A^2 + \parallel z^n - x^k \parallel_A^2) \\
&= \chi_k \parallel y - z^n \parallel_A^2 .
\end{aligned}
$$

Altogether, we obtain

$$a + b = \hat{l}^n(y) - \hat{l}^n(z^n) \geq \langle \tilde{e}^n, y - z^n \rangle + \chi_k \parallel y - z^n \parallel_A^2$$

and estimate (8.21) is established.

Now, a combination of the estimates (8.19), (8.20), and (8.21) with $y = z^{n+1}$ leads to

$$\begin{aligned}
\varphi(x^k) &\geq \hat{\varphi}^{n+1}(z^{n+1}) + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle \\
&= \hat{l}^{n+1}(z^{n+1}) + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle \\
&\geq \hat{l}^n(z^{n+1}) + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle \\
&\geq \hat{l}^n(z^n) + \left\langle \tilde{e}^n, z^{n+1} - z^n \right\rangle + \chi_k \parallel z^{n+1} - z^n \parallel_A^2 + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle \\
&\geq \hat{l}^n(z^n) + \left\langle \tilde{e}^n, z^{n+1} - z^n \right\rangle + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle . \qquad (8.23)
\end{aligned}$$

Omitting all error terms in the above inequality chain would directly show that $\{\hat{l}^n(z^n)\}_{n\geq k}$ is monotone increasing and bounded from above, thus convergent. In our situation, conditions (8.13), (8.14), and (8.16) on the error terms ensure the convergence of $\{\hat{l}^n(z^n)\}_{n\geq k}$ in (8.23). Indeed, if we apply Lemma A.4.4 to the inequalities

$$\begin{aligned}
\varphi(x^k) &\geq \hat{l}^{n+1}(z^{n+1}) + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle \\
&\geq \hat{l}^n(z^n) + \left\langle \tilde{e}^n, z^{n+1} - z^n \right\rangle + \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle
\end{aligned}$$

with $\bar{a} = \varphi(x^k)$, $a_n = \hat{l}^n(z^n)$, $b_n = \langle \tilde{e}^n, z^{n+1} - z^n \rangle$, and $c_n = \left\langle \tilde{e}^{n+1}, x^k - z^{n+1} \right\rangle$, we obtain that

$$\{\hat{l}^n(z^n)\}_{n\geq k} \text{ is convergent}$$

to some $l^* \in \mathbb{R}$. A further consequence is $\lim_{k\leq n\to\infty} b_n = 0$ (see Remark A.4.5). In view of the inequality chain (8.23) we also obtain the convergence of $\{\hat{l}^n(z^{n+1})\}_{n\geq k}$ to l^*.

With these preparations we are ready to prove statement (a). Consider again relation (8.21) and choose $y = z^{n+1}$. Then

$$\hat{l}^n(z^{n+1}) - \hat{l}^n(z^n) \geq \left\langle \tilde{e}^n, z^{n+1} - z^n \right\rangle + \chi_k \parallel z^{n+1} - z^n \parallel_A^2 . \qquad (8.24)$$

Thus, $\lim_{k\leq n\to\infty} \parallel z^{n+1} - z^n \parallel_A = 0$. In view of (3.3), this implies the convergence in Euclidean norm:

$$\lim_{k\leq n\to\infty} \parallel z^{n+1} - z^n \parallel = 0. \qquad (8.25)$$

So, statement (a) is proved.

Now, we turn to the proof of statement (b). The idea is to write

$$0 \leq \varphi(z^{n+1}) - \varphi^{n+1}(z^{n+1}) = \varphi(z^{n+1}) - \varphi(z^n) + \varphi(z^n) - \varphi^{n+1}(z^{n+1}) \qquad (8.26)$$

and to show that the right hand side converges to zero. This is done in three steps.

In the first step, we obtain from (C1), (C3), and the Cauchy-Schwarz inequality that

$$\varphi(z^{n+1}) - \varphi(z^n) \geq \varphi^{n+1}(z^{n+1}) - \varphi(z^n) \geq \left\langle s^n, z^{n+1} - z^n \right\rangle \geq - \parallel s^n \parallel \parallel z^{n+1} - z^n \parallel . \tag{8.27}$$

By (C1) and (C2) one has $l^n(x^k) \leq \varphi^{n+1}(x^k) \leq \varphi(x^k)$. This implies $\hat{l}^n(x^k) \leq \varphi(x^k)$. Involving relation (8.21) with $y = x^k$ we see that

$$\varphi(x^k) - \hat{l}^n(z^n) \geq \hat{l}^n(x^k) - \hat{l}^n(z^n) \geq \left\langle \tilde{e}^n, x^k - z^n \right\rangle + \chi_k \parallel x^k - z^n \parallel_A^2 .$$

Together with the fact that $\{\hat{l}^n(z^n)\}_{n\geq k}$ converges to l^* and $\left\{\left\langle \tilde{e}^n, x^k - z^n \right\rangle\right\}_{n\geq k}$ converges to zero, it follows that the sequence

$$\{z^n\}_{n\geq k} \text{ is bounded.}$$

Since $\partial\varphi$ is maximal monotone and $\mathrm{dom}(\varphi) = \mathrm{dom}(\partial\varphi) = \mathbb{R}^n$ we can deduce from Lemma A.2.2 and Theorem A.2.4 that $\partial\varphi$ is bounded on bounded subsets of $\mathbb{R}^n$. Since $s^n \in \partial\varphi(z^n)$ for all $n \geq k$, boundedness of $\{z^n\}_{n\geq k}$ implies that

$$\{s^n\}_{n\geq k} \text{ is bounded.}$$

In the second step, we extend (8.27) by an estimate of $\varphi(z^{n+1}) - \varphi(z^n)$ from above. According to the mean value theorem there exists y^n in the open line segment $]z^n, z^{n+1}[$ and there exists $c^n \in \partial\varphi(y^n)$ such that

$$\varphi(z^{n+1}) - \varphi(z^n) = \left\langle c^n, z^{n+1} - z^n \right\rangle .$$

Since $\{z^n\}_{n\geq k}$ is bounded, also $\bigcup_{n\geq k}]z^n, z^{n+1}[$ is bounded. So $\partial\varphi$ is bounded on the bounded set $\bigcup_{n\geq k}]z^n, z^{n+1}[$, which implies that

$$\{c^n\}_{n\geq k} \text{ is bounded.}$$

With the Cauchy-Schwarz inequality we get the estimate

$$\parallel c^n \parallel \parallel z^{n+1} - z^n \parallel \geq \left\langle c^n, z^{n+1} - z^n \right\rangle = \varphi(z^{n+1}) - \varphi(z^n). \tag{8.28}$$

In the third step, we can now combine (8.27) and (8.28) to obtain

$$\begin{aligned} \parallel c^n \parallel \parallel z^{n+1} - z^n \parallel &\geq \varphi(z^{n+1}) - \varphi(z^n) \\ &\geq \varphi^{n+1}(z^{n+1}) - \varphi(z^n) \\ &\geq - \parallel s^n \parallel \parallel z^{n+1} - z^n \parallel . \end{aligned}$$

Boundedness of $\{c^n\}_{n\geq k}$ and $\{s^n\}_{n\geq k}$ and the convergence of $\{\| z^{n+1} - z^n \|\}_{n\geq k}$ to zero imply

$$\lim_{k\leq n\to\infty}(\varphi(z^{n+1}) - \varphi(z^n)) = 0 \quad \text{and} \quad \lim_{k\leq n\to\infty}(\varphi^{n+1}(z^{n+1}) - \varphi(z^n)) = 0. \tag{8.29}$$

In view of (8.26), we now get

$$\lim_{k\leq n\to\infty}\varphi(z^{n+1}) - \varphi^{n+1}(z^{n+1}) = 0$$

and statement (b) is established.

Statement (c) has already been prepared in (8.6) where we derived

$$\tilde{e}^{n+1} \in \nabla\psi(x^k) + \partial_{\tilde{\epsilon}_{n+1}}\varphi(z^{n+1}) + \chi_k\nabla_I D(z^{n+1}, x^k).$$

With the setting $d^{n+1} = \tilde{e}^{n+1} - \nabla\psi(x^k) - \chi_k\nabla_I D(z^{n+1}, x^k)$ it immediately follows that $d^{n+1} \in \partial_{\tilde{\epsilon}_{n+1}}\varphi(z^{n+1})$.

It remains to prove statement (d), i.e., the convergence of $\{z^n\}_{n\geq k}$ to the solution of the auxiliary problem (8.3). Since $d^{n+1} \in \partial_{\tilde{\epsilon}_{n+1}}\varphi(z^{n+1})$, it follows for all $y \in \mathbb{R}^n$ that

$$\varphi(y) \geq \varphi(z^{n+1}) + \left\langle d^{n+1}, y - z^{n+1}\right\rangle - \tilde{\epsilon}_{n+1}. \tag{8.30}$$

For the solution $\bar{z}^k$ of (8.3) it holds that $0 \in \nabla\psi(x^k) + \partial\varphi(\bar{z}^k) + \chi_k\nabla_I D(\bar{z}^k, x^k)$, which is equivalent to

$$\varphi(y) \geq \varphi(\bar{z}^k) + \left\langle -\nabla\psi(x^k) - \chi_k\nabla_I D(\bar{z}^k, x^k), y - \bar{z}^k\right\rangle. \tag{8.31}$$

Setting $y = \bar{z}^k$ in (8.30) and $y = z^{n+1}$ in (8.31) and adding the two inequalities, we obtain

$$0 \geq \left\langle d^{n+1}, \bar{z}^k - z^{n+1}\right\rangle - \tilde{\epsilon}_{n+1} + \left\langle -\nabla\psi(x^k) - \chi_k\nabla_I D(\bar{z}^k, x^k), z^{n+1} - \bar{z}^k\right\rangle,$$

which can be equivalently transformed to

$$\tilde{\epsilon}_{n+1} \geq \left\langle d^{n+1} + \nabla\psi(x^k) + \chi_k\nabla_I D(\bar{z}^k, x^k), \bar{z}^k - z^{n+1}\right\rangle.$$

With the definition of d^{n+1} this can be rewritten as

$$\frac{1}{\chi_k}\tilde{\epsilon}_{n+1} \geq \left\langle \frac{1}{\chi_k}\tilde{e}^{n+1}, \bar{z}^k - z^{n+1}\right\rangle + \left\langle \nabla_I D(\bar{z}^k, x^k) - \nabla_I D(z^{n+1}, x^k), \bar{z}^k - z^{n+1}\right\rangle.$$

Since $D(\cdot, x^k)$ is strongly convex, there exists $m > 0$ with

$$\frac{1}{\chi_k}\tilde{\epsilon}_{n+1} \geq \frac{1}{\chi_k}\left\langle \tilde{e}^{n+1}, \bar{z}^k - z^{n+1}\right\rangle + m \parallel \bar{z}^k - z^{n+1} \parallel_A^2.$$

With regard to the assumptions on the error sequence $\{\tilde{e}^n\}$ we have

$$\lim_{k \leq n \to \infty} \frac{1}{\chi_k} \left\langle \tilde{e}^{n+1}, \bar{z}^k - z^{n+1} \right\rangle = 0$$

since χ_k is fixed. Together with part (b) it now follows that

$$\lim_{k \leq n \to \infty} \| \bar{z}^k - z^{n+1} \|_A = 0.$$

Thus, $\{z^{n+1}\}_{n \geq k}$ converges to $\bar{z}^k$ and part (d) is proved. □

8.2 Numerical realization of the LQPAP bundle method

To realize the LQPAP bundle method numerically, we have to take a closer look at some details. The following aspects need to be concretized:

- Choice of a method to solve the auxiliary problem (8.17).
- Choice of the sequence $\{\epsilon_k\}$.
- Choice and update of the lower approximation φ^{k+1}.
- Initialization and update of the regularization parameter χ_k.
- Realization of a stopping criterion.

First, we restrict our considerations to the case

$$\psi = 0,$$

where we can give a theoretical justification of certain implementations. The necessary extensions for the case $\psi \neq 0$ are discussed in Section 8.2.7.

Furthermore, also empirical aspects are taken into account, e.g., when choosing the parameter settings or when differing from theory. The considerations are based on works from Auslender/Teboulle [4], Hübner [44], Kiwiel [59], and Wright [89], and corresponding results are transferred to our situation or extended by new conclusions.

8.2.1 Primal-dual interior point method to solve the auxiliary problem

Transformation of the auxiliary problem. We summarize the ideas in [44, Section 6.2.1] to solve the auxiliary problem (8.17), which is equivalent to z^{k+1} being an inexact solution of the problem

$$\min_{y\in\mathbb{R}^n} \left\{\varphi^{k+1}(y) + \chi_k D(y, x^k)\right\}. \tag{8.32}$$

Let J^k be the set of bundle indices used to define φ^{k+1} as described in (8.12). Although J^k is a selection of indices from the set $\{1,\dots,k\}$, for simplicity and better writing we assume that $J^k = \{1,\dots,m\}$. The corresponding bundle is $\{(z^j, s^j) : j = 1,\dots,m\}$.

Because of the special structure of φ^{k+1} we can transform (8.32) to

$$\begin{aligned} \min_{(y,w)\in\mathbb{R}^n\times\mathbb{R}} & \left\{w + \chi_k D(y, x^k)\right\} \\ s.t. \quad & \varphi(z^j) + \left\langle s^j, y - z^j\right\rangle \le w \quad \forall j \in J^k \\ & \varphi^k(z^k) + \left\langle -\chi_{k-1}\nabla_I D(z^k, x^{k-1}), y - z^k\right\rangle \le w. \end{aligned} \tag{8.33}$$

With the variable $v = w - \varphi(x^k)$ we transform (8.33) to

$$\begin{aligned} \min_{(y,v)\in\mathbb{R}^n\times\mathbb{R}} & \left\{v + \chi_k D(y, x^k)\right\} \\ s.t. \quad & Sy - ev \le d, \end{aligned} \tag{8.34}$$

with $e = (1,\dots,1)^T \in \mathbb{R}^{m+1}$ and

$$S = \begin{bmatrix} (s^1)^T \\ \cdots \\ (s^m)^T \\ (\tilde{s}^k)^T \end{bmatrix} \in \mathbb{R}^{(m+1)\times n}, \quad d = Sx^k + \begin{bmatrix} \alpha_{k,1} \\ \cdots \\ \alpha_{k,m} \\ \tilde{\alpha}_k \end{bmatrix} \in \mathbb{R}^{m+1}. \tag{8.35}$$

Here, we use the notation

$$\begin{aligned} \tilde{s}^k &= -\chi_{k-1}\nabla_I D(z^k, x^{k-1}), \\ \alpha_{k,j} &= \varphi(x^k) - \varphi(z^j) - \left\langle s^j, x^k - z^j\right\rangle \quad \forall j \in J^k, \\ \tilde{\alpha}_k &= \varphi(x^k) - \varphi^k(z^k) - \left\langle \tilde{s}^k, x^k - z^k\right\rangle. \end{aligned}$$

Namely, $\tilde{s}^k$ is the aggregate subgradient and $\tilde{\alpha}_k$ the corresponding linearization error in x^k between φ and the linearization of φ^k in $(z^k, \tilde{s}^k)$. The values $\alpha_{k,j}$ $(j = 1,\dots,m)$ are the linearization errors in x^k between φ and the linearization of φ in (z^j, s^j).

Remark 8.2.1. *Like in [44, Section 6.2.1], we leave out the error vector $\tilde{e}^k$ in the aggregate subgradient. From a theoretical point of view it would be no problem to work with the error vector $\tilde{e}^k$ as before. We would just have to adapt the definition of the matrix S coming further down. This would not have any consequences on the following argumentation. From an implementational point of view we would have to determine a vector $\tilde{e}^k$ in the set $\partial\varphi^k(z^k) + \chi_{k-1}\nabla_I D(z^k, x^{k-1})$. Since φ^k is the maximum of affine*

functions, its subdifferential is the convex hull of the gradients of the active functions. In view of the condition $\| \tilde{e}^k \| \leq \delta_{k-1}$ *in (see (8.7)) an element* $\hat{s}^k_{\min} \in \partial\varphi^k(z^k)$ *of minimal norm is preferable to set* $\tilde{e}^k = \hat{s}^k_{\min} + \chi_{k-1}\nabla_I D(z^k, x^{k-1})$*. Nevertheless, the calculation of* $\hat{s}^k_{\min}$ *can only be done inexactly. This would bring up another error term. So, in order to avoid too much work in estimating all errors that occur in a real computation, we omit the error vector in the aggregate subgradient for simplicity.*

Karush-Kuhn-Tucker (KKT) conditions. Problem (8.34) is a convex optimization problem. The objective function is continuously differentiable on $\mathrm{int}(K) \times \mathbb{R}$, and the feasible set is polyhedral. For its solution we aim to apply a primal-dual interior point method. The corresponding necessary optimality conditions (Karush-Kuhn-Tucker conditions) are:

$$\chi_k \nabla_I D(y, x^k) + S^T \nu = 0, \tag{8.36}$$
$$1 - \langle e, \nu \rangle = 0, \tag{8.37}$$
$$Sy - ev - d \leq 0, \tag{8.38}$$
$$\langle Sy - ev - d, \nu \rangle = 0, \tag{8.39}$$
$$\nu \geq 0. \tag{8.40}$$

The vector $\nu \in \mathbb{R}^{m+1}_+$ corresponds to the Lagrange multipliers for the inequality conditions in (8.34). Note that no additional constraint qualification is needed because of the linearity of the constraints, and that the KKT conditions are also sufficient since the objective function is convex.

We define

$$\begin{aligned} t &= -Sy + ev + d, \\ T &= \mathrm{diag}(t_1, \ldots, t_{m+1}), \\ \mathcal{V} &= \mathrm{diag}(\nu_1, \ldots, \nu_{m+1}) \end{aligned}$$

and get the following conditions, which are equivalent to (8.36)–(8.40):

$$\chi_k \nabla_I D(y, x^k) + S^T \nu = 0, \tag{8.41}$$
$$1 - \langle e, \nu \rangle = 0, \tag{8.42}$$
$$Sy - ev + t - d = 0, \tag{8.43}$$
$$T\mathcal{V}e = 0, \tag{8.44}$$
$$\nu \geq 0, \quad t \geq 0. \tag{8.45}$$

The primal-dual method generates iterates (x^i, v^i, ν^i, t^i) that satisfy the bounds in (8.45) strictly, which is the interior point idea. Furthermore, the complementarity condition (8.44) will be disturbed using a parameter μ. This leads to the central path idea

of the primal-dual method. For more background we refer to Wright [89]. The KKT conditions with disturbed complementarity condition are:

$$\chi_k \nabla_I D(y, x^k) + S^T \nu = 0, \tag{8.46}$$
$$1 - \langle e, \nu \rangle = 0, \tag{8.47}$$
$$Sy - ev + t - d = 0, \tag{8.48}$$
$$T\mathcal{V}e - \mu e = 0, \tag{8.49}$$
$$\nu \geq 0, \quad t \geq 0. \tag{8.50}$$

Because of (8.49), it holds that

$$\mu = \frac{\langle \nu, t \rangle}{m+1},$$

and μ is considered as the duality measure.

Newton method. The primal-dual interior point method is based on a step of the Newton method to solve system (8.46)–(8.49) for a given μ. Then μ is scaled down and the next iterate is calculated with the Newton method. The perturbation with μ ensures that t and ν stay strictly positive.

To compute the Newton direction in a given iterate $(y, v, \nu, t) \in \operatorname{int}(K) \times \mathbb{R} \times \mathbb{R}^{m+1}_{++} \times \mathbb{R}^{m+1}_{++}$, we have to solve the Newton equation

$$\begin{bmatrix} \chi_k \nabla_I^2 D(y, x^k) & 0 & S^T & 0 \\ 0 & 0 & -e^T & 0 \\ S & -e & 0 & I \\ 0 & 0 & T & \mathcal{V} \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta v \\ \Delta \nu \\ \Delta t \end{bmatrix} = - \begin{pmatrix} \chi_k \nabla_I D(y, x^k) + S^T \nu \\ 1 - \langle \nu, e \rangle \\ Sy - ev + t - d \\ T\mathcal{V}e - \sigma \mu e \end{pmatrix}. \tag{8.51}$$

Here, the parameter $\sigma \in (0, 1]$ is the so-called centering parameter. For abbreviation we set

$$\begin{aligned} r_D(y, \nu) &= \chi_k \nabla_I D(y, x^k) + S^T \nu, \\ r_e(\nu) &= 1 - \langle \nu, e \rangle, \\ r_d(y, v, t) &= Sy - ev + t - d. \end{aligned}$$

It is possible to eliminate Δt in (8.51) and solve the transformed system

$$\begin{bmatrix} \chi_k \nabla_I^2 D(y, x^k) & 0 & S^T \\ 0 & 0 & -e^T \\ S & -e & -\mathcal{V}^{-1} T \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta v \\ \Delta \nu \end{bmatrix} = - \begin{pmatrix} r_D(y, v) \\ r_e(\nu) \\ r_d(y, v, t) - \mathcal{V}^{-1} r_{t\nu} \end{pmatrix}. \tag{8.52}$$

Then Δt is calculated by

$$\Delta t = -\mathcal{V}^{-1}(r_{t\nu} + T \Delta \nu)$$

with

$$r_{t\nu} = T\mathcal{V}e - \sigma\mu e.$$

System (8.52) is uniquely solvable. This can be seen after an equivalent transformation to

$$\begin{bmatrix} \chi_k \nabla_I^2 D(y, x^k) & 0 & -S^T \\ 0 & 0 & e^T \\ S & -e & \mathcal{V}^{-1}T \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta v \\ -\Delta\nu \end{bmatrix} = - \begin{pmatrix} r_D(y,\nu) \\ r_e(\nu) \\ r_d(y,v,t) - \mathcal{V}^{-1} r_{t\nu} \end{pmatrix}. \tag{8.53}$$

For $(\Delta_1, \Delta_2, \Delta_3)^T \in \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^{m+1}$ it holds

$$\begin{aligned} &\begin{bmatrix} \Delta_1^T & \Delta_2^T & \Delta_3^T \end{bmatrix} \begin{bmatrix} \chi_k \nabla_I^2 D(y, x^k) & 0 & -S^T \\ 0 & 0 & e^T \\ S & -e & \mathcal{V}^{-1}T \end{bmatrix} \begin{bmatrix} \Delta_1 \\ \Delta_2 \\ \Delta_3 \end{bmatrix} \\ &= \chi_k \Delta_1^T \nabla_I^2 D(y, x^k) \Delta_1 + \Delta_3^T \mathcal{V}^{-1} T \Delta_3. \end{aligned}$$

Since the iteration process will ensure $\nu_j > 0$ and $t_j > 0$ for all j, the diagonal entries of the diagonal matrix $\mathcal{V}^{-1}T$ will be positive and, therefore, $\Delta_3^T \mathcal{V}^{-1} T \Delta_3 > 0$ holds for any $\Delta_3 \in \mathbb{R}^{m+1}$. For each $x \in \operatorname{int}(K)$ the distance function $D(\cdot, x)$ is strictly convex. So, $\nabla_I^2 D(y, x^k)$ is positive semidefinite. Altogether, the matrix in the system (8.53) is positive definite and thus regular.

Update of the iterates – calculation of the step length. Having calculated the Newton direction $(\Delta y, \Delta v, \Delta\nu, \Delta t)$ with system (8.52), the next iterate of the primal-dual method is given by

$$\begin{aligned} (y^+, v^+, \nu^+, t^+) &= (y, v, \nu, t) + \tau(\Delta y, \Delta v, \Delta\nu, \Delta t), \\ \mu^+ &= \frac{\langle \nu^+, t^+ \rangle}{m+1}, \quad \tau > 0. \end{aligned}$$

According to the path-following idea, the iterates shall be restricted to a neighborhood of the central path. The neighborhood excludes points (ν, t) that are too close to the boundary of the nonnegative orthant. This helps to ensure that the search directions make at least minimal progress towards the solution.

It further has to be considered that the KKT conditions include the nonlinear equation (8.46). So, even if we start with a feasible point, i.e., an iterate satisfying equations (8.46)–(8.48), a step along the Newton direction $(\Delta x, \Delta v, \Delta\nu, \Delta t)$ may not preserve feasibility. Therefore, the infeasible interior point framework is used, which allows infeasible iterates and works simultaneously towards feasibility and optimality. Thus, the neighborhood used in the path-following idea is extended and defined as

$$\begin{aligned} N_{-\infty}(\xi, \eta) = \{(y, v, \nu, t) : &\parallel r_D(y, \nu) \parallel \leq \eta\mu, \ \parallel r_e(\nu) \parallel \leq \eta\mu, \\ &\parallel r_d(y, v, t) \parallel \leq \eta\mu, \ \nu_j t_j \geq \xi\mu, \ \forall j \in \{1, \ldots, m+1\}, \ y \in \operatorname{int}(K)\} \end{aligned}$$

with $\xi \in (0,1)$ and $\eta > 0$. The first three conditions ensure that the amount by which the equations (8.46)–(8.48) are violated decreases at least as rapidly as the duality measure μ. The fourth condition realizes the path-following idea. It keeps the pairwise products $\nu_i t_i$ roughly in balance and prevents the search directions from being distorted by components of (ν, t) that approach zero too quickly. The last condition ($y \in \text{int}(K)$) is added to ensure that the objective function in (8.34) is welldefined.

Moreover, an Armijo-like condition on μ is added demanding that μ decreases by at least some small fraction of the predicted decrease at every step. Altogether, the conditions on the step length τ are:

$$\begin{aligned}(y^+, v^+, \nu^+, t^+) &\in N_{-\infty}(\xi, \eta)\\ \mu^+ &\leq (1 - s\tau)\mu\end{aligned}$$

with $s \in (0,1)$.

For more information about infeasible primal-dual interior point algorithms and their application to convex programs see [89, Chapter 6, Chapter 8].

Determining an initial iterate. The expressions $r_e(\nu)$ and $r_d(y, v, t)$ are affine linear. So, if an iterate (y, v, ν, t) is chosen with $r_e(\nu) = 0$ and $r_d(y, v, t) = 0$, the next iterate (y^+, v^+, ν^+, t^+) will fulfill $r_e(\nu^+) = 0$ and $r_d(y^+, v^+, t^+) = 0$ as well. Indeed, in view of the second and third equation in (8.51) it holds for arbitrary $\tau > 0$

$$r_e(\nu^+) = r_e(\nu + \tau\Delta\nu) = 1 - \langle \nu + \tau\Delta\nu, e\rangle = r_e(\nu) - \tau\,\langle \Delta\nu, e\rangle = 0$$

and

$$\begin{aligned}r_d(y^+, v^+, t^+) &= S(y + \tau\Delta y) - e(\nu + \tau\Delta\nu) + (t + \tau\Delta t) - d\\ &= r_d(y, v, t) + \tau(S\Delta y - e\Delta\nu + \Delta t)\\ &= 0.\end{aligned}$$

A possible choice of $(y, v, \nu, t) \in N_{-\infty}(\xi, \eta)$ with $r_e(\nu) = r_d(y, v, t) = 0$ is the following. Given $x^k \in \text{int}(K)$, set, for instance,

$$
\begin{aligned}
&y = x^k,\\
&v = 0.1,\\
&t_j = \alpha_{k,j} + v > 0, \quad j = 1, \ldots, m+1,\\
&\nu_j = \frac{1}{t_j} / \sum_{i=1}^{m+1} \frac{1}{t_i} > 0, \quad j = 1, \ldots, m+1,\\
&\xi \in (0,1) \text{ arbitrary (e.g. } 10^{-3}),\\
&\eta = 10 \frac{\| r_D(y,\nu) \|}{\mu} > 0 \text{ with}\\
&\mu = \frac{\langle \nu, t \rangle}{m+1} = 1 / \sum_{j=1}^{m+1} \frac{1}{t_j}.
\end{aligned}
$$

Indeed, $\langle \nu, e \rangle = 1$, so that $r_e(\nu) = 0$. With (8.35) it holds

$$(Sy - ev + t - d)_j = (Sx^k)_j - 0.1 + \alpha_{k,j} + 0.1 - (Sx^k)_j - \alpha_{k,j} = 0$$

for all $j = 1, \ldots, m+1$, so that $r_d(y, v, t) = 0$. For arbitrary $\xi \in (0,1)$ it holds $\nu_j t_j = \mu \geq \xi\mu$. Finally, $\eta\mu = 10 \parallel r_D(y,\nu) \parallel \geq \parallel r_D(y,\nu) \parallel$ is valid due to the choice of η.

Pseudocode and comments on convergence. The primal-dual interior point method to solve auxiliary problem (8.17) is summarized in Algorithm 8.2.

We close this section with a comment on the convergence of the primal-dual method and the overall LQPAP bundle method.

We do not aim at giving a stringent convergence analysis for the described primal-dual method. A convergence proof of a similar method – without the requirement $y \in \text{int}(K)$ – can be found in [78].

Concerning the overall LQPAP bundle method remember condition (8.7), i.e.,

$$\parallel \tilde{e}^{k+1} \parallel \leq \delta_k,$$

which describes the desired accuracy of z^{k+1}. If the primal-dual method stops at iterate $(\bar{y}, \bar{v}, \bar{\nu}, \bar{t})$, we assign

$$z^{k+1} = \bar{y} \text{ and } v^{k+1} = \bar{v}.$$

Theoretically it is possible to calculate z^{k+1} as accurate as it is required by iteratively decreasing the accuracy parameters θ_μ and θ_r in the primal-dual method. However, numerical tests have shown that the influence of θ_μ and θ_r is insignificant. Thus, we can omit an adaptation of the parameters in our implementation.

Algorithm 8.2: Primal-dual interior point method

1. *(Initialization)* Choose scalars $\xi \in (0,1),\ \eta > 0,\ 0 < \underline{\sigma} < \overline{\sigma} \leq 1/2,\ s \in (0,1)$, $\theta_\mu > 0,\ \theta_r > 0$, and an initial iterate $(y, v, \nu, t) \in N_{-\infty}(\xi, \eta)$ with $r_e(\nu) = 0$ and $r_d(y, v, t) = 0$. Set $\mu = \langle t, \nu \rangle / (m+1)$.

2. *(Stopping criterion)* If $\mu \leq \theta_\mu$ and $\| r_D(y, \nu) \| \leq \theta_r$ then stop: (y, v) is an approximate solution of (8.34).

3. *(Calculate search direction)* Choose $\sigma \in [\underline{\sigma}, \overline{\sigma}]$ and calculate $(\Delta y, \Delta v, \Delta \nu, \Delta t)$ by solving

$$\begin{bmatrix} \chi_k \nabla_I^2 D(y, x^k) & 0 & S^T \\ 0 & 0 & -e^T \\ S & -e & -\mathcal{V}^{-1}T \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta v \\ \Delta \nu \end{bmatrix} = - \begin{pmatrix} r_D(y, v) \\ 0 \\ -\mathcal{V}^{-1} r_{t\nu} \end{pmatrix}$$

and setting

$$\Delta t = -\mathcal{V}^{-1}(r_{t\nu} + T\Delta\nu)$$

with

$$r_{t\nu} = T\mathcal{V}e - \sigma\mu e.$$

4. *(Calculate step length)* Let $\tau_0 \in (0, 1]$ and $\omega \in (0, 1)$. Choose the step length τ as the first element in the sequence $\tau_0, \omega\tau_0, \omega^2\tau_0, \ldots$, such that

$$\begin{aligned} \nu_i^+ t_i^+ &\geq \xi\mu^+, \\ \| r_D(y^+, \nu^+) \| &\leq \eta\mu^+, \\ \mu^+ &\leq (1 - s\tau)\mu, \\ y^+ &\in \operatorname{int}(K). \end{aligned}$$

5. *(Update)* Set

$$\begin{aligned} (y, v, \nu, t) &\leftarrow (y, v, \nu, t) + \tau(\Delta y, \Delta v, \Delta \nu, \Delta t), \\ \mu &= \langle \nu, t \rangle / (m+1). \end{aligned}$$

6. Go to step 2.

Alternative calculation of $\tilde{\epsilon}_{k+1}$. With the knowledge about the primal-dual method, an alternative way to calculate $\tilde{\epsilon}_{k+1}$ can be derived. With $\tilde{\epsilon}_{k+1}$ it is checked, whether a null or a serious step will be performed. According to the definition we have to calculate

$$\tilde{\epsilon}_{k+1} = \varphi(z^{k+1}) - \varphi^{k+1}(z^{k+1}). \tag{8.54}$$

An evaluation of function φ^{k+1} needs $|J^k| + 1$ function evaluations of φ because the maximum of $|J^k| + 1$ affine functions has to be determined. In view of the optimization problem (8.33) one obtains

$$\bar{w} = \varphi^{k+1}(\bar{y})$$

as the value of w in the objective function if $(\bar{y}, \bar{v}, \bar{\nu}, \bar{t})$ is the result of the primal-dual method. Furthermore, by the substitution $v = w - \varphi(x^k)$ one has

$$\bar{v} = \varphi^{k+1}(\bar{y}) - \varphi(x^k) \tag{8.55}$$

as the value of v. So, with $z^{k+1} = \bar{y}$ and $v^{k+1} = \bar{v}$ the value of $\tilde{\epsilon}_{k+1}$ can be computed as

$$\tilde{\epsilon}_{k+1} = \varphi(z^{k+1}) - v^{k+1} - \varphi(x^k) \tag{8.56}$$

alternatively to (8.54).

8.2.2 Adaptive choice of the sequence $\{\epsilon_k\}$

The sequence $\{\epsilon_k\}$ influences the choice of the outer approximation $\mathcal{Q}^k$ of the operator $\mathcal{Q}$. The inclusion $\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k}$ has to be fulfilled (see (3.15) in Chapter 3). In the situation of a nondifferentiable, convex optimization problem we have $\mathcal{Q}^k = \partial_{\epsilon_k}\varphi$. According to the convergence conditions for the LQPAP algorithm, the sequence $\{\epsilon_k\}$ has to fulfill

$$\epsilon_k \geq 0 \ \forall k \in \mathbb{N}_0, \text{ and } \sum_{k=0}^{\infty} \epsilon_k < +\infty. \tag{8.57}$$

In step 3 of Algorithm 8.1 it became clear that the value of ϵ_k influences whether a null or a serious step will follow. In the sense of the LQPAP scheme the sequence $\{\epsilon_k\}$ is determined a priori, i.e., before the algorithm starts. In the framework of the bundle method this sequence is used as follows: In the case of a serious step, the next element of the given sequence is taken for the next iteration. But in the case of a null step, the current element of the sequence is taken again for the next iteration.

Nevertheless, we prefer an adaptive choice of the sequence $\{\epsilon_k\}$. This makes sense since, if the current iteration point is far away from the solution or the algorithm makes good progress, it is not necessary that the approximation φ^{k+1} is improved within several null

steps. And, vice versa, if the algorithm does not make enough progress or if the iterates are close to the optimal point, a small ϵ_k is desired. The value of v can be taken as a measure for the progress of the algorithm because it represents the predicted descent, i.e., the difference between $\varphi^{k+1}(\bar{y})$ and $\varphi(x^k)$ (see (8.55)). Therefore, like in [44, Section 6.1.2] we propose to perform a serious step if

$$\tilde{\epsilon}_{k+1} \leq -\gamma_1 v^{k+1}$$

with $\gamma_1 \in (0,1)$. With (8.56) this is equivalent to

$$\varphi(z^{k+1}) \leq \varphi(x^k) + (1-\gamma_1)v^{k+1}. \tag{8.58}$$

In many papers on bundle methods a similar criterion is used for the determination of a serious step (see, e.g, [59, 86]).

For a current iterate x^k we denote $i(k) \in \mathbb{N}_0$ with $i(k) \geq k$ as the first index such that inequality (8.58) holds. It is then possible to define the sequence $\{\epsilon_k\}$ a posteriori as

$$\{\epsilon_k\}_{k\in\mathbb{N}_0} = \{-\gamma_1 v^{i(k)+1}\}_{k\in\mathbb{N}_0}. \tag{8.59}$$

The next lemma will show that for each current iterate x^k there indeed exists an index $i(k)$. Afterwards, we demonstrate that $\{\epsilon_k\}_{k\in\mathbb{N}_0}$ fulfills the conditions in (8.57). This will provide a theoretical justification of such a choice.

Lemma 8.2.2. *Let x^k be the current iterate of the LQPAP bundle method and no solution of problem (8.1). Then there exists an index $i(k) \in \mathbb{N}_0$ with $i(k) \geq k$ such that inequality (8.58) holds.*

Proof. Suppose that for all subsequent iterations inequality (8.58) is violated, i.e.,

$$\varphi(z^{n+1}) > \varphi(x^n) + (1-\gamma_1)v^{n+1} \quad \forall n \geq k.$$

Thus, only null steps will follow and $x^n = x^k$ for all $n \geq k$. With regard to (8.56) this implies

$$\varphi(z^{n+1}) > \varphi(x^k) + (1-\gamma_1)(\varphi(z^{n+1}) - \varphi(x^k) - \tilde{\epsilon}_{n+1})$$

respectively

$$\tilde{\epsilon}_{n+1} > -\gamma_1(\varphi(z^{n+1}) - \varphi(x^k) - \tilde{\epsilon}_{n+1}). \tag{8.60}$$

For a sequence of null steps Theorem 8.1.2 states that $\lim_{k\leq n\to\infty} \tilde{\epsilon}_{n+1} = 0$ and $\lim_{k\leq n\to\infty} z^{n+1} = \bar{z}^k$. Since φ is continuous on $\operatorname{int}(K)$ as a finite, convex function on $\mathbb{R}^n$, for $n \to \infty$ we obtain from (8.60) that $0 \geq -\gamma_1(\varphi(\bar{z}^k) - \varphi(x^k))$. With $\gamma_1 \in (0,1)$ the relation

$$\varphi(x^k) \leq \varphi(\bar{z}^k)$$

follows. On the other hand, due to the optimality of $\bar{z}^k$ for problem (8.3), we have

$$\varphi(x^k) \geq \varphi(\bar{z}^k) + \chi_k D(\bar{z}^k, x^k) \geq \varphi(\bar{z}^k).$$

This establishes

$$\varphi(x^k) = \varphi(\bar{z}^k),$$

which implies $x^k = \bar{z}^k$ since $\bar{z}^k$ is a unique solution. The necessary optimality condition for problem (8.3) together with $D(x^k, x^k) = 0$ now results in

$$0 \in \partial\varphi(x^k),$$

i.e., x^k is an optimal solution of (8.1). This is a contradiction. □

For the next proposition we assume that we have an exact solution (y^*, v^*, ν^*, t^*) of the KKT system (8.46)–(8.50) with $\mu = 0$.

Proposition 8.2.3. *For the sequence $\{\epsilon_k\}$ defined by (8.59) it holds that*

$$\epsilon_k \geq 0 \quad \forall k \in \mathbb{N}_0.$$

Proof. Let x^k be the current iterate. We assign for the next iteration of the algorithm

$$z^{k+1} = y^*, \ v^{k+1} = v^*, \text{ and } \nu^{k+1} = \nu^*.$$

Multiplying equation (8.48) with vector ν^{k+1} results in

$$\left\langle \nu^{k+1}, Sz^{k+1} - ev^{k+1} + t^* - d \right\rangle = 0. \tag{8.61}$$

We set $\alpha^k = (\alpha_{k,1}, \ldots, \alpha_{k,m}, \tilde{\alpha}_k)^T$ and apply (8.46), (8.47), and (8.49) with $\mu = 0$ to equivalently transform (8.61) to

$$\begin{aligned}
0 &= \left\langle S^T\nu^{k+1}, z^{k+1} \right\rangle + \left\langle \nu^{k+1}, -ev^{k+1} + t^* - d \right\rangle \\
&= \left\langle -\chi_k \nabla_I D(z^{k+1}, x^k), z^{k+1} \right\rangle + v^{k+1} \left\langle \nu^{k+1}, -e \right\rangle + \left\langle \nu^{k+1}, t^* - d \right\rangle \\
&= \left\langle -\chi_k \nabla_I D(z^{k+1}, x^k), z^{k+1} \right\rangle - v^{k+1} - \left\langle \nu^{k+1}, d \right\rangle \\
&= \left\langle -\chi_k \nabla_I D(z^{k+1}, x^k), z^{k+1} \right\rangle - v^{k+1} - \left\langle \nu^{k+1}, Sx^k + \alpha^k \right\rangle \\
&= \left\langle -\chi_k \nabla_I D(z^{k+1}, x^k), z^{k+1} \right\rangle - v^{k+1} - \left\langle S^T\nu^{k+1}, x^k \right\rangle - \left\langle \nu^{k+1}, \alpha^k \right\rangle \\
&= \left\langle -\chi_k \nabla_I D(z^{k+1}, x^k), z^{k+1} \right\rangle - v^{k+1} - \left\langle -\chi_k \nabla_I D(z^{k+1}, x^k), x^k \right\rangle - \left\langle \nu^{k+1}, \alpha^k \right\rangle \\
&= \left\langle -\chi_k \nabla_I D(z^{k+1}, x^k), z^{k+1} - x^k \right\rangle - v^{k+1} - \left\langle \nu^{k+1}, \alpha^k \right\rangle.
\end{aligned}$$

We obtain the following formula for the value of v^{k+1}:

$$v^{k+1} = \left\langle \chi_k \nabla_I D(z^{k+1}, x^k), x^k - z^{k+1} \right\rangle - \left\langle \nu^{k+1}, \alpha^k \right\rangle . \tag{8.62}$$

To further estimate the scalar product $\left\langle \chi_k \nabla_I D(z^{k+1}, x^k), x^k - z^{k+1} \right\rangle$, key property (3.14) is applied with $x = z^{k+1}$, $y = x^k$, and $z = x^k$. This results in

$$\begin{aligned} v^{k+1} &\leq \frac{3}{2}(\parallel x^k - x^k \parallel_A^2 - \parallel x^k - z^{k+1} \parallel_A^2) - \left\langle \nu^{k+1}, \alpha^k \right\rangle \\ &= -\frac{3}{2} \parallel x^k - z^{k+1} \parallel_A^2 - \left\langle \nu^{k+1}, \alpha^k \right\rangle \\ &\leq 0 \end{aligned} \tag{8.63}$$

because $\nu^{k+1} \geq 0$ and $\alpha^k \geq 0$. With $\gamma_1 \in (0,1)$ it is evident that $\epsilon_k = -\gamma_1 v^{i(k)+1} \geq 0$ for all $k \in \mathbb{N}_0$. □

Remark 8.2.4 (Case of inexact solutions). *We briefly discuss the case of an inexact solution of the KKT system (8.46)–(8.50). As explained before, the primal-dual interior point method is implemented without an adaptation of the accuracy parameters θ_μ and θ_r. Consequently, the calculated solution $(\bar{y}, \bar{v}, \bar{\nu}, \bar{t})$ does not solve the KKT system exactly, but it fulfills the following relations*

$$\begin{aligned} \chi_k \nabla_I D(\bar{y}, x^k) + S^T \bar{\nu} &= r_D(\bar{y}, \bar{\nu}), \\ \parallel r_D(\bar{y}, \bar{\nu}) \parallel &\leq \theta_r, \\ 1 - \langle e, \bar{\nu} \rangle &= 0, \\ S\bar{y} - e\bar{\nu} + \bar{t} - d &= 0, \\ \bar{T}\bar{\mathcal{V}}e - \mu e &= 0, \\ \mu &\leq \theta_\mu, \\ \bar{\nu} \geq 0, \quad \bar{t} &\geq 0. \end{aligned}$$

Using these relations to get a formula for v^{k+1}, we arrive at

$$v^{k+1} \leq \left\langle r_D(\bar{y}, \bar{\nu}), z^{k+1} - x^k \right\rangle + \theta_\mu - \frac{3}{2} \parallel x^k - z^{k+1} \parallel_A^2 - \left\langle \nu^{k+1}, \alpha^k \right\rangle .$$

Applying (3.3) and (A.2) with $\xi = 3a^2$ (see Appendix A.4), this can further be estimated as

$$\begin{aligned} v^{k+1} &\leq \frac{1}{6a^2}\theta_r^2 + \frac{3a^2}{2} \parallel z^{k+1} - x^k \parallel^2 + \theta_\mu - \frac{3a^2}{2} \parallel x^k - z^{k+1} \parallel^2 - \left\langle \nu^{k+1}, \alpha^k \right\rangle \\ &\leq \frac{1}{6a^2}\theta_r^2 + \theta_\mu. \end{aligned}$$

So, in the inexact case we can only state that v^{k+1} is less than or equal to some error term depending on θ_r and θ_μ . This is one source of numerical difficulties. They become apparent if test examples with known solutions are solved by the method.

Proposition 8.2.5. *The sequence $\{\epsilon_k\}$ defined by (8.59) is summable.*

Proof. With the definition of the sequence $\{i(k)\}_{k\in\mathbb{N}_0}$ it holds for all $k \in \mathbb{N}_0$ that

$$\varphi(z^{i(k)+1}) \leq \varphi(x^{i(k)}) + (1-\gamma_1)v^{i(k)+1}.$$

In the case of a serious step, iterate x^{k+1} is set to $z^{i(k)+1}$, whereas for all $k \leq l \leq i(k)$ one has $x^l = x^k$. Thus, for all $k \in \mathbb{N}_0$,

$$-v^{i(k)+1} \leq \frac{\varphi(x^k) - \varphi(x^{k+1})}{1-\gamma_1}.$$

For arbitrary $N \in \mathbb{N}$ it holds

$$\begin{aligned}
\sum_{k=0}^{N} \epsilon_k &= -\gamma_1 \sum_{k=0}^{N} v^{i(k)+1} \\
&\leq \gamma_1 \sum_{k=0}^{N} \frac{\varphi(x^k) - \varphi(x^{k+1})}{1-\gamma_1} \\
&= \gamma_1 \frac{\varphi(x^0) - \varphi(x^N)}{1-\gamma_1} \\
&\leq \gamma_1 \frac{\varphi(x^0) - \varphi(x^*)}{1-\gamma_1},
\end{aligned}$$

where x^* denotes a solution of problem (8.1). For $N \to \infty$ it follows immediately that

$$\sum_{k=0}^{\infty} \epsilon_k < \infty.$$

□

We summarize that the choice of the sequence $\{\epsilon_k\}$ according to (8.59) makes sense not only from a numerical point of view, but it is also theoretically justified. Thus, the decision rule for a serious step respectively null step is implemented as follows:

If $\varphi(z^{k+1}) \leq \varphi(x^k) + (1-\gamma_1)v^{k+1}$ then perform a serious step, otherwise perform a null step.

8.2.3 Choice and update of the lower approximation φ^{k+1}

The general considerations in this section are not specific for the LQPAP bundle method. The main aspects about the choice and update of φ^{k+1} are summarized from

the literature about bundle methods (see, e.g., [59, 86]) and special settings concerning the LQPAP bundle method are pointed out.

As mentioned in Section 8.1.2, we define the lower approximation φ^{k+1} as

$$\varphi^{k+1}(y) = \max\{l^k(y), \varphi(z^j) + \langle s^j, y - z^j \rangle : j \in J^k\},$$

where $J^k \subset \{1, \ldots, k\}$ and $k \in J^k$. The size of the index set J^k plays a crucial rule concerning the numerical performance of the method. The larger the number of indices in J^k, i.e., the more testpoints and subgradients are in the current bundle, the better the approximation of φ by φ^{k+1} and the less null steps are necessary to find a tolerable approximation. However, if $m = |J^k|$ is large, the dimension of the KKT matrix (see (8.52)) is large as well. This implies a huge numerical effort to calculate a Newton step. Therefore, it makes sense to keep the size of J^k bounded:

$$|J^k| \leq M, \quad M \geq 1.$$

For that purpose, it is common to clear the bundle in each iteration by removing all elements $j \in J^k$ with

$$\nu_j^{k+1} = 0.$$

This has the following background: The values $\nu_1^{k+1}, \ldots, \nu_m^{k+1}$ are the Lagrange multipliers for the first m inequality conditions in (8.34). The complementarity condition (8.39) implies that

$$(Sz^{k+1} - ev^{k+1} - d)_j < 0$$

is possible if $\nu_j^{k+1} = 0$. This is equivalent to

$$\varphi(z^j) + \langle s^j, z^{k+1} - z^j \rangle < w^{k+1}$$

with $w^{k+1} = v^{k+1} + \varphi(x^k)$ and means that the linear function $\varphi(z^j) + \langle s^j, \cdot - z^j \rangle$ has no impact on the approximation of φ in a neighborhood of x^k. So it can be discarded for the next iteration. Note that also the situation $(Sz^{k+1} - ev^{k+1} - d)_j = 0$ and $\nu_j^{k+1} = 0$ is possible, but even in this case it is conform to theory to remove the corresponding index.

To guarantee condition (C3), the element (z^{k+1}, s^{k+1}) is added to the bundle after each null or serious step. If the bundle is at its maximum size, we have to remove one element to give space for the new element (z^{k+1}, s^{k+1}). For that purpose, we look at the bundle elements (z^j, s^j) and the corresponding linearization errors α_j^k. The smaller α_j^k, the better the linear function $\varphi(z^j) + \langle s^j, \cdot - z^j \rangle$ describes the behavior of φ in a neighborhood of x^k. Thus, it makes sense to remove a bundle element with the largest linearization error.

In some descriptions of bundle methods the bundle is completely cleared after a serious step by setting $J^{k+1} = \{0\}$ (see, e.g., [4]). This is not necessary in view of the conditions

(C1)–(C3) and it even makes sense to use the information from earlier iterations, especially if the evaluation of the function values and the subgradients is expensive. Thus, we keep the bundle after a serious step.

The aggregate subgradient $\tilde{s}^k$ and its corresponding linearization error $\tilde{\alpha}_k$ play a special role. In iteration $k = 0$, $\tilde{s}^0$ and $\tilde{\alpha}_0$ are not existent. For $k = 1$ it holds

$$\tilde{s}^1 = -\chi_0 \nabla_I D(z^1, x^0) = \nu^1 s^0 = s^0$$

since ν^1 has only one component that must therefore be equal to one. The corresponding linearization error $\tilde{\alpha}_1$ is equal to $\alpha_{1,0}$. Thus, in iteration $k = 1$ the aggregate subgradient can be omitted since it would lead to a redundant inequality condition in problem (8.34). For that reason, $\tilde{s}^k$ and $\tilde{\alpha}_k$ are first determined for $k = 2$ and then updated after each iteration, i.e., $(\tilde{s}^k, \tilde{\alpha}_k)$ is substituted by $(\tilde{s}^{k+1}, \tilde{\alpha}_{k+1})$. By the definition of the aggregate subgradient and the KKT condition (8.46), we get

$$\tilde{s}^{k+1} = -\chi_k \nabla_I D(z^{k+1}, x^k) = \sum_{j \in J^k} \nu_j^{k+1} s^j + \nu_{m+1}^{k+1} \tilde{s}^k.$$

We point out that in contrast to other implementations of bundle methods, where the aggregate subgradient is removed after each serious step, we keep it in each iteration. This is also conform to the conditions (C1)–(C3).

Finally, we take a closer look at the linearization errors and describe how they are updated from iteration k to $k + 1$. We distinguish between null and serious steps. In iteration k we have

$$\begin{aligned} \alpha_{k,j} &= \varphi(x^k) - \varphi(z^j) - \left\langle s^j, x^k - z^j \right\rangle \quad \forall j \in J^k, \\ \tilde{\alpha}_k &= \varphi(x^k) - \varphi^k(z^k) - \left\langle \tilde{s}^k, x^k - z^k \right\rangle. \end{aligned}$$

In the case of a null step one has $x^{k+1} = x^k$ and therefore

$$\alpha_{k+1,j} = \alpha_{k,j} \quad \forall j \in J^k.$$

For the new bundle element (z^{k+1}, s^{k+1}) we get

$$\alpha_{k+1,k+1} = \varphi(x^k) - \varphi(z^{k+1}) - \left\langle s^{k+1}, x^k - z^{k+1} \right\rangle.$$

Furthermore, with equations (8.55) and (8.62) for v^{k+1} and the definition of $\tilde{s}^{k+1}$ it holds

$$\begin{aligned} \tilde{\alpha}_{k+1} &= \varphi(x^k) - \varphi^{k+1}(z^{k+1}) - \left\langle \tilde{s}^{k+1}, x^k - z^{k+1} \right\rangle \\ &= -v^{k+1} + \left\langle \chi_k \nabla_I D(z^{k+1}, x^k), x^k - z^{k+1} \right\rangle \\ &= \left\langle \nu^{k+1}, \alpha^k \right\rangle \\ &= \sum_{j \in J^k} \nu_j^{k+1} \alpha_{k,j} + \nu_{m+1}^{k+1} \tilde{\alpha}_k. \end{aligned}$$

In the case of a serious step the following update rules can be deduced:

$$\begin{aligned}
\alpha_{k+1,j} &= \varphi(x^{k+1}) - \varphi(z^j) - \left\langle s^j, x^{k+1} - z^j \right\rangle \\
&= \alpha_{k,j} + \varphi(x^{k+1}) - \varphi(x^k) - \left\langle s^j, x^{k+1} - x^k \right\rangle \quad \forall j \in J^k, \\
\tilde{\alpha}_{k+1} &= \varphi(x^{k+1}) - \varphi^{k+1}(z^{k+1}) - \left\langle \tilde{s}^{k+1}, x^{k+1} - z^{k+1} \right\rangle \\
&= \varphi(x^{k+1}) - \varphi(x^k) - v^{k+1} - \left\langle \tilde{s}^{k+1}, x^k - z^{k+1} \right\rangle \\
&\quad + \left\langle \tilde{s}^{k+1}, x^k - z^{k+1} \right\rangle - \left\langle \tilde{s}^{k+1}, x^{k+1} - z^{k+1} \right\rangle \\
&= \sum_{j \in J^k} \nu_j^{k+1} \alpha_{k,j} + \nu_{m+1}^{k+1} \tilde{\alpha}_k + \varphi(x^{k+1}) - \varphi(x^k) - \left\langle \tilde{s}^{k+1}, x^{k+1} - x^k \right\rangle \\
\alpha_{k+1,k+1} &= 0.
\end{aligned}$$

8.2.4 Initialization and update of the regularization parameter χ_k

Concerning the lower and upper bound for the sequence $\{\chi_k\}$, we refer to the general statements in Section 6.1.2.

An idea to adaptively calculate the initial value χ_0 is presented in Appendix A.6.4 for problems of Category 1. It can easily be transferred to the situation in this chapter by writing φ instead of ψ and $s^0 \in \partial\varphi(x^0)$ instead of $\nabla\psi(x^0)$.

Of course, we can use the simple update rule

$$\chi_{k+1} = \max\{\chi_0 r^{k+1}, \underline{\chi}\}, \quad \chi_0 \geq \underline{\chi}, \quad r \in (0,1)$$

to change χ_k after each serious step. However, in the context of bundle methods (see, e.g., [59]) or trust region methods (see, e.g., [77]) it is common to take the quality of the lower approximation φ^{k+1} into account.

If φ^{k+1} is a bad model for φ, we intend to keep the solution z^{k+1} of (8.32) close to the current iterate x^k. This is achieved with an appropriate large regularization parameter. On the other hand, a small regularizing effect of D is preferable if φ^{k+1} is a good approximation of φ. Thus, an adaptive update strategy for χ_k is searched such that the solution z^{k+1} is kept in a region where φ^{k+1} is close to φ.

It is standard to use the ratio between the actual descent and the predicted descent, i.e.,

$$\rho_k := \frac{\varphi(z^{k+1}) - \varphi(x^k)}{\varphi^{k+1}(z^{k+1}) - \varphi(x^k)}$$

as a value to decide whether φ^{k+1} is a good approximation or not. In Section 8.2.2 (see (8.58)) the test

$$\rho_k \geq (1 - \gamma_1)$$

is used as a criterion for a serious step. The following refinement of this test will give an update rule for the regularization parameter:

Let $0 < \gamma_2 < \gamma_1 < 1$ and $0 < \tau_3 < \tau_2 < 1 < \tau_1$ be given. The situation $\rho_k \geq (1 - \gamma_2)$ implies that the model function φ^{k+1} is close to φ, such that χ_k can be scaled down (using τ_3). If $(1 - \gamma_1) \leq \rho_k < (1 - \gamma_2)$, a serious step is performed but the stronger condition $\rho_k \geq (1 - \gamma_2)$ is violated. In this case, one can reduce χ_k slightly (using τ_2). In the case of a null step, i.e., $\rho_k < (1 - \gamma_1)$, φ^{k+1} is a bad model for φ and therefore χ_k should be enlarged (using τ_1). Following the description in [59], we further use a counter c_{SS} to remember the number of consecutive serious steps (c_{SS} positive) or consecutive null steps (c_{SS} negative). This introduces some inertia that smooths out the updating procedure. More precisely this means:

- If $\rho_k \geq (1 - \gamma_2)$ and more than two consecutive serious steps have occurred then reduce χ_k with factor τ_3.
- If there were more than four consecutive serious steps but the stronger condition $\rho_k \geq (1 - \gamma_2)$ is violated then reduce χ_k with factor τ_2.
- If more than four consecutive null steps occurred then increase χ_k with factor τ_1.

Algorithm 8.3 describes the updating procedure in detail.

Algorithm 8.3: Updating procedure for the sequence $\{\chi_k\}$

if *(serious step)* **then**
  if $\varphi(z^{k+1}) \leq \varphi(x^k) + (1 - \gamma_2)v^{k+1}$ *and* $c_{SS} \geq 2$ **then**
    $\chi_{k+1} = \tau_3 \chi_k$;
  else if $c_{SS} \geq 4$ **then**
    $\chi_{k+1} = \tau_2 \chi_k$;
  end
  if $\chi_{k+1} < \underline{\chi}$ **then** $\chi_{k+1} = \underline{\chi}$;
  $c_{SS} = \max\{1, c_{SS} + 1\}$;
  if $\chi_{k+1} \neq \chi_k$ **then** $c_{SS} = 1$;
else *(null step)*
  if $c_{SS} \leq -4$ **then**
    $\chi_{k+1} = \tau_1 \chi_k$;
  if $\chi_{k+1} > \bar{\chi}$ **then** $\chi_{k+1} = \bar{\chi}$;
  $c_{SS} = \min\{c_{SS} - 1, -1\}$;
  if $\chi_{k+1} \neq \chi_k$ **then** $c_{SS} = -1$;
end

8.2.5 Realization of a stopping criterion

We now turn to the question of how to decide if the current iterate x^k is an approximate solution of the given problem (8.1). Consider the case that

$$v^{k+1} = 0.$$

Then the estimate in (8.63) implies that $x^k = z^{k+1}$. In view of (8.56), this leads to $\tilde{\epsilon}_{k+1} = 0$. Since z^{k+1} is an inexact solution of problem (8.17), it follows immediately with (8.6) that

$$\tilde{e}^{k+1} \in \partial\varphi(x^k),$$

i.e., x^k is an approximate solution of (8.1). Taking into account that $v^{k+1} \leq 0$ for all k, it is reasonable to terminate the LQPAP bundle method if

$$-v^{k+1} \leq \theta$$

with a small $\theta > 0$.

8.2.6 The overall LQPAP bundle algorithm

We summarize the considerations concerning the numerical realization of the LQPAP bundle method in Algorithm 8.4.

8.2.7 Extensions for the case $\psi \neq 0$

The argumentation in Sections 8.2.1, 8.2.3, and 8.2.4 can easily be extended to the case $\psi \neq 0$. However, an adaptation of the proofs of Lemma 8.2.2 and Proposition 8.2.3 is not possible, because this would require an estimation of an inner product of the type $\langle \psi(x), x - y \rangle$ which cannot be given in this generality. Nevertheless, if one considers the settings in Sections 8.2.2 and 8.2.5 as heuristics, the algorithm can still be used if the changes described in this section are taken into account.

The primal-dual interior point method (see Section 8.2.1) has to be extended such that it solves auxiliary problems of the type

$$\min_{y \in \mathbb{R}^n} \left\{ \left\langle \nabla\psi(x^k), y - x^k \right\rangle + \varphi^{k+1}(y) + \chi_k D(y, x^k) \right\}.$$

For that purpose, we change the definition of $\tilde{s}^k$ to

$$\tilde{s}^k = -\nabla\psi(x^k) - \chi_{k-1} \nabla_I D(z^k, x^{k-1})$$

Algorithm 8.4: LQPAP bundle algorithm

1. *(Initialization)* Choose an initial iterate $x^0 \in \operatorname{int}(K)$, a stopping parameter $\theta > 0$, a tolerance parameter $\gamma_1 \in (0,1)$, an initial regularization parameter $\chi_0 \geq \underline{\chi}$, a subgradient $s^0 \in \partial\varphi(x^0)$, and a maximal number $M \geq 1$ of bundle elements. Set $z^0 = x^0$, $\alpha_{0,0} = 0$, $J^0 = \{0\}$, $m = |J^0|$, $k := 0$.

2. *(Solution of the bundle auxiliary problem)*
Compute $(z^{k+1}, v^{k+1}, \nu^{k+1}, t^{k+1}) \in \operatorname{int}(K) \times \mathbb{R} \times \mathbb{R}_+^{m+1} \times \mathbb{R}_+^{m+1}$ with the primal-dual interior point method of Section 8.2.1. Then (z^{k+1}, v^{k+1}) is the solution of the k-th bundle auxiliary problem (8.34).

3. *(Clear set of bundle indices)* Remove from J^k all indices j with $\nu_j^{k+1} = 0$, set $m = |J^k|$.

4. *(Update aggregate subgradient)*
if $k = 1$ **then**
$\tilde{s}^{k+1} = \sum_{j \in J^k} \nu_j^{k+1} s^j, \quad \tilde{\alpha}_{k+1} = \sum_{j \in J^k} \nu_j^{k+1} \alpha_{k,j}$.
if $k \geq 2$ **then**
$\tilde{s}^{k+1} = \sum_{j \in J^k} \nu_j^{k+1} s^j + \nu_{m+1}^{k+1} \tilde{s}^k, \quad \tilde{\alpha}_{k+1} = \sum_{j \in J^k} \nu_j^{k+1} \alpha_{k,j} + \nu_{m+1}^{k+1} \tilde{\alpha}_k$.

5. *(Stopping criterion)* **if** $-v^{k+1} \leq \theta$ **then** stop: x^k is an approximate solution of (8.1).

6. *(Decision serious step/null step)*
if $\varphi(z^{k+1}) \leq \varphi(x^k) + (1-\gamma_1) v^{k+1}$ **then**
Set $x^{k+1} = z^{k+1}$. Choose $s^{k+1} \in \partial\varphi(x^{k+1})$.
Update the linearization errors:
$\alpha_{k+1,j} = \alpha_{k,j} + \varphi(x^{k+1}) - \varphi(x^k) - \langle s^j, x^{k+1} - x^k \rangle \quad \forall j \in J^k$,
$\alpha_{k+1,k+1} = 0$.
if $k \geq 1$ **then**
$\tilde{\alpha}_{k+1} \leftarrow \tilde{\alpha}_{k+1} + \varphi(x^{k+1}) - \varphi(x^k) - \langle \tilde{s}^{k+1}, x^{k+1} - x^k \rangle$.
else
Set $x^{k+1} = x^k$. Choose $s^{k+1} \in \partial\varphi(z^{k+1})$.
Update the linearization errors:
$\alpha_{k+1,j} = \alpha_{k,j} \quad \forall j \in J^k$,
$\alpha_{k+1,k+1} = \varphi(x^k) - \varphi(z^{k+1}) - \langle s^{k+1}, x^k - z^{k+1} \rangle$.
end

7. *(Update χ_k)* Choose a new regularization parameter χ_{k+1} according to Algorithm 8.3.

8. *(Update J^k)* If $|J^k| = M$, remove one element from J^k with the largest linearization error. Set $J^{k+1} = J^k \cup \{k+1\}$.

9. Set $k := k+1$ and go to step 2.

and write the KKT conditions with disturbed complementarity condition as

$$\nabla\psi(x^k) + \chi_k \nabla_I D(y, x^k) + S^T\nu = 0, \tag{8.64}$$
$$1 - \langle e, \nu\rangle = 0, \tag{8.65}$$
$$Sy - ev + t - d = 0, \tag{8.66}$$
$$T\mathcal{V}e - \mu e = 0, \tag{8.67}$$
$$\nu \geq 0, \quad t \geq 0. \tag{8.68}$$

Thus, in Algorithm 8.2 the Newton equation has to be solved with

$$r_D(y, v) = \nabla\psi(x^k) + \chi_k \nabla_I D(y, x^k) + S^T\nu.$$

Concerning the choice and update of φ^{k+1} (see Section 8.2.3) no changes are necessary.

If $\psi \neq 0$ it is important to set

$$\underline{\chi} = \frac{1}{2a^2\gamma} + 10^{-3}$$

as discussed in Section 6.1.2. The idea for the calculation of χ_0 (see Appendix A.6.4) can be adapted by taking $s^0 + \nabla\psi(x^0)$ instead of $\nabla\psi(x^0)$. The adaptive update procedure for $\{\chi_k\}$ described in Section 8.2.4 is independent of ψ and therefore requires no changes.

8.3 Academic test examples

The numerical performance of the LQPAP bundle method is tested with examples of the type

$$\begin{aligned} &\min\ \varphi(x) \\ &\text{s.t. } Ax \leq b, \end{aligned}$$

where $\varphi : \mathbb{R}^n \to \mathbb{R}$ is a nondifferentiable, convex function. In most cases, φ is of the form

$$\varphi(x) = \max\{f_k(x) : k = 1, \ldots, n_\varphi\}, \tag{8.69}$$

where $f_k : \mathbb{R}^n \to \mathbb{R}$, $k = 1, \ldots, n_\varphi$, are differentiable, convex functions. As a consequence, an element of $\partial\varphi(x)$ is easy to calculate because for each given x, any active index $j \leq n_\varphi$ (i.e., an index where the maximum in (8.69) is attained) yields a subgradient $\nabla f_j(x) \in \partial\varphi(x)$.

The examples are taken from the collections in [44, 56, 59, 67] and one example is constructed to have multiple solutions. If the restriction matrix of the examples from

literature does not have full column rank, we add some upper or lower bounds on the variables. For each example we list the objective function φ, A and b or the corresponding constraint functions $c_i(x) = (Ax - b)_i$, the dimension n, the number of constraints p, the solution set X^* or the unique solution x^* (if known), the optimal value φ^*, and one or more strict feasible initial points x^0 with their objective values. In all examples, except Example 8.3.8, the objective function is nondifferentiable at the optimal solution.

Furthermore, a comparison to the BrPAP bundle method (see BrεRPPA in [44]) will be given. For that purpose, our implementation was extended to Bregman distances analogously to Section 6.1.5.

The two-dimensional examples are chosen only to get an impression of the geometrical behavior of the algorithm. For these examples we plot the level sets of the objective function, the feasible set, and the paths of the iterates for both methods.

8.3.1 Two-dimensional examples

Example 8.3.1 (Constrained Demyanov, [44]).

$$\begin{aligned}
&\varphi(x) = \max\{f_1(x), f_2(x), f_3(x)\}, \quad x \in \mathbb{R}^2,\\
&f_1(x) = 5x_1 + x_2,\\
&f_2(x) = x_1^2 + x_2^2 + 4x_2,\\
&f_3(x) = -5x_1 + x_2,
\end{aligned}$$

$$A = \begin{pmatrix} 1 & -1 \\ 1 & 1 \\ -1 & 1 \\ -1 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 3 \\ 3 \\ 3 \\ 3 \end{pmatrix},$$

$n = 2$, $p = 4$, $x_1^0 = (-2, 0)^T$, $\varphi(x_1^0) = 10$, $x_2^0 = (0, 2.5)^T$, $\varphi(x_2^0) = 16.25$, $x_3^0 = (1, 1)^T$, $\varphi(x_3^0) = 6$, $x^* = (0, -3)^T$, $\varphi^* = -3$.

Example 8.3.2 (Constrained Mifflin, [44]).

$$\varphi(x) = -x_1 + 3\max\{x_1^2 + x_2^2 - 1, 0\}, \quad x \in \mathbb{R}^2,$$

$$A = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} -1 \\ 1 \end{pmatrix},$$

$n = 2$, $p = 2$, $x_1^0 = (0.9, 1.7)^T$, $\varphi(x_1^0) = 7.2$, $x_2^0 = (0, 1.8)^T$, $\varphi(x_2^0) = 6.72$, $x_3^0 = (0.2, \sqrt{1 - 0.2^2})^T$, $\varphi(x_3^0) = -0.2$, $x^* = (1, 0)^T$, $\varphi^* = -1$.

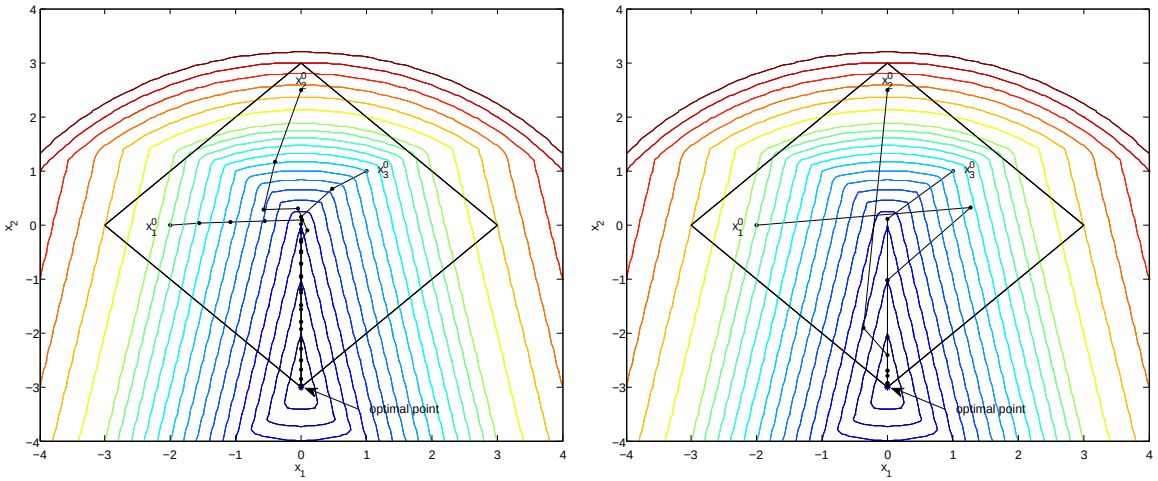
Example 8.3.3 (Multiple solutions).

$$\varphi(x) = \max\{-4x_1 - x_2 - 5, x_1^2 + x_2 + 3\}, \quad x \in \mathbb{R}^2,$$

$$A = \begin{pmatrix} 4 & 1 \\ -\frac{1}{6} & 1 \\ \frac{3}{5} & -1 \end{pmatrix}, \quad b = \begin{pmatrix} -5 \\ -\frac{5}{6} \\ 5 \end{pmatrix},$$

$n = 2$, $p = 3$, $x_1^0 = (-5, -7.8)^T$, $\varphi(x_1^0) = 22.8$, $x_2^0 = (-5, -6.5)^T$, $\varphi(x_2^0) = 21.5$, $x_3^0 = (-5, -1.7)^T$, $\varphi(x_3^0) = 26.3$, $X^* = \{(x_1, x_2) \in \mathbb{R}^2 : x_1 \in [2-\sqrt{6}, 0], x_2 = -4x_1 - 5\}$, $\varphi^* = 0$.

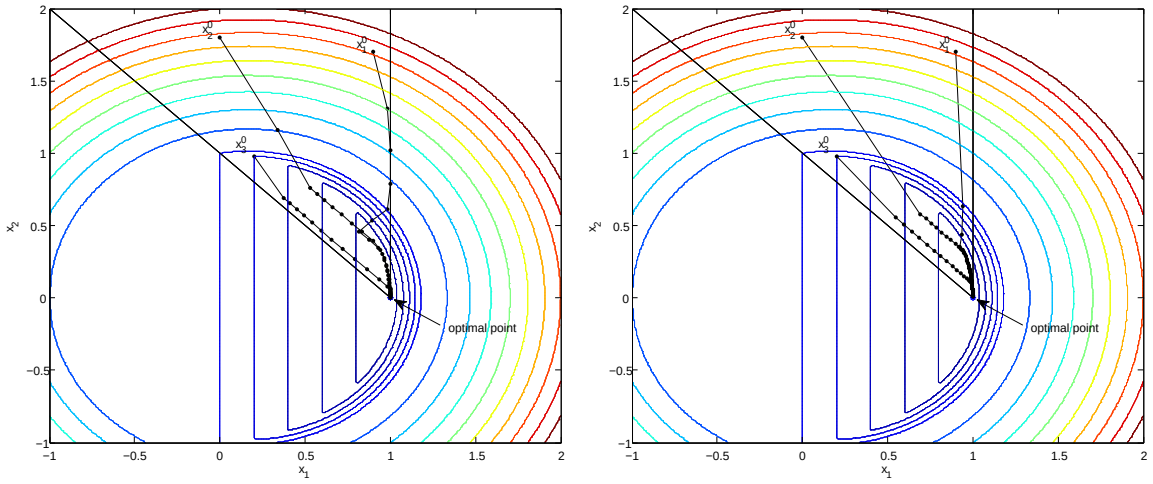
Figures 8.1–8.3 show that both methods succeed to reach an optimal point independently of the chosen initial point (with one exception in Figure 8.3 with the LQPAP method). We like to note that only exemplary paths of the iterates are shown where the sequence of regularization parameters might not be adapted towards best performance.



(a) LQPAP method (b) BrPAP method

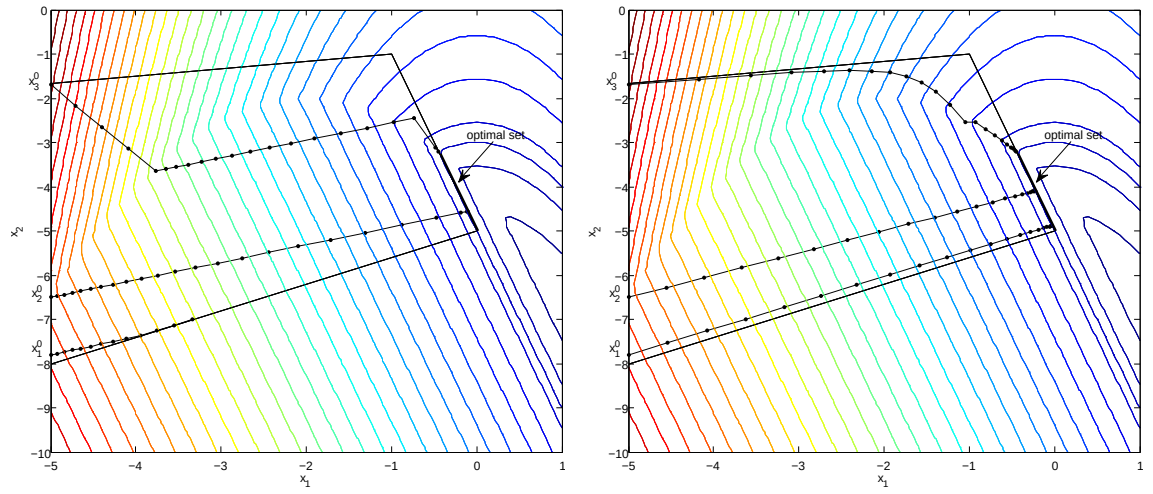
Figure 8.1. Example 8.3.1: Exemplary paths of the iterates for different initial points.

We comment on two observations. The first one is about the proximity of the initial point to the boundary. If the initial point lies close to the boundary (like x_1^0 in Figures 8.2 and 8.3) the LQPAP bundle method can fail to keep the iterates away from the



(a) LQPAP method (b) BrPAP method

Figure 8.2. Example 8.3.2: Exemplary paths of the iterates for different initial points.



(a) LQPAP method (b) BrPAP method

Figure 8.3. Example 8.3.3: Exemplary paths of the iterates for different initial points.

boundary. A better behavior can be observed with the BrPAP method. This effect was already discussed in Sections 6.3.1 and 6.4. The second observation concerns nondifferentiability. The different paths of the iterates for initial point x_3^0 in Figure 8.3 are interesting. Whereas the iterates generated by the LQPAP bundle method tend towards the interior of the feasible set and pass the line of nondifferentiability after few iterations, the iterates of the BrPAP bundle method lie close to the boundary and pass this line much later. It is an interesting and open question if the line of nondifferentiability has an influence in this context.

8.3.2 Higher-dimensional examples

Example 8.3.4 (Constrained MaxQuad, [59]).

$$\begin{aligned}
\varphi(x) &= \max\left\{\left\langle A^k x, x\right\rangle - \left\langle b^k, x\right\rangle : k = 1, \dots, 5\right\}, \quad x \in \mathbb{R}^{10},\\
(A^k)_{ij} &= e^{i/j}\cos(ij)\sin(k) = (A^k)_{ji},\\
(A^k)_{ii} &= \frac{i}{10}|\sin(k)| + \sum_{j\neq i}|(A^k)_{ij}|,\\
(b^k)_i &= e^{i/k}\sin(ik),\\
c_j(x) &= -x_j - 0.05, \quad j = 1, \dots, 10,\\
c_{10+j}(x) &= x_j - 0.05, \quad j = 1, \dots, 10,\\
c_{21}(x) &= \sum_{i=1}^{10} x_i - 0.05,
\end{aligned}$$

$n = 10$, $p = 21$, $x^0 = (0, \dots, 0)^T \in \mathbb{R}^{10}$, $\varphi(x^0) = 0$, $\varphi^* = -0.36816644175$.

Example 8.3.5 (Constrained Wong2, [67]).

$$\begin{aligned}
\varphi(x) &= \max\left\{f_k(x) : k = 1, \dots, 6\right\}, \quad x \in \mathbb{R}^{10},\\
f_1(x) &= x_1^2 + x_2^2 + x_1x_2 - 14x_1 - 16x_2 + (x_3 - 10)^2 + 4(x_4 - 5)^2 + (x_5 - 3)^2 +\\
&\quad + 2(x_6 - 1)^2 + 5x_7^2 + 7(x_8 - 11)^2 + 2(x_9 - 10)^2 + (x_{10} - 7)^2 + 45,\\
f_2(x) &= f_1(x) + 10(3x_1 - 2)^2 + 4(x_2 - 3)^2 + 2x_3^2 - 7x_4 - 120),\\
f_3(x) &= f_1(x) + 10(5x_1^2 + 8x_2 + (x_3 - 6)^2 - 2x_4 - 40),\\
f_4(x) &= f_1(x) + 10(0.5(x_1 - 8)^2 + 2(x_2 - 4)^2 + 3x_5^2 - x_6 - 30),\\
f_5(x) &= f_1(x) + 10(x_1^2 + 2(x_2 - 2)^2 - 2x_1x_2 + 14x_5 - 6x_6),\\
f_6(x) &= f_1(x) + 10(-3x_1 + 6x_2 + 12(x_9 - 8)^2 - 7x_{10}),\\
c_1(x) &= 4x_1 + 5x_2 - 3x_7 + 9x_8 - 105,\\
c_2(x) &= 10x_1 - 8x_2 - 17x_7 + 2x_8,\\
c_3(x) &= -8x_1 + 2x_2 + 5x_9 - 2x_{10} - 12,\\
c_j(x) &= x_{j-1} - 100, \ j = 4, \dots, 10,
\end{aligned}$$

$n = 10$, $p = 10$, $x^0 = (2, 3, 5, 5, 1, 2, 7, 3, 6, 10)^T$, $\varphi(x^0) = 753$,
$x^* \approx (2.17, 2.36, 8.77, 5.09, 0.99, 1.43, 1.32, 9.82, 8.27, 8.36)^T$, $\varphi^* \approx 24.306209$.

Example 8.3.6 (Constrained MAD8 $n = 20$, [67]).

$$\begin{aligned}
\varphi(x) &= \max\{f_k(x) : k = 1, \ldots, 2n-2\}, \quad x \in \mathbb{R}^n,\\
f_1(x) &= x_1^2 + x_2 + x_3 + \ldots + x_n - 1,\\
f_2(x) &= x_1 + x_2^2 + x_3 + \ldots + x_n - 1,\\
f_3(x) &= x_1 + 2x_2^2 + x_3 + \ldots + x_n - 1,\\
&\ldots\\
f_k(x) &= x_1 + x_2 + x_3 + \ldots + x_{(k+2)/2}^2 + \ldots + x_n - 1, \ k \ \textit{even}\\
f_{k+1}(x) &= x_1 + x_2 + x_3 + \ldots + 2x_{(k+2)/2}^2 + \ldots + x_n - 1, \ k \ \textit{even}\\
&\ldots\\
f_{2n-2}(x) &= x_1 + x_2 + x_3 + \ldots + x_n^2 - 1,\\
c_j(x) &= -x_j + 0.5, \ j = 1 \ldots, n/2,\\
c_j(x) &= -x_j - 1, \ j = n/2 + 1, \ldots, n,
\end{aligned}$$

$n \in \mathbb{N}$ *even (here* $n = 20$*),* $p = n$, $x^0 = (100, \ldots, 100)^T \in \mathbb{R}^n$, $\varphi(x^0) = 21899$, $x_i^* = 0.5$ $(i = 1, \ldots, n/2)$, $x_i^* = -1$ $(i = n/2 + 1, \ldots, n)$, $\varphi^* = -3$.

Example 8.3.7 (Constrained MAXQ $n = 20$, [56]).

$$\begin{aligned}
\varphi(x) &= \max\{x_i^2 : i = 1, \ldots, n\}, \quad x \in \mathbb{R}^n,\\
c_j(x) &= -x_j + 0.1, \quad j = 1, \ldots, n, \ j \ \textit{even},\\
c_j(x) &= x_j - \frac{n}{2}, \quad j = 1, \ldots, n, \ j \ \textit{odd},\\
c_{n+\frac{j}{2}}(x) &= x_j - 1.1, \quad j = 1, \ldots, n, \ j \ \textit{even},\\
x_i^0 &= 1.0999, \quad i = 1, \ldots, n/2, \ i \ \textit{even},\\
x_i^0 &= i, \quad i = 1, \ldots, n/2, \ i \ \textit{odd},\\
x_i^0 &= 0.1001, \quad i = n/2 + 1, \ldots, n, \ i \ \textit{even},\\
x_i^0 &= -i, \quad i = n/2 + 1, \ldots, n, \ i \ \textit{odd},\\
x_i^* &= 0.1, \quad i = 1, \ldots, n, \ i \ \textit{even},\\
x_i^* &= 0, \quad i = 1, \ldots, n, \ i \ \textit{odd},
\end{aligned}$$

$n \in \mathbb{N}$ *even (here* $n = 20$*),* $p = n + n/2$, $\varphi(x^0) = 361$, $\varphi^* = 0.01$.

Example 8.3.8 (Constrained MXHILB, [56]).

$$\begin{aligned}
\varphi(x) &= \max\left\{\left|\sum_{i=1}^{n}\frac{x_i}{k+i-1}\right| : k=1,\dots,n\right\},\\
c_j(x) &= -x_j + 0.1, \quad j=1,\dots,n,\ j\ \textit{even},\\
c_j(x) &= -x_j, \quad j=1,\dots,n,\ j\ \textit{odd},\\
c_{n+\frac{j}{2}}(x) &= x_j - 1.1, \quad j=1,\dots,n,\ j\ \textit{even},\\
x_i^* &= 0.1,\ i=1,\dots,n,\ i\ \textit{even},\\
x_i^* &= 0,\ i=1,\dots,n,\ i\ \textit{odd},
\end{aligned}$$

$n \in \mathbb{N}$ *(here* $n = 50$*),* $p = n + n/2$*,* $x^0 = (1,\dots,1)^T \in \mathbb{R}^n$*,* $\varphi(x^0) \approx 4.4992053$*,* $\varphi^* \approx 0.1907979$*.*

Example 8.3.9 (Constrained MAD8, $n = 100$**).** *Like Example 8.3.6, but with* $n = 100$*,* $\varphi(x^0) = 29899$*,* $\varphi^* = -23$*.*

Example 8.3.10 (Constrained MAXQ, $n = 100$**).** *Like Example 8.3.7, but with* $n = 100$*,* $\varphi(x^0) = 9801$*,* $\varphi^* = 0.01$*.*

8.3.3 Numerical results for nondifferentiable examples

The following parameter settings were used in the implementation: In the (outer) LQ-PAP/BrPAP bundle method we choose $\gamma_1 = 0.9$, $\theta = 10^{-5}$, and $M = n + 2$ ($M = 2n$ in Example 8.3.5). For the adaptive update of χ_k we use the parameters as in [44], i.e., $\gamma_2 = 0.5$, $\tau_1 = 2$, $\tau_2 = \frac{10}{11}$, $\tau_3 = \frac{2}{3}$. In the (inner) primal-dual method we set $\xi = 10^{-3}$, $\sigma = 0.5$, $\theta_\mu = 10^{-8}$, $\theta_r = 10^{-6}$. The numerical experience shows that it is reasonable to set the maximal number of inner iterations to 100. Additionally, the strategy of under-relaxation (see Section 6.4) is taken into account as a possibility to improve the results.

In the tables we denote

χ_0:	initial value of the regularization parameter,
r:	decreasing factor to update $\chi_{k+1} = \chi_0 r^{k+1}$,
t:	parameter of under-relaxation,
#iter:	number of iterations (i.e., serious steps plus null steps),
#ss:	number of serious steps,
#pdipm:	total number of iterations of the primal-dual interior point method,
#φ:	number of objective function evaluations,
φ_{calc}:	calculated optimal value,
$\lvert\varphi_{calc} - \varphi^*\rvert$:	distance between calculated and known optimal value.

The number of subgradient evaluations is equal to #iter since one subgradient is calculated and added to the bundle in every null or serious step. For the two-dimensional examples the last listed initial point is chosen for the computation.

For a comparison of the methods we measure their efficiency in terms of the accuracies of the calculated optimal values. For Tables 8.1 and 8.2, the values for $\chi_0 \in \{0.01, 0.1, 1, 10, 100\}$, $r \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$, and $t \in \{0.5, 1\}$ were experimentally adapted towards best accuracy. This is possible because for all examples the optimal values are known.

Example		$\{\chi_k\}$		u.relax.	LQPAP bundle method					
No.	Name	χ_0	r	t	#iter	#ss	#pdipm	$\#\varphi$	φ_{calc}	$\lvert\varphi_{calc} - \varphi^*\rvert$
8.3.1	Demyanov	0.01	0.7	1.0	6	4	162	16	-3.00000	1.08e-09
8.3.2	Mifflin	0.01	0.7	1.0	3	3	161	9	-1.00000	1.11e-16
8.3.3	Mult. sol.	0.01	0.3	1.0	4	4	183	12	0.00000	8.88e-16
8.3.4	MaxQuad	10.00	0.9	0.5	26	19	766	71	-0.36816	3.08e-06
8.3.5	Wong2	100.00	0.1	0.5	212	26	9729	450	24.30644	2.26e-04
8.3.6	MAD8	1.00	0.9	0.5	75	49	2716	199	-2.99996	3.54e-05
8.3.7	MAXQ	10.00	0.9	1.0	70	45	2278	185	0.01000	5.89e-13
8.3.8	MXHILB	0.01	0.1	1.0	4	4	115	12	0.19080	2.09e-06
8.3.9	MAD8	0.01	0.5	0.5	30	30	1719	90	-22.99993	7.23e-05
8.3.10	MAXQ	0.10	0.1	0.5	254	50	10249	558	0.01000	4.55e-06

Table 8.1. Results for the LQPAP bundle method applied to nondifferentiable convex problems.

Example		$\{\chi_k\}$		u.relax.	BrPAP bundle method					
No.	Name	χ_0	r	t	#iter	#ss	#pdipm	$\#\varphi$	φ_{calc}	$\lvert\varphi_{calc} - \varphi^*\rvert$
8.3.1	Demyanov	10.00	0.7	1.0	14	13	320	41	-3.00000	5.44e-09
8.3.2	Mifflin	0.01	0.9	1.0	2	2	47	6	-1.00000	1.11e-16
8.3.3	Mult. sol.	0.10	0.1	1.0	2	2	152	6	0.00000	8.88e-16
8.3.4	MaxQuad	1.00	0.9	0.5	26	19	938	71	-0.36809	7.24e-05
8.3.5	Wong2	100.00	0.9	0.5	252	65	7748	569	24.30634	1.34e-04
8.3.6	MAD8	100.00	0.9	1.0	98	57	2855	253	-3.00000	1.02e-06
8.3.7	MAXQ	100.00	0.9	1.0	102	76	2943	280	0.01000	2.12e-06
8.3.8	MXHILB	0.10	0.3	1.0	5	5	365	15	0.19494	4.14e-03
8.3.9	MAD8	100.00	0.9	1.0	158	55	6852	371	-23.00000	1.55e-06
8.3.10	MAXQ	10.00	0.9	1.0	337	67	11529	741	0.01002	2.28e-05

Table 8.2. Results for the BrPAP bundle method applied to nondifferentiable convex problems.

For problems with unknown solution it is of course reasonable to apply the adaptive initialization and update strategies for the sequence $\{\chi_k\}$ together with a robustification via under-relaxation. The performance of the methods when using this setting is presented in Tables 8.3 and 8.4.

Example		$\{\chi_k\}$	u.relax.	LQPAP bundle method					
No.	Name		t	#iter	#ss	#pdipm	#φ	φ_{calc}	$\lvert\varphi_{calc} - \varphi^*\rvert$
8.3.1	Demyanov	adap.	0.5	44	36	1143	124	-3.00000	3.35e-06
8.3.2	Mifflin	adap.	0.5	48	33	2104	129	-0.99998	1.94e-05
8.3.3	Mult. sol.	adap.	0.5	34	34	869	102	0.00000	3.91e-06
8.3.4	MaxQuad	adap.	0.5	26	19	877	71	-0.36816	7.43e-06
8.3.5	Wong2	adap.	0.5	101	68	2916	270	142.53131	1.18e+02
8.3.6	MAD8	adap.	0.5	129	104	4179	362	-2.99991	8.54e-05
8.3.7	MAXQ	adap.	0.5	125	96	4113	346	0.01001	5.01e-06
8.3.8	MXHILB	adap.	0.5	32	32	1090	96	0.19473	3.94e-03
8.3.9	MAD8	adap.	0.5	241	141	5858	623	-22.96178	3.82e-02
8.3.10	MAXQ	adap.	0.5	972	645	24520	2589	0.01000	4.33e-06

Table 8.3. Results for the LQPAP bundle method when using adaptive initialization and update of χ_k.

Example		$\{\chi_k\}$	u.relax.	BrPAP bundle method					
No.	Name		t	#iter	#ss	#pdipm	#φ	φ_{calc}	$\lvert\varphi_{calc} - \varphi^*\rvert$
8.3.1	Demyanov	adap.	0.5	36	28	870	100	-2.99999	6.42e-06
8.3.2	Mifflin	adap.	0.5	48	44	1045	140	-0.99999	8.96e-06
8.3.3	Mult. sol.	adap.	0.5	34	34	842	102	0.00000	2.68e-06
8.3.4	MaxQuad	adap.	0.5	44	39	1129	127	-0.36813	3.37e-05
8.3.5	Wong2	adap.	0.5	566	310	14457	1442	24.30652	3.11e-04
8.3.6	MAD8	adap.	0.5	196	171	6277	563	-2.99999	5.57e-06
8.3.7	MAXQ	adap.	0.5	53	44	1315	150	1.20978	1.20e+00
8.3.8	MXHILB	adap.	0.5	47	47	1473	141	0.19290	2.10e-03
8.3.9	MAD8	adap.	0.5	278	165	8574	721	-23.00000	4.11e-06
8.3.10	MAXQ	adap.	0.5	467	309	12125	1243	1.20978	1.20e+00

Table 8.4. Results for the BrPAP method when using adaptive initialization and update of χ_k.

Before we summarize the results we like to note that (like in the previous numerical tests) the practical efficiency of both methods strongly depends on an appropriate management of the regularization parameter, especially in examples of higher-dimension. The results of our experiments with different choices of χ_0 and r are very inhomogeneous and often only few parameter settings lead to satisfactory results. Again, the reason is that the iterates approach the boundary too quickly. As in Section 6.4, under-relaxation can improve the situation.

Now, we compare the reached accuracies in Tables 8.1 and 8.2. For each example, the LQPAP and the BrPAP bundle method compute similarly accurate solutions, but there is a tendency towards slightly better results with the LQPAP bundle method (see Examples 8.3.7, 8.3.8). The range of accuracy is mostly 10^{-5} or better with exceptions in Example 8.3.5 (LQPAP) and Examples 8.3.5, 8.3.8 (BrPAP). In examples, where both methods reach the same range of accuracy, a significant difference in the number of needed iterations cannot be observed.

The adaptive initialization and update strategy for χ_k proves to work well in most examples. A failure (with an accuracy of less than 10^{-2}) occurs in Examples 8.3.5, 8.3.9 with the LQPAP bundle method and in Examples 8.3.7, 8.3.10 with the BrPAP bundle method. The other examples can be solved with an accuracy of at least 10^{-3}, but which is mostly lower than with a best choice of the parameters.

8.4 Summary

In this chapter we considered linearly constrained variational inequalities $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ with $\mathcal{F} = \nabla\psi$ and $\mathcal{Q} = \partial\varphi$, where ψ is a convex, differentiable function and φ is a convex, nondifferentiable function. For the solution of the corresponding LQPAP auxiliary problems we developed the LQPAP bundle method, which exploits the possibility to approximate $\partial\varphi$ by $\partial_\epsilon\varphi$ by working with piecewise linear, lower approximations of the nonsmooth function φ. Well-definedness and convergence of this method was proved under certain error conditions. Details for the numerical realization were presented for the case $\psi = 0$, especially a primal-dual interior point method for the solution of the bundle auxiliary problems was described and concrete proposals for the choice of certain parameters were given. The method was tested with different nonsmooth academic test examples and compared to the BrPAP bundle method. A significant difference between both methods could not be observed in the numerical performance. In most examples, the methods succeeded to compute an optimal value with an accuracy of at least 10^{-5}. Also the described adaptive update strategies for the parameters proved to work well. Nevertheless, the effectiveness of both methods highly depends on a suitable choice of the regularization parameter. As in Chapter 6, under-relaxation can improve the results of the LQPAP method.

9. Summary and Outlook

This thesis contributes to theoretical as well as numerical investigations of solution methods for monotone variational inequalities (VIs). A structured analysis of existing regularization methods provides the basis for the development of a new solution method – the logarithmic-quadratic proximal auxiliary problem method (LQPAP method).

Our theoretical analysis of the LQPAP method leads to a convergence proof under common assumptions. The logarithmic-quadratic distance establishes an interior point effect that simplifies the structure of the LQPAP auxiliary problems because they can be considered as unconstrained ones. Thus, this function not only has a regularization but also a penalization effect. By combining the proximal point algorithm (PPA) with the auxiliary problem principle (APP), the advantages of both methods can be exploited. The APP offers the possibility to solve nonsymmetric VIs by a sequence of optimization problems, while the PPA requires weaker monotonicity assumptions on the given operator. With respect to the numerical practicability, inexact solutions of the auxiliary problems are allowed using a summable-error criterion that is easy to implement. Furthermore, outer operator approximations based on the ϵ-enlargement are considered. This simplifies the numerical solution of VIs with multi-valued operators since, for example, bundle-techniques can be applied. Our verification that the logarithmic-quadratic distance is self-concordant motivates to apply the Newton method for the solution of the auxiliary problems.

The auxiliary operator $\mathcal{L}^k$, originally introduced to unify the convergence analysis of descent and decomposition algorithms, can be easily included into the LQPAP scheme under a co-coercivity condition on $\mathcal{F} - \mathcal{L}^k$. From a numerical point of view, however, it is difficult to find auxiliary operators which ensure this condition. For the special case of an affine operator $\mathcal{F}$ with a diagonally dominant matrix, a suitable proposition is given. For other standard choices of the auxiliary operator there proves to be no particular benefit in our context.

The LQPAP method is applied to linearly constrained, differentiable and nondifferentiable convex optimization problems, as well as to nonsymmetric VIs. Doing so, we encounter a discrepancy between the theoretical freedom in the choice of the sequence of regularization parameters and the numerical behavior of the method. Our general ob-

servation is that the performance of the LQPAP method as well as the BrPAP method highly depends on an suitable choice of the sequence of regularization parameters. Tests with different sequences of regularization parameters show that there can be choices which are not able to prevent the iterates from tending too early towards the boundary of the feasible set, so that a further progress of the algorithm is difficult or even impossible. A comparison of the Hesse matrices of the logarithmic-quadratic distance and the Bregman distance illustrate their different characteristics when a sequence of iterates approaches the boundary. Against this background, the under-relaxation strategy is presented as a possibility to robustify the LQPAP method. Similar improvements with the BrPAP method cannot be observed.

For differentiable, convex optimization problems it is evaluated that a combination of the Armijo step size rule with the self-concordance step size rule can reduce the number of function evaluations in the Newton method. A further advantage of self-concordance cannot be recognized, since the efficiency of the Newton method is only realized in some few iterations before the algorithm terminates. The adaptive choice of an initial value for the regularization parameter proves to work well.

For nonsymmetric VIs, test problems with known solutions are generated with a geometric and an analytic approach. To this aim, the Lagrange function of a convex optimization problem is build and modified such that the corresponding saddle-point problem includes a co-coercive operator. With appropriate linear transformations we are able to construct problems with known multiple solutions. Such ideas have so far not been presented in literature. For this class of problems as well as for symmetric VIs that are solved by an auxiliary problem principle approach, it turns out that the computed solutions can be quite inaccurate. A reason for this behavior is that in the auxiliary problems the operator $\mathcal{F}$ is fixed at the current iterate, which implies a loss of information. This drawback can hardly be compensated by a careful choice of the regularization parameters, and possible improvements have to be found and analyzed in the future.

The solution of nondifferentiable, convex optimization problems with the LQPAP method succeeds with the help of the bundle-technique. A structured procedure to compute the solutions of the LQPAP auxiliary problems is given, which was so far only done for a Bregman-function based proximal method. The main result in this context is Theorem 8.1.2, which shows that after a finite number of null steps a serious step will follow. Also, adaptive update strategies for the sequence of regularization parameters are taken into account and prove to work in most cases.

The numerical comparison of the LQPAP and the BrPAP method is based on the solution of several test problems. It turns out that none of the methods is superior to the other.

As an outlook we point out some directions for further investigation.

For the solution of the LQPAP auxiliary problems we proposed and established certain methods (Newton method, resp. bundle method in combination with a primal-dual interior point method). It is not clear if other solution methods are more suitable, e.g., to cope with iterates lying close to the boundary. In view of the presented adaptive strategies for the regularization parameters and the introduced under-relaxation strategy, it would be of interest to extend these ideas to develop a more sophisticated control of the regularization parameters.

For the special case of $K = \mathbb{R}^n_+$ the ideas in Auslender/Teboulle [4] and Hübner [44] could be used to solve the LQPAP bundle auxiliary problems with a dual approach. This can exploit the advantage that the Fenchel conjugate of the logarithmic-quadratic distance function can explicitly be calculated.

A further interesting investigation would be the usage of a relative error criterion as introduced in Burachik/Svaiter [13] for generalized proximal point methods. It is also an open task to analyze the convergence rate of the LQPAP method (e.g., similar to Auslender/Teboulle/Ben-Tiba [5]). Additionally, it would be interesting to include the ideas of Burachik/Lopes/da Silva [10] who recently proposed an infeasible logarithmic-quadratic function based proximal method allowing that $\text{int}(K) = \emptyset$ by introducing a perturbation of K.

A. Appendix

The Appendix contains additional information to some sections of the thesis. We recall basic definitions for (convex) functions and some properties of multi-valued operators. Further, basic properties of logarithmic-quadratic distance functions are proved. Also some auxiliary results about the convergence of sequences of numbers are given. The largest part of the Appendix consists of supplementaries to the test examples of Chapters 6 and 7 and to the numerical experiments mentioned in Chapter 6. Especially, detailed explanations about the setup of the experiments will be given as well as all tables and graphics on which our summarizing remarks in Chapter 6 are based on.

A.1 Elements of convex analysis

An important example of a maximal monotone operator is the subdifferential of a convex function. For that reason, basic definitions and some concepts of convexity are recalled.

Let $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a function. The effective domain of φ is the set

$$\mathrm{dom}(\varphi) = \{x \in \mathbb{R}^n : \varphi(x) < +\infty\}.$$

The function φ is said to be proper if its effective domain is nonempty. We say that φ is lower semicontinuous at some $x \in \mathbb{R}^n$ if for any sequence $\{x^k\} \to x$ it holds that

$$\liminf_{k\to\infty} \varphi(x^k) \geq \varphi(x).$$

The function φ is called upper semicontinuous at $x \in \mathbb{R}^n$ if $-\varphi$ is lower semicontinuous at x.

Definition A.1.1 (Notions of convexity). *Let $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a function and $K \subset \mathbb{R}^n$ a convex set.*

(a) φ is convex on K if for all $x, y \in K$ and $\lambda \in [0, 1]$ it holds

$$\varphi(\lambda x + (1-\lambda)y) \leq \lambda\varphi(x) + (1-\lambda)\varphi(y).$$

(b) φ *is strictly convex on* K *if for all* $x, y \in K$, $x \neq y$, *and* $\lambda \in (0,1)$ *it holds*

$$\varphi(\lambda x + (1-\lambda)y) < \lambda\varphi(x) + (1-\lambda)\varphi(y).$$

(c) φ *is strongly convex with modulus* $\kappa > 0$ *on* K, *if for all* $x, y \in K$, $\lambda \in [0,1]$ *it holds*

$$\varphi(\lambda x + (1-\lambda)y) \leq \lambda\varphi(x) + (1-\lambda)\varphi(y) - \frac{\kappa}{2}\lambda(1-\lambda) \parallel x - y \parallel^2 .$$

(d) φ *is called (strictly, strongly) concave if* $-\varphi$ *is (strictly, strongly) convex.*

A convex function φ is continuous on $\mathrm{int}(\mathrm{dom}(\varphi))$ but not necessarily differentiable. Convex functions are subdifferentiable in the following sense:

Definition A.1.2 (subdifferential, ϵ-subdifferential).

For a proper, convex function $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ *the subdifferential at* $x \in \mathrm{dom}(\varphi)$ *is defined as*

$$\partial\varphi(x) = \{s \in \mathbb{R}^n : \varphi(y) - \varphi(x) - \langle s, y - x\rangle \geq 0 \quad \forall y \in \mathbb{R}^n\}.$$

For a proper, convex function $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ *and* $\epsilon \geq 0$ *the* ϵ*-subdifferential at* $x \in \mathrm{dom}(\varphi)$ *is defined as*

$$\partial_\epsilon\varphi(x) = \{s \in \mathbb{R}^n : \varphi(y) - \varphi(x) - \langle s, y - x\rangle \geq -\epsilon \quad \forall y \in \mathbb{R}^n\}.$$

Lemma A.1.3 ([41], Remark 4.1.7, [80], Section 23, Theorem 25.1). *Let* $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ *be a proper, convex function and* $x \in \mathrm{dom}(\varphi)$. *Then the following statements hold:*

(a) $\mathrm{dom}(\varphi) \supset \mathrm{dom}(\partial\varphi) \supset \mathrm{int}(\mathrm{dom}(\varphi))$.

(b) $\partial\varphi(x) = \partial_0\varphi(x)$ *and* $\partial_{\epsilon_1}\varphi(x) \subseteq \partial_{\epsilon_2}\varphi(x)$ *for* $0 \leq \epsilon_1 \leq \epsilon_2$.

(c) The set $\partial\varphi(x)$ *is closed and convex.*

(d) The set $\partial\varphi(x)$ *is compact if and only if* $x \in \mathrm{int}(\mathrm{dom}(\varphi))$.

(e) $\partial\varphi(x) = \{\nabla\varphi(x)\}$ *if* φ *is finite and differentiable at* x.

(f) Let $\varphi_1, \ldots, \varphi_m$ *be proper, convex functions on* $\mathbb{R}^n$. *Then,*

$$\sum_{i=1}^{m} \partial\varphi_i(x) \subset \partial\left(\sum_{i=1}^{m} \varphi_i\right)(x).$$

Equality holds if, e.g., $\bigcap_{i=1}^{m} ri(\mathrm{dom}(\varphi_i)) \neq \emptyset$.

A.2 Properties of multi-valued (maximal monotone) operators

A multi-valued (also called set-valued) operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ maps a point $x \in \mathbb{R}^n$ to a set $\mathcal{T}(x) \subset \mathbb{R}^n$. Some continuity and boundedness properties of a multi-valued operator are defined as follows:

Definition A.2.1 ([33], Definition 2.1.16, and [9]). *An operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is said to be*

(a) closed at a point $x \in \mathrm{dom}(\mathcal{T})$ if the situation $\{x^k\} \to x$, $\{y^k\} \to y$, $y^k \in \mathcal{T}(x^k)$ for all k, implies $y \in \mathcal{T}(x)$.

(b) lower semicontinuous at a point $x \in \mathrm{dom}(\mathcal{T})$ if for every open set $\mathcal{U}$ such that $\mathcal{T}(x) \cap \mathcal{U} \neq \emptyset$ there exists an open neighborhood $\mathcal{N}$ of x such that $\mathcal{T}(y) \cap \mathcal{U} \neq \emptyset$ for each $y \in \mathcal{N}$.

(c) upper semicontinuous at a point $x \in \mathrm{dom}(\mathcal{T})$ if for every open set $\mathcal{V}$ containing $\mathcal{T}(x)$ there exists an open neighborhood $\mathcal{N}$ of x such that $\mathcal{T}(y) \subset \mathcal{V}$ for each $y \in \mathcal{N}$.

(d) continuous at a point $x \in \mathrm{dom}(\mathcal{T})$ if $\mathcal{T}$ is both lower and upper semicontinuous at x.

(e) locally bounded at a point $x \in \mathrm{dom}(\mathcal{T})$ if there exists an open neighborhood $\mathcal{N}$ of x such that the set $\bigcup_{y \in \mathcal{N} \cap \mathrm{dom}(\mathcal{T})} \mathcal{T}(y)$ is bounded.

(f) bounded on bounded sets if for all bounded set $Q \subset \mathbb{R}^n$ with $cl(Q) \subset \mathrm{int}(\mathrm{dom}(\mathcal{T}))$ it holds that $\bigcup_{y \in Q} T(y)$ is bounded.

(g) locally hemi-bounded at a point $\bar{y} \in \mathrm{dom}(\mathcal{T})$ if for each $y \in \mathrm{dom}(\mathcal{T})$, $y \neq \bar{y}$ there exists a number $\bar{t}(\bar{y}, y) > 0$ such that $\bar{y} + t(y - \bar{y}) \in \mathrm{dom}(\mathcal{T})$ holds for $0 \leq t \leq \bar{t}(\bar{y}, y)$ and the set

$$\bigcup_{0 < t \leq \bar{t}(\bar{y}, y)} \mathcal{T}(\bar{y} + t(y - \bar{y})) \text{ is bounded.}$$

Some statements on the above properties are:

Lemma A.2.2 ([33], [9]). *Let $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ and $x \in \mathrm{dom}(\mathcal{T})$.*

(a) If $\mathcal{T}$ is closed at x then $\mathcal{T}(x)$ is a closed set. Conversely, if $\mathcal{T}(x)$ is a closed set and $\mathcal{T}$ is upper semicontinuous at x then $\mathcal{T}$ is closed at x.

(b) $\mathcal{T}$ is closed at every $x \in \mathbb{R}^n$ if and only if $\mathrm{gph}(\mathcal{T})$ is a closed set.

(c) If $\mathcal{T}$ is lower semicontinuous at x then $x \in \operatorname{int}(\operatorname{dom}(\mathcal{T}))$.

(d) If $\mathcal{T}$ is upper semicontinuous at x then for every $\epsilon > 0$ there exists an open neighborhood $\mathcal{N}$ of x such that $\mathcal{T}(y) \subseteq \mathcal{T}(x) + B_\epsilon(0)$ for all $y \in \mathcal{N}$ (where $B_\epsilon(0) = \{x \in \mathbb{R}^n : \| x \| < \epsilon\}$).

(e) If $\mathcal{T}$ is locally bounded then it is also bounded on bounded sets.

The next statements hold for maximal monotone, multi-valued operators.

Lemma A.2.3 ([91], p. 852). *An operator $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is maximal monotone, if $\mathcal{T}$ is monotone and it follows from $(x, u) \in \mathbb{R}^n \times \mathbb{R}^n$ and $\langle u - v, x - y \rangle \geq 0$ for all $(y, v) \in \operatorname{gph}(\mathcal{T})$, that $(x, u) \in \operatorname{gph}(\mathcal{T})$. In other words, for a maximal monotone operator $\mathcal{T}$ it holds*

$$\mathcal{T}(x) = \{u \in \mathbb{R}^n : \langle u - v, x - y \rangle \geq 0 \quad \forall (y, v) \in \operatorname{gph}(\mathcal{T})\}.$$

Theorem A.2.4 ([79], Theorem 1). *If $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$ is maximal monotone then $\mathcal{T}$ is locally bounded at each $x \in \operatorname{int}(\operatorname{dom}(\mathcal{T}))$, whereas $\mathcal{T}$ is not locally bounded at any boundary point of* $\operatorname{dom}(\mathcal{T})$.

Theorem A.2.5 ([34], Theorem 12.3.3). *Let $\mathcal{T} : \mathbb{R}^n \to 2^{\mathbb{R}^n}$. The following statements are equivalent.*

(a) $\mathcal{T}$ is maximal monotone.

(b) $\mathcal{T}$ is monotone and $\operatorname{rge}(I + \mathcal{T}) = \mathbb{R}^n$.

(c) For each $\lambda > 0$ the resolvent operator $(I + \lambda\mathcal{T})^{-1}$ is nonexpansive and further $\operatorname{dom}((I + \lambda\mathcal{T})^{-1}) = \mathbb{R}^n$.

A.3 Basic properties of logarithmic quadratic distance functions

Lemma A.3.1. *Consider for parameters $\nu > \mu > 0$ the logarithmic-quadratic distance function*

$$d_{LQ}^{\nu,\mu} : \mathbb{R}^p \times \mathbb{R}^p_{++} \to \mathbb{R} \cup \{+\infty\},$$
$$d_{LQ}^{\nu,\mu}(u, v) := \begin{cases} \sum_{i=1}^p \frac{\nu}{2}(u_i - v_i)^2 + \mu\left(v_i^2 \log \frac{v_i}{u_i} + u_i v_i - v_i^2\right) & \text{if } u \in \mathbb{R}^p_{++} \\ +\infty & \text{otherwise.} \end{cases} \tag{A.1}$$

Then, for every $v \in \mathbb{R}^p_{++}$, function $d^{\nu,\mu}_{LQ}(\cdot, v)$ is a nonnegative, proper, lower semicontinuous, convex function with $dom(d^{\nu,\mu}_{LQ}(\cdot, v)) = \mathbb{R}^p_{++}$, and it holds $d^{\nu,\mu}_{LQ}(u, v) = 0$ if and only if $u = v$.

Proof. Nonnegative: For every $i = 1, \ldots, p$ and $u, v \in \mathbb{R}^p_{++}$ it is clear that $\frac{\nu}{2}(u_i - v_i)^2 \geq 0$. Since $\mu > 0$, it remains to show that $\left(v_i^2 \log \frac{v_i}{u_i} + u_i v_i - v_i^2\right)$ is nonnegative. The last term is equivalent to

$$v_i^2 \left(\frac{u_i}{v_i} - \log \frac{u_i}{v_i} - 1\right).$$

Substituting $t := \frac{u_i}{v_i}$, it suffices to show that

$$t - \log(t) - 1$$

is nonnegative for $t > 0$. In view of the analytical properties of the logarithm function, this is directly clear since $\log(t) \leq t - 1$ for all $t > 0$.
Proper: For all $u, v \in \mathbb{R}^p_{++}$ one has $d^{\nu,\mu}_{LQ}(u, v) < +\infty$. Thus, $\{u \in \mathbb{R}^p : d^{\nu,\mu}_{LQ}(u, v) < +\infty\} \neq \emptyset$ for all fixed $v \in \mathbb{R}^p_{++}$. Clearly, $\mathrm{dom}(d^{\nu,\mu}_{LQ}(\cdot, v)) = \mathbb{R}^p_{++}$.
Lower semicontinuous: Function $d^{\nu,\mu}_{LQ}(\cdot, v)$ is obviously continuous at every $u \in \mathbb{R}^p_{++}$. Further, $d^{\nu,\mu}_{LQ}(\cdot, v)$ has constant value $+\infty$ for every $u \notin \mathbb{R}^p_+$. Now, let $u \in \mathrm{bd}(\mathbb{R}^p_+)$ and $\{u^k\}$ be a sequence in $\mathbb{R}^p$ converging to u. Then there exists $j \in \{1, \ldots, p\}$ with $u_j = 0$. Thus, in view of the logarithm term in $d^{\nu,\mu}_{LQ}(u^k, v)$, the summand for $i = j$ tends to infinity for $k \to \infty$. Hence,

$$\liminf_{u^k \to u} d^{\nu,\mu}_{LQ}(u^k, v) = +\infty \geq +\infty = d^{\nu,\mu}_{LQ}(u, v).$$

Convex: Fix $v \in \mathbb{R}^p_{++}$. It suffices to show that $d^{\nu,\mu}_{LQ}(\cdot, v)$ is convex on $\mathbb{R}^p_{++}$. For every $u \in \mathbb{R}^p_{++}$ the quadratic term in $d^{\nu,\mu}_{LQ}(u, v)$ is obviously convex. For the second term one has

$$\underbrace{\mu}_{>0} \left(\underbrace{v_i^2}_{\text{const}} \underbrace{(\log(v_i)}_{\text{const}} \underbrace{- \log(u_i))}_{\text{convex}} + \underbrace{u_i v_i}_{\text{linear}} \underbrace{- v_i^2}_{\text{const}} \right),$$

which shows that it is convex.
Distance property: It is clear that $u = v$ implies $d^{\nu,\mu}_{LQ}(u, v) = 0$. On the other hand, if $d^{\nu,\mu}_{LQ}(u, v) = 0$ then every summand has to be zero because all summands are nonnegative. Hence, the quadratic term implies that $u_i = v_i$ for all $i = 1, \ldots, p$. □

A.4 Convergence of sequences of numbers and elementary calculus

An auxiliary result from elementary calculus used in Chapter 3 is

Lemma A.4.1. *The following inequalities are valid:*

$$\langle x, y\rangle \leq \frac{1}{2\xi} \parallel x \parallel^2 + \frac{\xi}{2} \parallel y \parallel^2 \quad \forall x, y \in \mathbb{R}^n,\ \xi > 0. \tag{A.2}$$

$$1 \leq (1-r)^{-1} \leq 1 + 2r \leq 2 \quad \forall 0 \leq r \leq \frac{1}{2}. \tag{A.3}$$

Proof. (A.2) is a consequence of Fenchel's inequality for the function $f(y) = \frac{\xi}{2} \parallel y \parallel^2$ and its conjugate function $f^*(x) = \frac{1}{2\xi} \parallel x \parallel^2$. (A.3) is simple calculus.

Polyak's statement about the convergence of sequences of numbers is applied in Theorem 3.4.3. It reads as follows.

Lemma A.4.2 ([76], Lemma 2.2.2). *Let $\{v_k\}$ be a nonnegative sequence of numbers satisfying*

$$v_{k+1} \leq (1 + \alpha_k)v_k + \beta_k,$$

with $\alpha_k \geq 0,\ \beta_k \geq 0,\ \sum_{k=1}^{\infty} \alpha_k < \infty,\ \sum_{k=1}^{\infty} \beta_k < \infty$. Then $\{v_k\}$ is convergent.

An extension of the above result is

Lemma A.4.3 ([61], Lemma 7). *Assume that $\{a^k\}$, $\{b^k\}$, $\{c^k\}$, $\{d^k\}$ are sequences of nonnegative numbers. If the relation*

$$a^{k+1} \leq (1 + b^k)a^k + c^k - d^k$$

is valid and $\sum_{k=0}^{\infty} \max\{b^k, c^k\} < \infty$, then the sequence $\{a^k\}$ is convergent and further $\sum_{k=0}^{\infty} d^k < \infty$ also holds true.

In Theorem 8.1.2 we apply the following lemma which is based on Lemma A.4.3.

The notation $r^+ := \max\{r, 0\}$ and $r^- := \min\{r, 0\}$ is used to denote the positive respectively negative part of some $r \in \mathbb{R}$. Then $r^+ \geq 0$, $r^- \leq 0$, and $r = r^+ + r^-$.

Lemma A.4.4. *Given are the sequences* $\{a_n\}, \{b_n\}, \{c_n\} \in \mathbb{R}^{\mathbb{N}}$ *and a constant* $\bar{a} \in \mathbb{R}$. *Suppose that for all* $n \in \mathbb{N}$ *the following relation holds*

$$\bar{a} \geq a_{n+1} + c_n \geq a_n + b_n + c_n. \tag{A.4}$$

Then, under the conditions

$$\lim_{n\to\infty} c_n = 0 \quad \textit{and} \quad \sum_{n=1}^{\infty} -b_n^- < +\infty,$$

the sequence $\{a_n\}$ *is convergent.*

Proof. In view of the second inequality in (A.4) one has $-(a_{n+1}+c_n) \leq -(a_n+b_n+c_n)$ and thus

$$\bar{a} - (a_{n+1} + c_n) \leq \bar{a} - (a_n + b_n + c_n).$$

With $u_n := \bar{a} - a_n$ this can be transformed to

$$u_{n+1} - c_n \leq u_n - b_n - c_n.$$

It is also obvious that

$$0 \leq \bar{a} - a_{n+1} - c_n = u_{n+1} - c_n.$$

Consequently,

$$c_n^+ + c_n^- = c_n \leq u_{n+1} \leq u_n - b_n$$

and therefore

$$c_n^- \leq c_n^+ + c_n^- \leq u_{n+1} \leq u_n - (b_n^+ + b_n^-).$$

Since $\lim_{n\to\infty} c_n = 0$, also $\lim_{n\to\infty} c_n^- = 0$. Thus, $\{c_n^-\}$ is bounded and there exists $\underline{c} \leq 0$ with $c_n^- \geq \underline{c}$ for all n. It follows that

$$0 \leq u_{n+1} - \underline{c} \leq u_n - \underline{c} - b_n^+ - b_n^-.$$

With $g_n := u_n - \underline{c}$ we have

$$0 \leq g_{n+1} \leq g_n - b_n^+ - b_n^-.$$

Now, the convergence of the sequence $\{g_n\}$ follows with Lemma A.4.3. This is equivalent to the convergence of $\{a_n\}$. □

Remark A.4.5. *(a) A further consequence of the situation in Lemma A.4.4 is that* $\sum_{n=0}^{\infty} b_n^+ < +\infty$, *which implies that* $\sum_{n=0}^{\infty} |b_n| = \sum_{n=0}^{\infty} b_n^+ + b_n^- < +\infty$. *Thus, the assumption on the sequence* $\{b_n\}$ *in Lemma A.4.4 is stronger than requiring that* $\sum_{n=0}^{\infty} b_n$ *exists and is finite.*

(b) Instead of requiring $\lim_{n\to\infty} c_n = 0$ *one could use the weaker assumption that there exists* $\underline{c} \leq 0$ *with* $c_n^- \geq \underline{c}$ *for all* n.

A.5 Data of high-dimensional test examples in Chapter 6

This section contains additional information to the high-dimensional test examples which are mentioned in Chapter 6.

A.5.1 Data for Example 6.2.3

$$\psi(x) = \left\langle D^T D x, x \right\rangle - 2 \left\langle Dx, d \right\rangle + \| d \|^2,$$

$$D = \begin{pmatrix} -74 & 80 & 18 & -11 & -4 \\ 14 & -69 & 21 & 28 & 0 \\ 66 & -72 & -5 & 7 & 1 \\ -12 & 66 & -30 & -23 & 3 \\ 3 & 8 & -7 & -4 & 1 \\ 4 & -12 & 4 & 4 & 0 \end{pmatrix}, \quad d = \begin{pmatrix} 51 \\ -61 \\ -56 \\ 69 \\ 10 \\ -12 \end{pmatrix},$$

$$A = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -10 & -10 & 3 & -5 & -4 \\ 8 & -1 & 2 & 5 & -3 \\ -8 & 1 & -2 & -5 & 3 \\ 4 & 2 & -3 & 5 & -1 \end{pmatrix}, \quad b = \begin{pmatrix} 5 \\ -20 \\ 40 \\ -1 \\ 30 \end{pmatrix},$$

$n = 5, p = 5, x^0 = (-1.5, 3.5, 0.5, 4.0, -2.0)^T, \psi(x^0) = 182799.25, x^* = (1, 2, -1, 3, -4)^T,$
$\psi^* = 0$, $\mathrm{cond}(D^T D) = 1.1769 \cdot 10^6$.

A.5.2 Data for Example 6.2.4

$$\psi(x) = x^T C x + d^T x + e^T x,$$

$$C = \begin{pmatrix} 30 & -20 & -10 & 32 & -10 \\ -20 & 39 & -6 & -31 & 32 \\ -10 & -6 & 10 & -6 & -10 \\ 32 & -31 & -6 & 39 & -20 \\ -10 & 32 & -10 & -20 & 30 \end{pmatrix}, \quad d = \begin{pmatrix} 4 \\ 8 \\ 10 \\ 6 \\ 2 \end{pmatrix}, \quad e = \begin{pmatrix} -15 \\ -27 \\ -36 \\ -18 \\ -12 \end{pmatrix},$$

$$A = \begin{pmatrix} 16 & -2 & 0 & -1 & 0 \\ 0 & 2 & 0 & -4 & -2 \\ 3.5 & 0 & -2 & 0 & 0 \\ 0 & 2 & 0 & 4 & 1 \\ 0 & 9 & 2 & -1 & 2.8 \\ -2 & 0 & 4 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 2 & 1 \\ -1 & -2 & -3 & -4 & -5 \\ -1 & -1 & -1 & -1 & -1 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \quad b = \begin{pmatrix} 40 \\ 2 \\ 0.25 \\ 4 \\ 4 \\ 1 \\ 40 \\ 60 \\ -5 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

$n = 5$, $p = 15$, $x^0 = (0.1, 0.1, 0.1, 0.1, 1)^T$, $\psi(x^0) = 11.96$,
$x^* \approx (0.3, 0.322547, 0.4, 0.4017501, 0.2495811)^T$, $\psi^* = -23.0448869$, $\lambda_{\min}(C) = 0$.

A.5.3 Data for Example 6.2.5.a

$$\psi(x) = \frac{1}{2}\langle Cx, x\rangle + \langle d, x\rangle, \quad x \in \mathbb{R}^n,$$

$$C = \begin{pmatrix} 440 & 59 & 62 & -60 & -81 & 21 & 22 & 92 & -20 & -19 \\ 59 & 409 & 22 & 21 & 30 & 43 & 41 & 50 & 99 & -40 \\ 62 & 22 & 491 & 65 & -57 & -20 & -23 & 96 & -48 & 90 \\ -60 & 21 & 65 & 418 & -51 & 72 & 46 & -53 & 33 & -8 \\ -81 & 30 & -57 & -51 & 600 & 84 & 77 & -81 & 93 & -42 \\ 21 & 43 & -20 & 72 & 84 & 479 & -89 & -23 & 34 & -83 \\ 22 & 41 & -23 & 46 & 77 & -89 & 364 & 0 & -40 & 16 \\ 92 & 50 & 96 & -53 & -81 & -23 & 0 & 473 & 6 & -69 \\ -20 & 99 & -48 & 33 & 93 & 34 & -40 & 6 & 466 & -85 \\ -19 & -40 & 90 & -8 & -42 & -83 & 16 & -69 & -85 & 459 \end{pmatrix},$$

$$d = (84, 21, 40, 49, -23, -50, -93, -6, 29, -44)^T,$$

$$A = \begin{pmatrix} 4 & 27 & 53 & 38 & 35 & 9 & 10 & -70 & -42 & 40 \\ -51 & 97 & -90 & 76 & 20 & 27 & -67 & -24 & -62 & -21 \\ -40 & -59 & 45 & 85 & -31 & 14 & -1 & 64 & -95 & -83 \\ 30 & 51 & 40 & -84 & -27 & 85 & 7 & -66 & -10 & -57 \\ 78 & 77 & -8 & -3 & -66 & 73 & -60 & -34 & -51 & -50 \\ 72 & -6 & 16 & -74 & 59 & -66 & 25 & 93 & 74 & -55 \\ -58 & -68 & -32 & -49 & -1 & -64 & -95 & 61 & 6 & 41 \\ -20 & 62 & -66 & 77 & -29 & -51 & -36 & -56 & 83 & 51 \\ 78 & -5 & -20 & -61 & 55 & 50 & 7 & 100 & 95 & 9 \\ -49 & -77 & 84 & -76 & -53 & -60 & -35 & -87 & 17 & 11 \\ 93 & 75 & -55 & 9 & 69 & 97 & 20 & -15 & -76 & 26 \\ 24 & 27 & -28 & -37 & 63 & 42 & -28 & -19 & 85 & 97 \\ -67 & -81 & -35 & -24 & 69 & -65 & -73 & -20 & 19 & 27 \\ 65 & 82 & -83 & 58 & -26 & 72 & 83 & -78 & 77 & 20 \\ 31 & -93 & 3 & 68 & -23 & 82 & 28 & -15 & -15 & 82 \\ 9 & -92 & 67 & 36 & 72 & 92 & 32 & 23 & 21 & 14 \\ -50 & 98 & 81 & -17 & -7 & 14 & 35 & 98 & -86 & -33 \\ -92 & 37 & 45 & 29 & 14 & 13 & 49 & -56 & 85 & 91 \\ -53 & -25 & -23 & -57 & 39 & -65 & 68 & -29 & 28 & -12 \\ -28 & 1 & -40 & 23 & 92 & 3 & 3 & -47 & -79 & 20 \end{pmatrix},$$

$$b = (72, 68, 22, 9, 28, 87, 56, 47, 44, 78, 66, 66, 17, 44, 51, 38, 49, 35, 78, 39)^T,$$

$n = 10$, $p = 20$, $x^0 = (0, \ldots, 0)^T$, $\psi(x^0) = 0$, $x^* \approx (-0.24696, -0.07834, -0.06959, -0.17925, -0.05713, 0.22185, 0.34456, 0.11154, -0.01301, 0.13069)^T$, $\psi^* \approx -43.14856$, $\mathrm{cond}(C) = 4.6428$.

A.5.4 Data for Example 6.2.6.a

$$\psi(x) = \frac{1}{2}\langle Cx, x\rangle + \langle d, x\rangle, \quad x \in \mathbb{R}^n,$$

$$C = \begin{pmatrix} 388 & 79 & -20 & 87 & -43 & 29 & -20 & 6 & 60 & -43 \\ 79 & 579 & -75 & 72 & 23 & 99 & 97 & 31 & 75 & 24 \\ -20 & -75 & 536 & 60 & 89 & -49 & -80 & -59 & -25 & -74 \\ 87 & 72 & 60 & 427 & 44 & 14 & 5 & 80 & -16 & 43 \\ -43 & 23 & 89 & 44 & 468 & -26 & 7 & -96 & 55 & -77 \\ 29 & 99 & -49 & 14 & -26 & 365 & -54 & 11 & 4 & -77 \\ -20 & 97 & -80 & 5 & 7 & -54 & 390 & -50 & 37 & -38 \\ 6 & 31 & -59 & 80 & -96 & 11 & -50 & 514 & 82 & -96 \\ 60 & 75 & -25 & -16 & 55 & 4 & 37 & 82 & 454 & 97 \\ -43 & 24 & -74 & 43 & -77 & -77 & -38 & -96 & 97 & 577 \end{pmatrix},$$

$$d = (-27, 94, -19, -14, 10, 21, -93, -6, -15, -50)^T$$

$$A = -I_n,$$

$$b = 0 \in \mathbb{R}^n.$$

$n = 10$, $p = 10$, $x^0 = (10, \ldots, 10)^T$, $\psi(x^0) = 263110$, $x^* \approx (0.10422, 0, 0.11335, 0, 0.00354, 0.02135, 0.29423, 0.07935, 0, 0.14486)^T$, $\psi^* \approx -19.78359$, $\mathrm{cond}(C) = 6.4193$.

A.6 Numerical experiments with differentiable, convex test problems

In this section detailed numerical experiments with the LQPAP and the BrPAP method applied to the test examples of Chapter 6 are presented. They are concerned with the combination of the Armijo- and the self-concordance step size rules, the properties of the Newton decrements, the modeling according to Category 1b, and the adaptive initialization of χ_0. Finally, several graphics demonstrate the influence of under-relaxation on the LQPAP method.

A.6.1 Combination of Armijo- and self-concordance rule reduces number of function evaluations

Table A.1 presents the results for the strategy to use the Armijo rule for the Newton step sizes until $\lambda_j < \lambda^*$ holds for some Newton decrement λ_j, and to switch to the self-concordance rule afterwards.

Example		$\{\chi_k\}$		LQPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.01	0.1	3	33	224	1.00000	0.00e+00
6.2.2	Second 2-dim example	0.01	0.7	5	47	260	0.22874	2.78e-17
6.2.3	Schittkowski no. 268	0.01	0.1	40	83	6	0.00000	2.40e-06
6.2.4	Modified Colville	0.01	0.1	3	49	451	-23.04489	6.81e-07
6.2.5.a	Random $n = 10, p = 20$	0.01	0.3	6	52	167	-43.12260	2.60e-02
6.2.5.b	Random $n = 100, p = 150$	0.01	0.1	5	49	89	-36.98940	3.43e-02
6.2.6.a	Random $n = 10$	0.10	0.5	4	66	671	-19.78359	3.95e-11
6.2.6.b	Random $n = 100$	10.00	0.5	5	203	2363	-19.68023	5.56e-08

Table A.1. Results for the LQPAP method using a switch from Armijo to self-concordance step sizes in the Newton method.

It can be seen that the number of outer (LQPAP) iterations is the same as in Table 6.1 and that the number of inner (Newton) iterations is mostly the same (in Examples 6.2.1, 6.2.2, 6.2.4, 6.2.5.a, 6.2.6.a one has 1-4 iterations less than in Table 6.1). Concerning the number $\#\psi$ of function evaluations the combination of the step size strategies results in less evaluations than the sole use of the Armijo step size rule. This indicates that a switch to the self-concordance step sizes saves possibly expensive function evaluations.

A.6.2 Verification of the properties of the Newton decrement

Let x^0 be the initial iterate and χ_0 be the initial regularization parameter of the LQPAP method. Consider the first auxiliary problem

$$\min_{y \in \mathbb{R}^n} \left\{ \psi(y) + \chi_0 D(y, x^0) \right\}. \tag{A.5}$$

Denote $F(y) = \psi(y) + \chi_0 D(y, x^0)$ and let ϑ_0 be the self-concordance parameter of F. Iteration index j is used to number the Newton iterates. Let λ_j denote the corresponding Newton decrements. The properties of the Newton method with self-concordance step size to solve (A.5) are (see Theorem 4.3.2)

(a) $\{\lambda_j > \lambda'\} \Rightarrow$
$\{F(y^{j+1}) \leq F(y^j) - \frac{4}{\vartheta_0^2}(\lambda_j - \log(1+\lambda_j)) \leq F(y^j) - \frac{4}{\vartheta_0^2}(\lambda' - \log(1+\lambda'))\}$,

(b) $\{\lambda' \geq \lambda_j \geq \lambda_*\} \Rightarrow$
$\left\{\lambda_{j+1} \leq \frac{6\lambda_j - \lambda_j^2 - 1}{4} < \lambda_j\right\}$ and $\left\{1 - \lambda_{j+1} \geq \frac{5-\lambda_j}{4}(1-\lambda_j) \geq \frac{5-\lambda'}{4}(1-\lambda_k)\right\}$,

(c) $\{\lambda_j < \lambda_*\} \Rightarrow$
$\left\{\lambda_{j+1} \leq \left(\frac{\lambda_j}{1-\lambda_j}\right)^2 < \frac{\lambda_j}{2}\right\}$.

For Example 6.2.3, Table A.2 presents a verification of the above relations. To shorten the table we only list the Newton iterations for $j \geq 200$. For the different cases (a)–(c) the values occurring in the corresponding inequalities are given. The last column shows if the relation is true (1) or false (0). Tables A.3 and A.4 correspond to Examples 6.2.6.a and 6.2.6.b, respectively.

In all cases the properties of the Newton method prove to be true.

j	Case	λ_j	$F(y^{j+1})$	$F(y^j)$ $-\frac{4}{\vartheta_k^2}(\lambda_j - \log(1+\lambda_j))$	$F(y^j)$ $-\frac{4}{\vartheta_k^2}(\lambda' - \log(1+\lambda'))$	Relation
200	a)	14.79	780.45	791.69	887.31	1
201	a)	13.853	679.03	689.84	778.35	1
202	a)	12.92	585.13	595.48	676.94	1
203	a)	11.992	498.68	508.55	583.03	1
204	a)	11.069	419.63	429	496.58	1
205	a)	10.152	347.93	356.76	417.54	1
206	a)	9.2417	283.5	291.76	345.84	1
207	a)	8.3394	226.26	233.91	281.41	1
208	a)	7.4464	176.09	183.11	224.16	1
209	a)	6.5648	132.88	139.21	174	1
210	a)	5.697	96.451	102.05	130.78	1
211	a)	4.8463	66.61	71.429	94.354	1
212	a)	4.0174	43.087	47.08	64.514	1
213	a)	3.2167	25.519	28.648	40.99	1
214	a)	2.4538	13.408	15.655	23.422	1
215	a)	1.7434	6.0493	7.4446	11.311	1
216	a)	1.1079	2.4415	3.1073	3.9525	1
j	Case	λ_j	λ_{j+1}	$(6\lambda_j - \lambda_j^2 - 1)/4$	λ_j	Relation
217	b)	0.5823	0.40953	0.53868	0.5823	1
218	b)	0.40953	0.18159	0.32237	0.40953	1
j	Case	λ_j	λ_{j+1}	$\lambda_j/(1-\lambda_j)$	$\lambda_j/2$	Relation
219	c)	0.18159	1.5312e-08	0.049232	0.090796	1

Table A.2. Properties of the Newton decrement for Example 6.2.3, iteration $k = 0$.

j	Case	λ_j	$F(y^{j+1})$	$F(y^j)$ $-\frac{4}{\vartheta_k^2}(\lambda_j - \log(1+\lambda_j))$	$F(y^j)$ $-\frac{4}{\vartheta_k^2}(\lambda' - \log(1+\lambda'))$	Relation
200	a)	31.076	4825.3	4845.6	5119.1	1
201	a)	30.098	4538.7	4558.7	4822.7	1
202	a)	29.12	4261.8	4281.5	4536.1	1
203	a)	28.144	3994.7	4014.1	4259.2	1
204	a)	27.167	3737.3	3756.4	3992.1	1
205	a)	26.191	3489.7	3508.4	3734.7	1
206	a)	25.215	3251.8	3270.2	3487.1	1
207	a)	24.24	3023.6	3041.7	3249.2	1
208	a)	23.265	2805.1	2822.8	3021	1
209	a)	22.291	2596.4	2613.7	2802.6	1
210	a)	21.316	2397.3	2414.3	2593.8	1
211	a)	20.343	2208	2224.5	2394.8	1
212	a)	19.369	2028.3	2044.4	2205.4	1
213	a)	18.395	1858.4	1874	2025.7	1
214	a)	17.422	1698.1	1713.3	1855.8	1
215	a)	16.448	1547.5	1562.2	1695.5	1
216	a)	15.474	1406.5	1420.8	1544.9	1
217	a)	14.499	1275.3	1289	1404	1
218	a)	13.522	1153.7	1166.8	1272.7	1
219	a)	12.545	1041.8	1054.3	1151.2	1
220	a)	11.565	939.65	951.51	1039.3	1
221	a)	10.582	847.16	858.33	937.07	1
222	a)	9.5974	764.36	774.79	844.58	1
223	a)	8.6105	691.26	700.89	761.78	1
224	a)	7.6239	627.8	636.57	688.68	1
225	a)	6.6414	573.89	581.72	625.22	1
226	a)	5.669	529.36	536.18	571.31	1
227	a)	4.7141	493.92	499.65	526.78	1
228	a)	3.7857	467.16	471.72	491.34	1
229	a)	2.8964	448.44	451.79	464.57	1
230	a)	2.065	436.85	438.99	445.86	1
231	a)	1.3205	430.99	432.06	434.27	1
j	Case	λ_j	λ_{j+1}	$(6\lambda_j - \lambda_j^2 - 1)/4$	λ_j	Relation
232	b)	0.70487	0.56992	0.68309	0.70487	1
233	b)	0.56992	0.3855	0.52368	0.56992	1
234	b)	0.3855	0.14334	0.29109	0.3855	1
j	Case	λ_j	λ_{j+1}	$\lambda_j/(1-\lambda_j)$	$\lambda_j/2$	Relation
235	c)	0.14334	0.0017828	0.027996	0.071669	1
236	c)	0.0017828	3.7493e-07	3.1899e-06	0.00089142	1

Table A.3. Properties of the Newton decrement for Example 6.2.6.a, iteration $k = 0$.

j	Case	λ_j	$F(y^{j+1})$	$F(y^j)$ $-\frac{4}{\vartheta_k^2}(\lambda_j - \log(1+\lambda_j))$	$F(y^j)$ $-\frac{4}{\vartheta_k^2}(\lambda' - \log(1+\lambda'))$	Relation
200	a)	18.213	4.8662e+05	4.8817e+05	5.0317e+05	1
201	a)	17.166	4.7084e+05	4.7235e+05	4.8636e+05	1
202	a)	16.119	4.5611e+05	4.5756e+05	4.7058e+05	1
203	a)	15.071	4.4242e+05	4.4382e+05	4.5585e+05	1
204	a)	14.025	4.2977e+05	4.311e+05	4.4216e+05	1
205	a)	12.981	4.1815e+05	4.1942e+05	4.2951e+05	1
206	a)	11.939	4.0756e+05	4.0877e+05	4.1789e+05	1
207	a)	10.902	3.98e+05	3.9913e+05	4.073e+05	1
208	a)	9.8712	3.8945e+05	3.9051e+05	3.9774e+05	1
209	a)	8.8489	3.819e+05	3.8289e+05	3.8919e+05	1
210	a)	7.838	3.7535e+05	3.7625e+05	3.8165e+05	1
211	a)	6.8421	3.6976e+05	3.7057e+05	3.7509e+05	1
212	a)	5.8659	3.6512e+05	3.6583e+05	3.6951e+05	1
213	a)	4.9152	3.6139e+05	3.6198e+05	3.6486e+05	1
214	a)	3.9976	3.5851e+05	3.59e+05	3.6113e+05	1
215	a)	3.1232	3.5644e+05	3.5681e+05	3.5825e+05	1
216	a)	2.3053	3.5508e+05	3.5533e+05	3.5618e+05	1
217	a)	1.5633	3.5431e+05	3.5445e+05	3.5482e+05	1
218	a)	0.92492	3.5398e+05	3.5404e+05	3.5405e+05	1
j	Case	λ_j	λ_{j+1}	$(6\lambda_j - \lambda_j^2 - 1)/4$	λ_j	Relation
219	b)	0.43033	0.20548	0.34919	0.43033	1
j	Case	λ_j	λ_{j+1}	$\lambda_j/(1-\lambda_j)$	$\lambda_j/2$	Relation
220	c)	0.20548	0.0014287	0.066887	0.10274	1
221	c)	0.0014287	7.1819e-08	2.0471e-06	0.00071437	1

Table A.4. Properties of the Newton decrement for Example 6.2.6.b, iteration $k = 0$.

A.6.3 Modeling according to Category 1b is unfavorable

To model the test examples of Section 6.2 according to Category 1b, we begin with the determination of $\underline{\chi}$ according to (6.13) and (6.17), respectively. Since all objective functions ψ are convex-quadratic, we can write their gradients in the form $\nabla\psi(x) = Cx+d$ and determine the modulus of co-coercivity as $\gamma = 1/\parallel C \parallel_2$ (see Lemma 5.4.7). Parameter a is calculated with Lemma 6.1.1 as $a = (\lambda_{\min}(A^TA))^{-1}$. Table A.5 specifies the (approximate) values for γ, a, and $\underline{\chi}$. Since the values for γ are in most cases very small (and the values for a do not compensate this by being sufficiently large), the values for $\underline{\chi}$ are rather large. For that reason, is is not reasonable to start with $\chi_0 \gg \underline{\chi}$ and decrease it with some $r \in (0,1)$ because this would lead to steps from x^k to x^{k+1} that are too small. Thus, we set $\chi_k = \underline{\chi}$ for all k in all examples.

Example	γ	a	$\underline{\chi}$ (LQPAP)	$\underline{\chi}$ (BrPAP)
6.2.1	5.00e-01	2.00e+00	0.251	0.501
6.2.2	1.00e-04	1.00e+00	5000.001	2500.001
6.2.3	1.66e-05	8.17e-08	4.51e+18	1.50e+04
6.2.4	4.58e-03	2.57e+00	16.469	54.561
6.2.5.a	1.22e-03	1.02e+02	0.039	203.587
6.2.5.b	1.59e-04	1.36e+02	0.169	1567.094
6.2.6.a	1.25e-03	1.00e+00	396.974	198.487
6.2.6.b	1.58e-04	1.00e+00	3152.639	1576.320

Table A.5. Values for $\underline{\chi}$ when modeling with Category 1b.

First, we set $\mathcal{L}^k = 0$ and present the results in Tables A.6 and A.7. In the examples marked by $(*)$ the methods fail to calculate an approximately good optimal solution because the accuracies are worse than 10^{-2}. On the one hand, this can be due to the large values for $\underline{\chi}$, which imply a strong regularization by the distance function. This can cause step sizes near zero, and the algorithm makes no advance and stops. On the other hand, also examples with rather small values for $\underline{\chi}$ do not show the performance as in Tables 6.1 and 6.2. An obvious reason is that ψ is only linear approximated in Category 1b, which can hardly be compensated by the regularization term.

Now, it is interesting to see if the usage of a nonzero auxiliary operator $\mathcal{L}^k$ can improve the above results. In view of Section 5.4.3, we will only consider those examples where $\nabla\psi(x) = Cx + d$ is given with a diagonally dominant matrix C. Then, $\mathcal{L}^k$ is defined as $\mathcal{L}^k(x) = Bx$ with B according to Lemma 5.4.16. Examples where B results to be the zero matrix or where $B = C$ will also not be considered. The remaining examples are Examples 6.2.2, 6.2.5.a, and 6.2.6.a with values for γ, a, and $\underline{\chi}$ as given in Table A.8.

The results of the LQPAP and the BrPAP method as given in Tables A.9 and A.10 show that there is no significant improvement compared to Tables A.6 and A.7. So, an advantage of using a nonzero auxiliary operator $\mathcal{L}^k$ cannot be observed in the tested examples.

Example		$\{\chi_k\}$		LQPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.251	1.0	5	51	355	1.00000	9.28e-14
6.2.2	Second 2-dim example	5000.001	1.0	132784	872130	1.18e+07	0.22874	3.26e-08
6.2.3	Schittkowski no. 268	4.51e+18	1.0	27	338	3971	9625.01039	$9625.01^{(*)}$
6.2.4	Modified Colville	16.469	1.0	10	68	486	-19.47036	$3.57^{(*)}$
6.2.5.a	Rand $n = 10, p = 20$	0.039	1.0	18	116	711	-39.68351	$3.46^{(*)}$
6.2.5.b	Rand $n = 100, p = 150$	0.169	1.0	43	184	831	-30.47879	$6.54^{(*)}$
6.2.6.a	Random $n = 10$	396.974	1.0	8	81	418	2785.64974	$2805.43^{(*)}$
6.2.6.b	Random $n = 100$	3152.639	1.0	19	122	465	47.02924	$66.71^{(*)}$

Table A.6. Results for the LQPAP method when modeling the problems according to Category 1b.

Example		$\{\chi_k\}$		BrPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.501	1.0	5	30	59	1.00000	1.90e-07
6.2.2	Second 2-dim example	2500.001	1.0	38872	147815	1327572	0.25452	$2.58\text{e-}02^{(*)}$
6.2.3	Schittkowski no. 268	1.5e+04	1.0	31874	162560	2245870	0.85338	$8.53\text{e-}01^{(*)}$
6.2.4	Modified Colville	54.561	1.0	172	793	4742	-22.98408	$6.08\text{e-}02^{(*)}$
6.2.5.a	Random $n = 10, p = 20$	203.587	1.0	4244	13114	25921	-42.87079	$2.78\text{e-}01^{(*)}$
6.2.5.b	Random $n = 100, p = 150$	1567.094	1.0	3023	49551	1240367	-28.43274	$8.59^{(*)}$
6.2.6.a	Random $n = 10$	198.487	1.0	2	30	182	39.01280	$58.80^{(*)}$
6.2.6.b	Random $n = 100$	1576.320	1.0	311	1336	4814	-19.63622	$4.40\text{e-}02^{(*)}$

Table A.7. Results for the BrPAP method when modeling the problems according to Category 1b.

Example	γ	a	$\underline{\chi}$ (LQPAP)	$\underline{\chi}$ (BrPAP)
6.2.2	50.00e+00	1.00e+00	0.011	0.006
6.2.5.a	1.24e-03	1.02e+02	0.039	202.139
6.2.6.a	1.27e-03	1.00e+00	394.937	197.469

Table A.8. Values for $\underline{\chi}$ when modeling with Category 1b and $\mathcal{L}^k = Bx$.

Example		$\{\chi_k\}$		LQPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.2	Second 2-dim example	0.011	1.0	5	43	291	0.22874	1.39e-14
6.2.5.a	Random $n = 10, p = 20$	0.039	1.0	18	101	529	-39.74002	3.41
6.2.6.a	Random $n = 10$	394.937	1.0	8	71	472	2768.98425	2788.76

Table A.9. Results for the LQPAP method when modeling the problems according to Category 1b with $\mathcal{L}^k = Bx$.

Example		$\{\chi_k\}$		BrPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.2	Second 2-dim example	0.006	1.0	2	38	281	2.74972	2.52
6.2.5.a	Random $n = 10, p = 20$	202.139	1.0	4227	13035	24618	-42.87291	2.76e-01
6.2.6.a	Random $n = 10$	197.469	1.0	2	31	190	44.04312	6.38

Table A.10. Results for the BrPAP method when modeling the problems according to Category 1b with $\mathcal{L}^k = Bx$.

A.6.4 Adaptive χ_0 as an alternative

In [44, Section 6.2.4.] an adaptive initialization strategy for χ_0 is presented in the context of a bundle method for the BrPPA. To transfer this idea to our situation we linearize function f^0 in x^0 and consider

$$\min_{x \in \mathbb{R}^n} \left\{ \left\langle \nabla f^0(x^0), x - x^0 \right\rangle + \chi_0 D(x, x^0) \right\}. \tag{A.6}$$

Note that $\nabla f^0(x^0) = \nabla \psi(x^0)$ for both Categories 1a and 1b. The first Newton iterate of this problem, i.e.,

$$\tilde{y}^1 = x^0 - \frac{1}{\chi_0} [\nabla_I^2 D(x^0, x^0)]^{-1} \nabla \psi(x^0)$$

is taken as an approximation for the solution x^1 of (A.6). Now, χ_0 is determined such that $\tilde{y}^1$ stays feasible. Condition $A\tilde{y}^1 \leq b$ is equivalent to

$$\chi_0 (Ax^0 - b) \leq A[\nabla_I^2 D(x^0, x^0)]^{-1} \nabla \psi(x^0),$$

which, in view of $Ax^0 < b$, can be transformed to

$$\chi_0 \geq \max \left\{ \frac{(A[\nabla_I^2 D(x^0, x^0)]^{-1} \nabla \psi(x^0))_j}{(Ax^0 - b)_j} : j = 1, \ldots, p \right\} =: \underline{\chi}_1.$$

This may result in a too small value for χ_0, especially if the start iterate is far away from the boundary such that $Ax^0 \ll b$. Thus, it is further required that $\| \tilde{y}^1 - x^0 \| \leq 1$. This is equivalent to the condition

$$\chi_0 \geq \| \nabla_I^2 D(x^0, x^0)]^{-1} \nabla \psi(x^0) \| =: \underline{\chi}_2. \tag{A.7}$$

Finally, the bounds $\underline{\chi}$ and $\overline{\chi}$ have to be respected. Altogether, we propose the following adaptive initial value for the regularization parameter:

$$\chi_0 = \min\{\max\{\underline{\chi}_1, \underline{\chi}_2, \underline{\chi}\}, \overline{\chi}\}$$

with $\underline{\chi} = 10^{-3}$ and $\overline{\chi} = 10^6$.

It remains to choose a decreasing factor $r \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$. It is determined such that the performance of the LQPAP respectively BrPAP method is best. The results are presented in Tables A.11 and A.12. A comparison with Tables 6.1 and 6.2 shows that the accuracies of the calculated solutions are comparable, whereas the iteration numbers are mostly higher. In some examples the determined values of χ_0 are quite large (in the range of $10^3 - 10^6$). This indicates that condition (A.7) is very restrictive.

Example		$\{\chi_k\}$		LQPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.4107543	0.1	4	39	326	1.00000	1.59e-14
6.2.2	Second 2-dim example	1332.6548156	0.1	5	45	421	0.22874	1.38e-16
6.2.3	Schittkowski no. 268	1e+6	0.1	48	113	130	0.00000	2.42e-06
6.2.4	Modified Colville	4.2214806	0.1	5	333	2764	-23.04488	3.10e-07
6.2.5.a	Random $n = 10, p = 20$	0.0077806	0.1	5	43	318	-43.10092	4.76e-02
6.2.5.b	Random $n = 100, p = 150$	0.0193623	0.1	5	65	903	-36.94648	7.72e-02
6.2.6.a	Random $n = 10$	6141.8760525	0.1	7	79	597	-19.78358	3.92e-07
6.2.6.b	Random $n = 100$	162133.8106565	0.1	8	232	2395	-19.68023	4.06e-07

Table A.11. Results for the LQPAP method with adaptive χ_0.

Example		$\{\chi_k\}$		BrPAP method				
No.	Name	χ_0	r	#iter	#New	$\#\psi$	ψ_{calc}	$\lvert\psi_{calc} - \psi^*\rvert$
6.2.1	First 2-dim example	0.4730659	0.1	3	31	155	1.00000	0
6.2.2	Second 2-dim example	3413.0774882	0.1	7	47	180	0.22874	1.37e-11
6.2.3	Schittkowski no. 268	1e+6	0.9	199	631	1435	0.00000	2.31e-06
6.2.4	Modified Colville	11.8079047	0.7	10	62	215	-22.98991	5.49e-02
6.2.5.a	Random $n = 10, p = 20$	0.6927731	0.7	13	73	220	-43.14853	3.15e-05
6.2.5.b	Random $n = 100, p = 150$	0.3766576	0.1	5	48	282	-37.02359	1.41e-04
6.2.6.a	Random $n = 10$	184256.2815754	0.9	82	364	586	-19.74961	3.39e-02
6.2.6.b	Random $n = 100$	1e+6	0.9	102	439	698	-19.67286	7.36e-03

Table A.12. Results for the BrPAP method with adaptive χ_0.

A.6.5 Under-relaxation robustifies the LQPAP method

Performance graphics. The figures presented in this section show that the under-relaxation strategy introduced in Section 6.4 improves the performance of the LQPAP method. The method becomes more robust with respect to different choices of $\{\chi_k\}$.

Figures A.1–A.8 compare the reached accuracies of the LQPAP algorithm with and without under-relaxation for different parameter sets $\{\chi_0, r\}$. These parameter sets are numbered in Table A.13. There are five groups of parameter sets, each one correspond-

ing to a different value of $\chi_0 \in \{0.01, 0.1, 1, 10, 100\}$. Within a group, the values for $r \in \{0.9, 0.7, 0.5, 0.3, 0.1\}$ are distinguished.

No.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
χ_0	0.01	0.01	0.01	0.01	0.01	0.1	0.1	0.1	0.1	0.1	1	1	1	1	1
r	0.9	0.7	0.5	0.3	0.1	0.9	0.7	0.5	0.3	0.1	0.9	0.7	0.5	0.3	0.1

No.	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**
χ_0	10	10	10	10	10	100	100	100	100	100
r	0.9	0.7	0.5	0.3	0.1	0.9	0.7	0.5	0.3	0.1

Table A.13. Numbering of parameter sets.

The values of the ordinate correspond to the range of the deviation $|\psi_{calc} - \psi^*|$. The lower a point in the graph, the more accurate is the calculated solution. The value 10^{-17} represents all deviations where MATLAB® outputs the value 0. Values in the range of 10^{-16} to 10^{-14} possibly lie beyond machine precision. Blue lines correspond to the standard LQPAP algorithm (i.e., without under-relaxation, $t = 1.0$) and red lines correspond to the LQPAP algorithm with under-relaxation ($t = 0.5$). As an additional information the number of iterations (#iter) corresponding to a parameter set is listed. The average value of iterations (Avg.) over all parameter settings is also given.

In Examples 6.2.2 and 6.2.6.b the under-relaxation strategy always results in a worse accuracy compared to the standard LQPAP algorithm. In Example 6.2.3 the accuracies for $t = 1.0$ and $t = 0.5$ are similar. All other examples show the desired robustification: Using the standard LQPAP algorithm there are outliers where the accuracy of the calculated solution is in the range of 10^{-2} to 10^{1}, whereas the accuracies reached with the under-relaxation strategy mostly stay at the same range over all parameter settings. For example, in Examples 6.2.4 and 6.2.6.a the accuracies reached with the under-relaxation strategy are about 10^{-4} over all parameter settings. On the other hand, there are 13 situations in Example 6.2.4 and 5 situations in Example 6.2.6.a where the standard LQPAP algorithms reaches a worse accuracy.

Concerning the iteration numbers it is clear that consistently more iterations are needed when using under-relaxation. The iteration numbers are about factor two or three (sometimes five) higher than in the standard LQPAP algorithm.

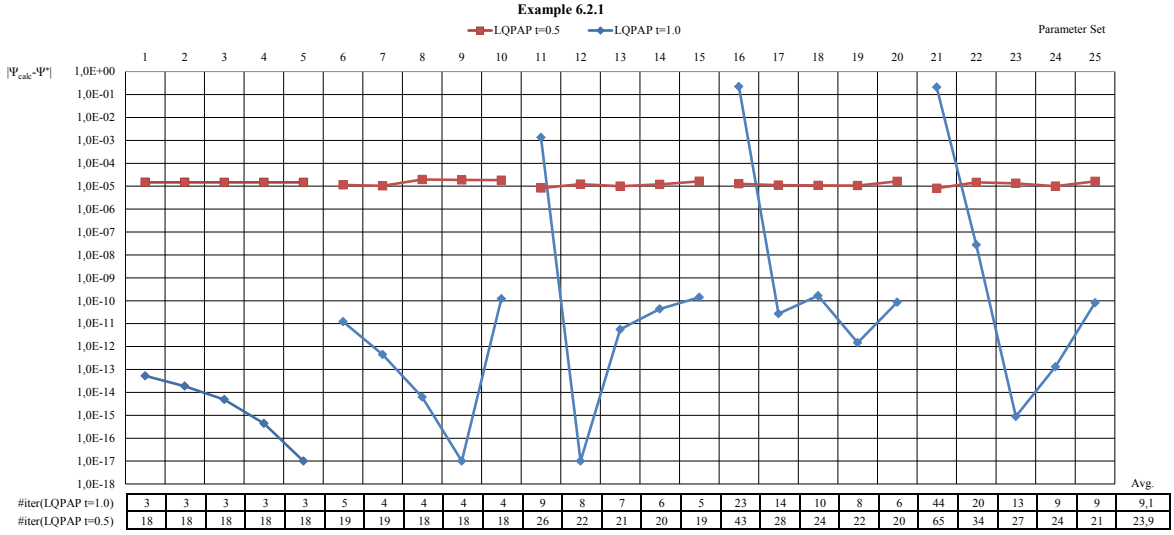


Figure A.1. Example 6.2.1: LQPAP method with and without under-relaxation.

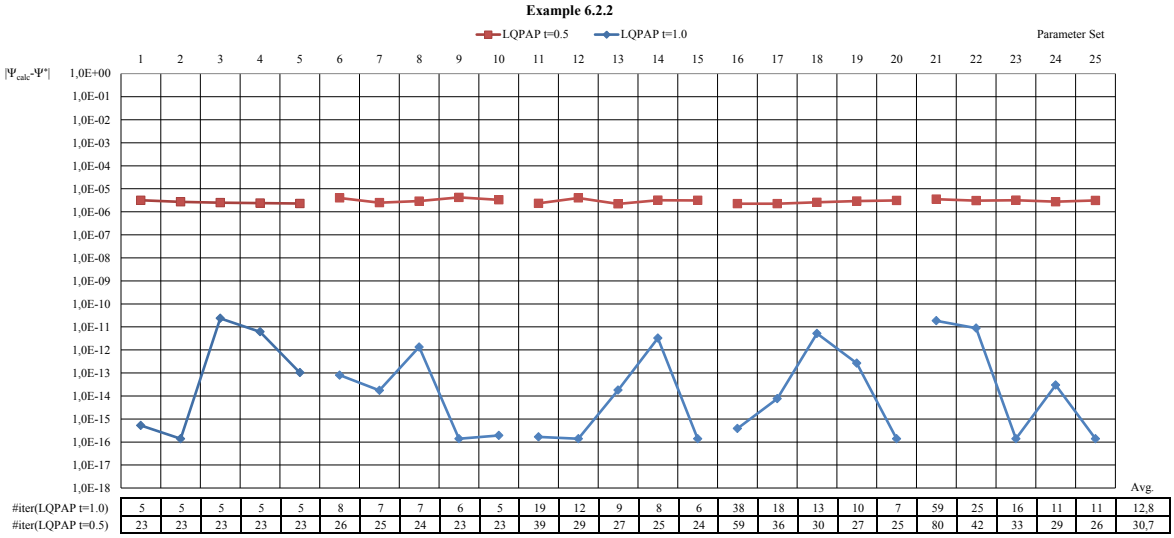
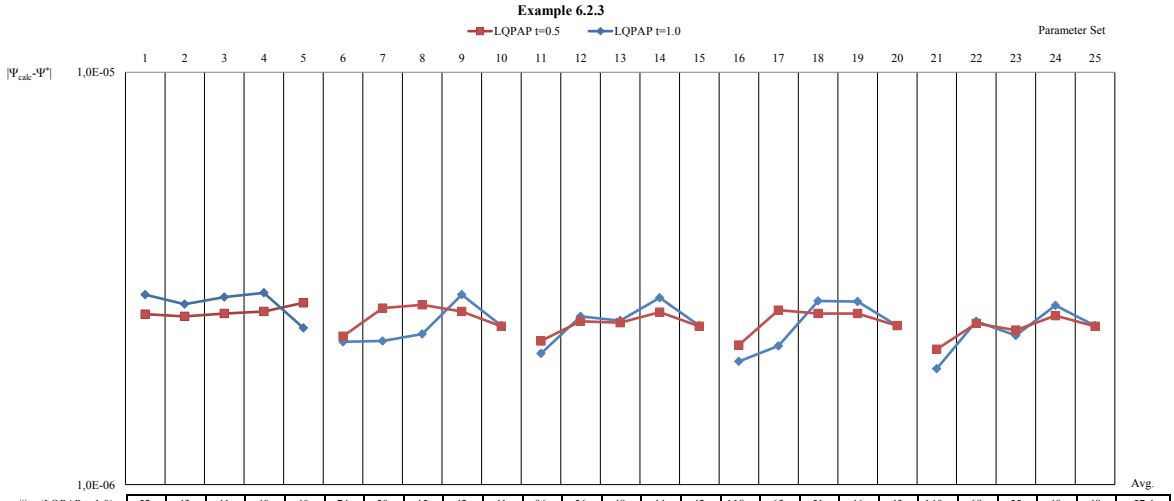
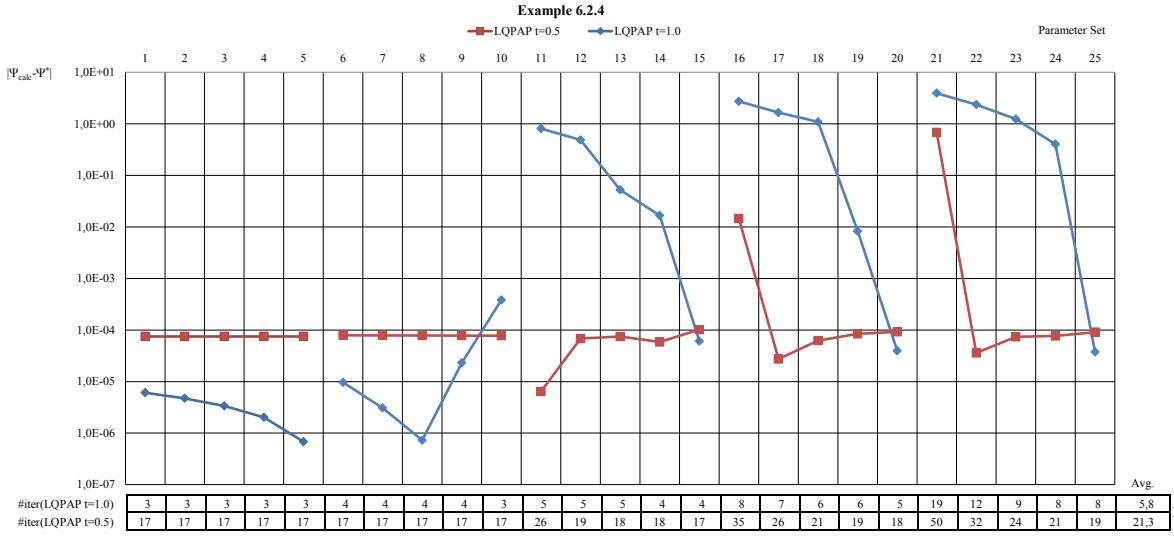


Figure A.2. Example 6.2.2: LQPAP method with and without under-relaxation.



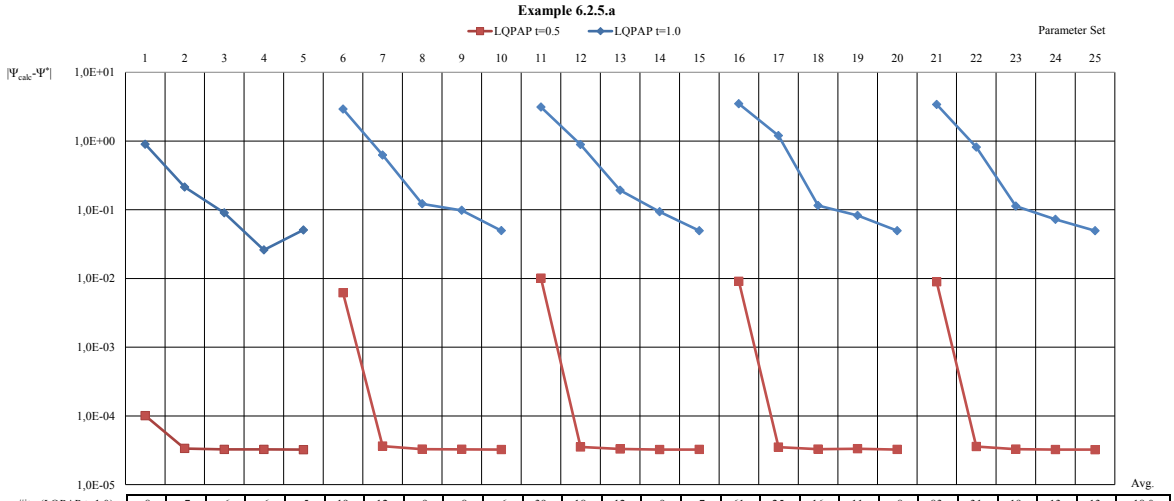
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
#iter(LQPAP t=1.0)	52	43	41	40	40	74	50	45	42	41	96	56	48	44	42	118	63	51	46	43	140	69	55	48	48	57,4
#iter(LQPAP t=0.5)	93	84	82	81	80	115	90	85	83	82	137	97	89	85	83	159	103	92	87	84	181	110	96	89	85	98,1

Figure A.3. Example 6.2.3: LQPAP method with and without under-relaxation.



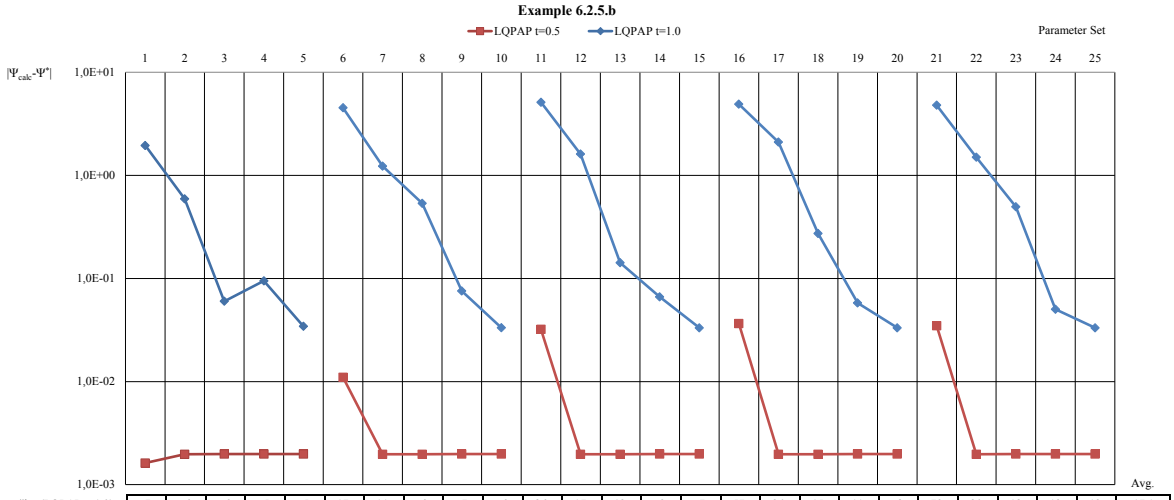
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
#iter(LQPAP t=1.0)	3	3	3	3	3	4	4	4	4	3	5	5	5	4	4	8	7	6	6	5	19	12	9	8	8	5,8
#iter(LQPAP t=0.5)	17	17	17	17	17	17	17	17	17	17	26	19	18	18	17	35	26	21	19	18	50	32	24	21	19	21,3

Figure A.4. Example 6.2.4: LQPAP method with and without under-relaxation.



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
#iter(LQPAP t=1.0)	8	7	6	6	5	19	12	9	8	6	39	18	12	9	7	61	25	16	11	8	83	31	19	13	13	18,0
#iter(LQPAP t=0.5)	32	30	29	29	28	47	34	33	30	29	68	41	35	32	30	89	48	39	33	31	111	54	42	36	32	41,7

Figure A.5. Example 6.2.5.a: LQPAP method with and without under-relaxation.



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
#iter(LQPAP t=1.0)	7	6	6	5	5	17	11	9	7	6	36	17	12	9	7	57	24	15	11	8	79	30	18	13	13	17,1
#iter(LQPAP t=0.5)	29	26	25	25	24	43	32	28	27	25	63	38	31	29	26	86	45	35	31	27	107	51	39	33	28	38,1

Figure A.6. Example 6.2.5.b: LQPAP method with and without under-relaxation.

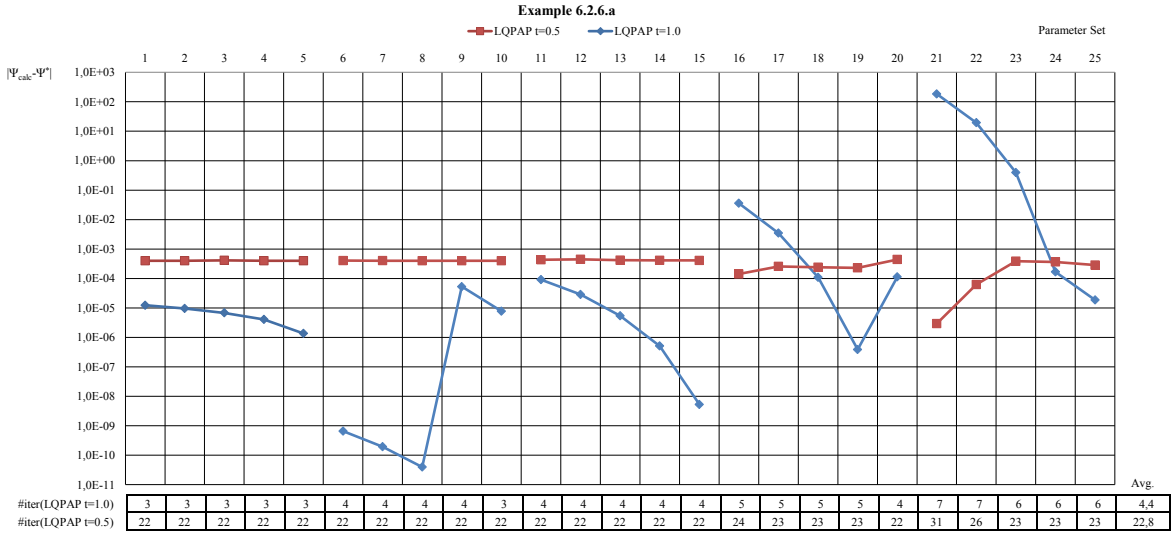


Figure A.7. Example 6.2.6.a: LQPAP method with and without under-relaxation.

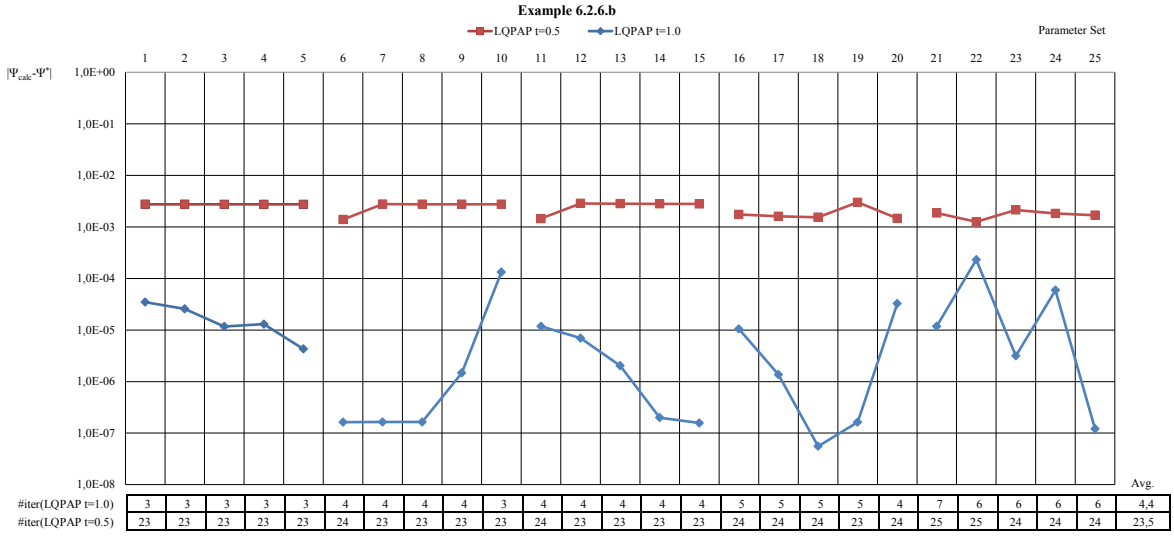


Figure A.8. Example 6.2.6.b: LQPAP method with and without under-relaxation.

Influence of the proximity to the boundary and to optimality. To explain the different situations observed in the performance graphics, it is helpful to analyze the behavior of the iterates with respect to their proximity to the boundary in relation to their proximity to optimality. We present three characteristic figures. In each figure a specific example and a specific parameter set is fixed. For a sequences $\{x^k\}$ of LQPAP iterates the points

$$\big(\| x^k - x^* \|, \min\{(b - Ax^k)_i : i = 1, \ldots, p\}\big)_{k=1,2,\ldots}$$

are plotted as a graph. The blue lines correspond to the case $t = 1.0$, and the red lines correspond to the case $t = 0.5$.

Figure A.9 belongs to a situation where the standard LQPAP algorithm calculates a solution of higher accuracy than the LQPAP algorithm using under-relaxation. Here, both sequences of iterates approach the optimal point and the boundary in the same manner. But with under-relaxation, the stopping criterion takes effect earlier and prevents a higher accuracy of the calculated solution.

This is not always the case as can be seen in Figure A.10. Both sequences of iterates behave similar with respect to their proximity to the boundary and to optimality. The same accuracies are reached. In Example 6.2.3 this is the case for all parameter sets and explains the appearance of the corresponding performance graphic in Figure A.3.

Finally, Figure A.11 represents the desired effect of under-relaxation. It prevents the iterates from tending to early towards the boundary and, thus, a higher accuracy of the calculated solution can be reached.

Switching strategy as an outlook. It would be interesting to analyze the influence of the relaxation parameter $t \in (0, 1)$ on the performance of the LQPAP method and to find an optimal choice. Furthermore, one can think of a switching strategy where under-relaxation is only used until a certain proximity to the boundary is reached. This positively influences the path of the iterates in the first iterations, while using the standard LQPAP algorithm in the last iterations can help to reach a higher accuracy. Figure A.12 shows that this is a promising strategy in comparison to the usage of a fixed under-relaxation parameter. The violet line presents the accuracies when switching from $t = 0.5$ to $t = 1.0$ if $\min\{(b - Ax^k)_i : i = 1, \ldots, p\} < 10^{-3}$. A more detailed analysis is left for further investigation.

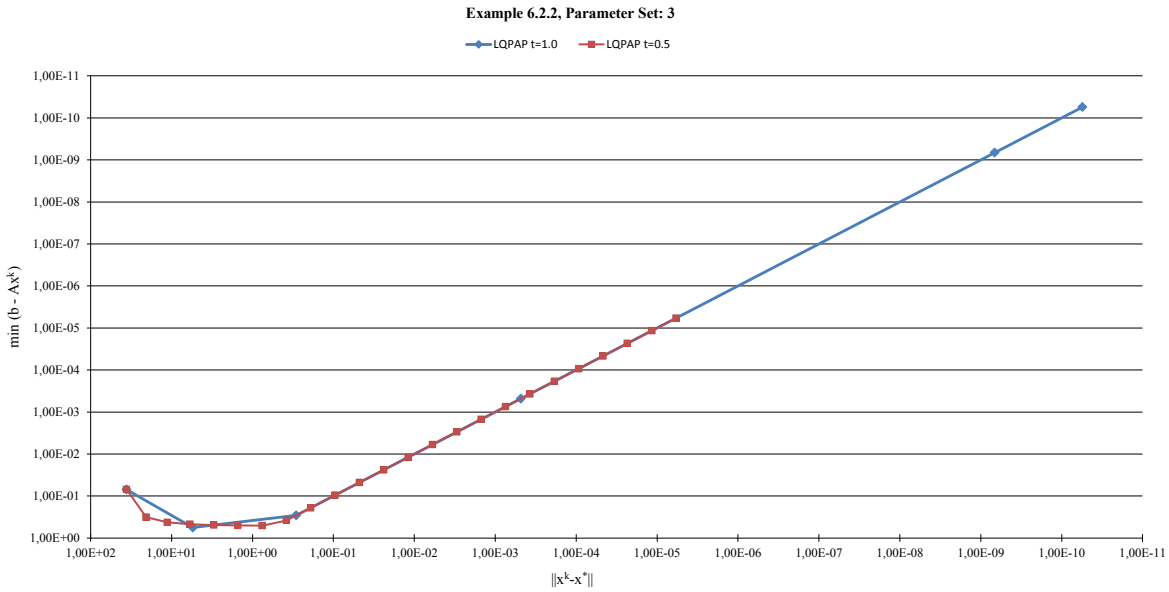


Figure A.9. Under-relaxation reaches less accuracy.

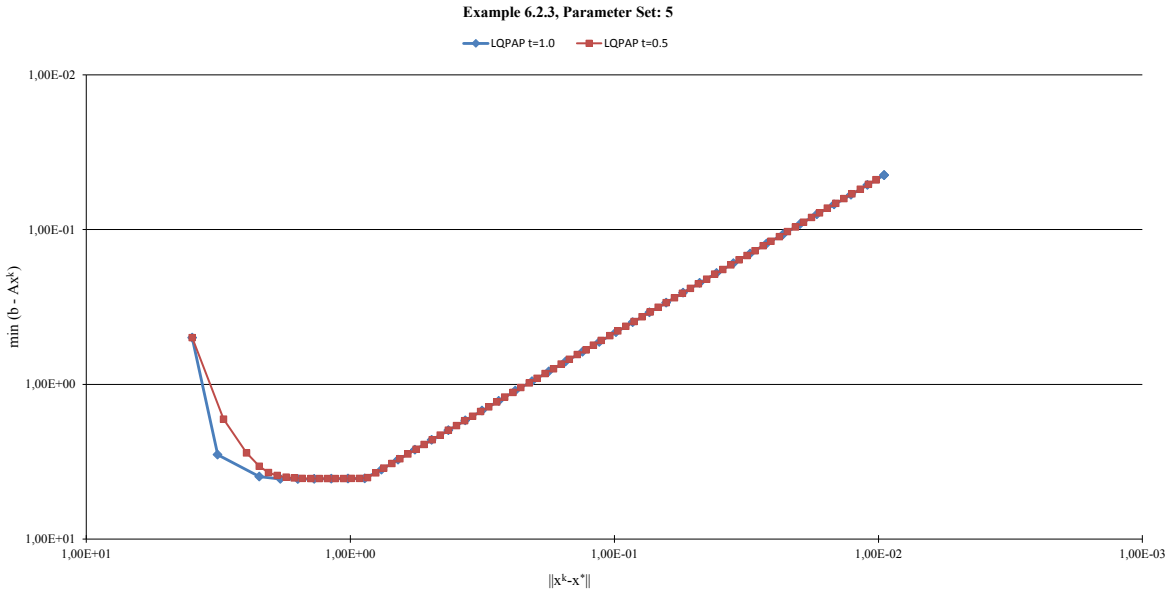


Figure A.10. Under-relaxation reaches similar accuracy.

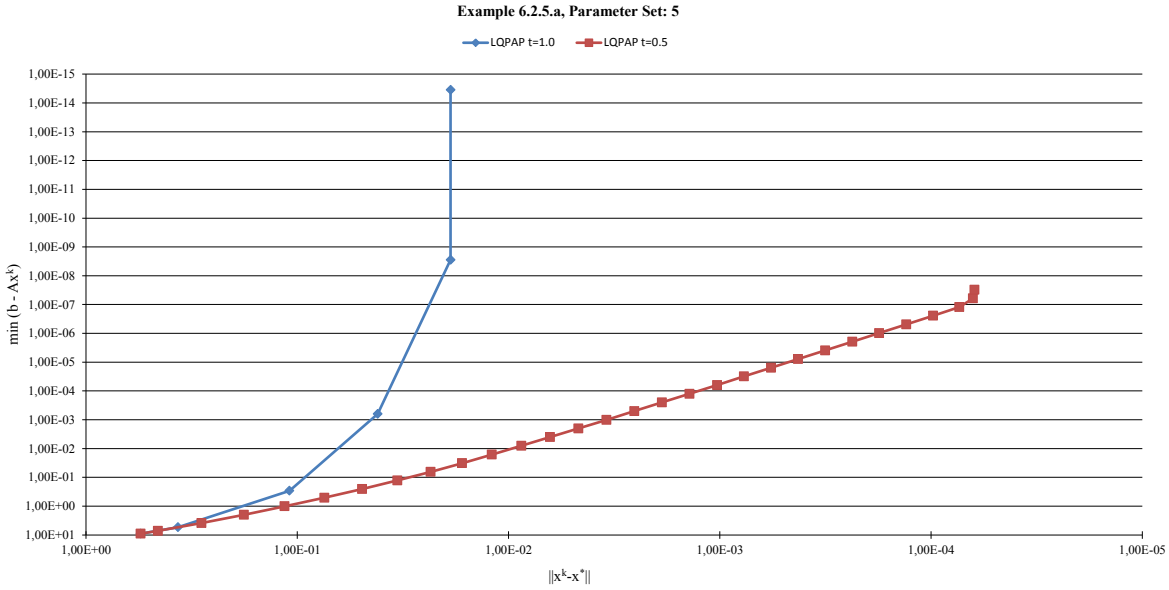


Figure A.11. Under-relaxation improves the relation between the proximity to the boundary and to optimality.

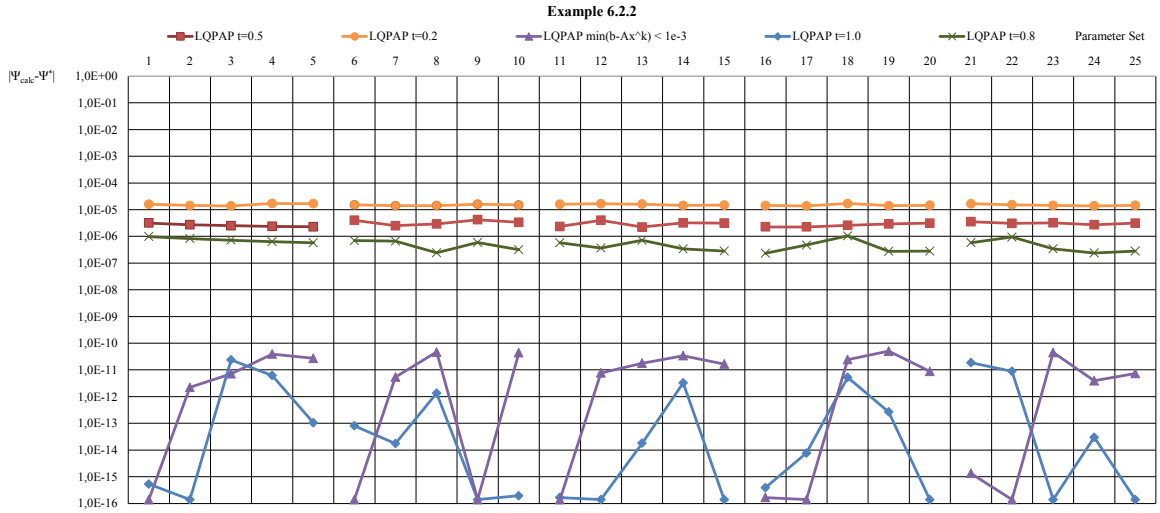


Figure A.12. Example 6.2.2: Influence of t and switching idea.

A.7 Generation of high-dimensional examples with the Lagrange approach

We describe the general process for generating an example with the Lagrange approach presented in Section 7.2.2.

We start with a randomly generated matrix $C_1 \in \mathbb{R}^{r\times r}$ which has integer entries in the interval $[-100, 100]$. We continue with its symmetric part $C_2 = 0.5(C_1 + C_1^T)$ and make it positive definite by adding $B = (-\lambda_{\min}(C_2) + 0.1)I_r$. Set $\tilde{C} = C_2 + B$. Vector $\tilde{d} \in \mathbb{R}^r$ is randomly generated with integer entries in $[-100, 100]$. Matrix $\tilde{A} \in \mathbb{R}^{p\times r}$ (with $p > r$) is randomly generated with entries in $[-100, 100]$ such that it has full column rank. Vector $\tilde{b} \in \mathbb{R}^p$ is randomly generated with entries in $[1, 100]$. Thus, the zero vector is a strict feasible point. The resulting optimization problem is solved by the MATLAB® routine fmincon and the dual solution is determined with the KKT system. If the primal solution lies in the interior of the feasible set we restart the generation process until we obtain a problem where the solution lies at the boundary of the feasible set. Now, the values for $p_\kappa \geq r$ and $p_\lambda > 0$, with $p_\kappa + p_\lambda = p$, are chosen to define a splitting of the constraints. Doing so, it has to be ensured that A_κ has full column rank. Finally, $s > 0$ is chosen to define the modified Lagrange function.

Example A.7.1. *For $r = 10$ and $p = 20$ the following data was generated:*

$$\tilde{C} = C_2 + B,$$

$$C_2 = \begin{pmatrix} 63.0 & 6.5 & -22.0 & 62.0 & 7.0 & -62.5 & 3.0 & 38.5 & 31.0 & 4.0 \\ 6.5 & 94.0 & -1.0 & -48.5 & 18.0 & -18.0 & -32.5 & 17.0 & 62.0 & 1.5 \\ -22.0 & -1.0 & 70.0 & 21.0 & 44.5 & 41.5 & 25.0 & 20.5 & 24.0 & -30.0 \\ 62.0 & -48.5 & 21.0 & -91.0 & -11.0 & -1.0 & 39.5 & -44.0 & 50.0 & -18.5 \\ 7.0 & 18.0 & 44.5 & -11.0 & -63.0 & -39.0 & 33.5 & 57.5 & 62.5 & 69.0 \\ -62.5 & -18.0 & 41.5 & -1.0 & -39.0 & -0.0 & 92.0 & -31.0 & -13.0 & -64.5 \\ 3.0 & -32.5 & 25.0 & 39.5 & 33.5 & 92.0 & 9.0 & -66.5 & -9.5 & -17.0 \\ 38.5 & 17.0 & 20.5 & -44.0 & 57.5 & -31.0 & -66.5 & -50.0 & 37.0 & -5.5 \\ 31.0 & 62.0 & 24.0 & 50.0 & 62.5 & -13.0 & -9.5 & 37.0 & -24.0 & -42.0 \\ 4.0 & 1.5 & -30.0 & -18.5 & 69.0 & -64.5 & -17.0 & -5.5 & -42.0 & -33.0 \end{pmatrix},$$

$$B = \mathit{diag}(192.36867461, \ldots, 192.36867461),$$

$$\tilde{d} = (-68, 59, -38, 6, -67, 20, -47, 31, 38, 50)^T,$$

$$\tilde{A} = \begin{pmatrix}
-10 & -14 & -17 & -53 & 86 & -58 & 19 & 93 & -79 & -63 \\
-83 & 82 & -90 & -29 & 55 & -40 & -48 & 9 & 31 & -52 \\
-54 & -64 & 81 & 64 & -3 & -6 & 21 & 4 & -1 & 77 \\
83 & -47 & 89 & -97 & -13 & -54 & 42 & -54 & 56 & -94 \\
-70 & -71 & -2 & -91 & -11 & 69 & -56 & -2 & 43 & -2 \\
65 & -73 & -2 & -66 & -39 & -61 & -77 & 25 & 81 & -66 \\
8 & 74 & -32 & 30 & 2 & -55 & -41 & 36 & 78 & 96 \\
99 & 16 & 80 & 46 & 2 & -66 & -36 & -21 & -33 & 43 \\
-84 & 10 & -26 & 30 & 64 & -54 & -15 & -27 & 40 & 0 \\
-11 & -71 & -78 & -10 & 59 & -13 & 2 & 98 & -60 & -6 \\
-79 & 71 & 56 & 9 & 29 & -38 & -83 & -92 & -94 & -88 \\
92 & 24 & -22 & -41 & -24 & 85 & -48 & 77 & 49 & 36 \\
-99 & -30 & -52 & 49 & 62 & -14 & 60 & 83 & 0 & -92 \\
55 & 3 & -19 & -62 & 7 & -63 & -94 & 59 & -4 & -86 \\
63 & -20 & -81 & 37 & -30 & 81 & 86 & -80 & 81 & 4 \\
74 & -85 & -74 & -63 & 88 & 96 & 46 & -48 & 22 & -81 \\
-83 & -52 & 88 & -26 & 75 & -12 & -2 & -33 & 24 & 64 \\
-20 & -75 & 91 & 25 & 10 & -78 & 16 & 36 & 72 & 64 \\
-48 & -63 & 15 & 56 & 24 & -48 & -53 & -73 & 61 & 44 \\
60 & -52 & -88 & -84 & 17 & -18 & -8 & 44 & 15 & -70
\end{pmatrix},$$

$$\tilde{b} = (66, 52, 97, 65, 80, 46, 44, 83, 9, 14, 18, 40, 83, 81, 7, 41, 53, 42, 66, 63)^T.$$

The primal and dual solutions are (approximately) determined as

$$\tilde{x} = (0.25081810, -0.09485588, 0.15541982, -0.02615318, 0.25295678, -0.20253054, 0.23047599, -0.09638734, -0.20858479, -0.13300297)^T,$$

$$\tilde{y} = (0, 0, 0, 0.15620580, 0, 0, 0, 0, 0, 0.19429457, 0.29623410, 0, 0, 0, 0, 0.24015519, 0, 0, 0, 0)^T.$$

To split the constraints we set $p_\kappa = 15$, $p_\lambda = 5$, choose $s = 2$, and obtain a variational inequality with dimension $n = 15$, and $p = 20$ restrictions. The optimal solution is

$$x^* = (0.25081810, -0.09485588, 0.15541982, -0.02615318, 0.25295678, -0.20253054, 0.23047599, -0.09638734, -0.20858479, -0.13300297, 0.24013181, 0, 0, 0, 0)^T.$$

An initial point in the interior of the feasible set is, e.g.,

$$x^0 = (x_1^0, x_2^0) \quad \text{with } x_1^0 = (0, \ldots, 0) \in \mathbb{R}^{10},\ x_2^0 = (10, \ldots, 10) \in \mathbb{R}^5.$$

Example A.7.2. *Another test example was randomly generated with $r = 100$, $p = 150$, $p_\kappa = 120$, and $p_\lambda = 30$. As an initial point we take*

$$x^0 = (x_1^0, x_2^0) \quad \text{with } x_1^0 = (0, \ldots, 0) \in \mathbb{R}^{100},\ x_2^0 = (10, \ldots, 10) \in \mathbb{R}^{30}.$$

This example is mentioned here such that it can be refered to in the tables of results.

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