Nonconvex All-Quadratic Global Optimization Problems:

Solution Methods, Application and Related Topics

Dissertation

Abstract

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Trier, 1999

ABSTRACT

The main aim of the present dissertation is the development and the theoretical as well as the numerical examination of solution methods for so-called *nonconvex all-quadratic optimization problems*, i.e., for problems of type

$$\begin{aligned} \min\ x^T Q^0 x + (d^0)^T x & \\ x^T Q^l x + (d^l)^T x + c^l \ \leq\ 0 & \qquad l = 1, \ldots, p \\ x\ \in P\ \ , & \end{aligned} \tag{QP}$$

with $Q^l \in \mathbb{R}^{n \times n}$ symmetric, $d^l \in \mathbb{R}^n$ ($l = 0, \ldots, p$), $c^l \in \mathbb{R}$ ($l = 1, \ldots, p$) and $P = \{x \in \mathbb{R}^n : Ax \leq b\}$ a non-empty, full-dimensional polytope with $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$.

In the first chapter some applications of this type of global optimization problems are presented. Furthermore, some basic concepts in the field of global optimization as well as solution approaches for Problem (QP) known from the literature are discussed in short. With the description of the construction of randomly generated test examples, which are used for the numerical examination of different solution methods discussed within the thesis, we conclude the first chapter.

In Chapter 2 we discuss an indirect approach for solving (QP). We do not develop an algorithm to determine an optimal solution of Problem (QP). We present several approaches for solving certain so-called *unary problems*. Each problem of type (QP) is equivalent to a unary problem, as we will see in this chapter. Thus, we can use algorithms for solving unary problems in order to detect optimal solutions of quadratic problems. This idea is due to Ramana [Ram93, Chapter 7]. Since the outer approximation (cutting plane) algorithm introduced by Ramana for solving unary problems cannot be guaranteed to be convergent, we present new approaches overcoming this theoretical deficiency. The resulting algorithms are combinations of linear outer approximations and branch-and-bound like subdivisions of the feasible region of the considered unary problem. In Chapter 2 we give, in particular, an explicit formulation of a so-called *regular* n-simplex with all its vertices on the boundary of the unit sphere $B = \{x \in \mathbb{R}^n : \|x\|_2 \leq 1\}$. The theoretical properties of such an n-simplex were known before (see, e.g., [Som29, Sle69, GKL95]) , but – to the author's knowledge – such a set has not yet been constructed. Unfortunately,

we have to recognize that this indirect solution method for (QP) is not applicable in practice. Only small dimensional all-quadratic problems can be solved with acceptable computational effort via the solution of the equivalent unary problem.

Chapter 3 deals with a direct approach for solving (QP). This method shows a significantly better performance than the foregoing indirect one. Beside the rectangular branch-and-bound algorithm introduced in [AKLV95] our simplicial method belongs to the rare approaches in the literature, which consider Problem (QP) directly. Other solution approaches for all-quadratic problems mostly interpret this type of programs as a special instance of a more general problem class, like bilinear problems [AK92], polynomial problems [ST92], problems involving biconvex functions [FV93], general d.c. problems (see Chapter 4) or – as we did in Chapter 3 – unary problems [Ram93].

The development of the proposed new algorithm was motivated by the work of Al-Khayyal et al. [AKLV95]. The branch-and-bound method for solving problems of type (QP) introduced in [AKLV95] is based on a rectangular subdivision of the feasible region of (QP) and exploits the convex and concave envelopes of the two-dimensional bilinear function xy on a rectangle $R \subset \mathbb{R}^2$. By using a simplicial partitioning strategy and the convex envelope of a concave function on an n-simplex, we obtain a simplicial branch-and-bound scheme involving mainly linear programming subproblems. The numerical comparison of our new approach with the rectangular branch-and-bound method by Al-Khayyal et al. shows that the simplex algorithm often outperforms the rectangular algorithm.

In the definition of the simplicial branch-and-bound algorithm in Chapter 3 we use the so-called *bisection* for subdividing an n-simplex. Because of the special property of this subdivision strategy, it is a so-called *exhaustive* subdivision rule, the convergence of the presented approach can be ensured. The convergence is meant in the sense that each accumulation point of a sequence generated by the proposed algorithm is an optimal solution of Problem (QP). Some authors favor another subdivision rule in simplicial branch-and-bound methods, the so-called ω-*subdivision rule*. This strategy is not necessarily exhaustive, and the convergence of an algorithm using this rule was still an open question.

In Chapter 4 we give an answer to this question. We consider a generalization of Problem (QP). We assume that the nonlinear functions involved in the global optimization problem under examination are d.c., i.e., the difference of two convex functions, not necessarily quadratic. After presenting an algorithm, which is a generalization of the simplicial branch-and-bound method introduced in Chapter 3 and which is applicable to the generalized problem class, we examine the convergence of this approach with respect to different subdivision rules. The convergence of the simplicial branch-and-bound scheme using the ω-subdivision rule can only be guaranteed for optimization problems with a d.c. objective function and with concave constraints. We present in Chapter 4 a counterexample showing that the presented method using this rule does not converge in general. In view of our theoretical results we are non the less able to develop a new convergent subdivision strategy – combining ω-subdivision and bisection. The numerical performance of some variants of this mixed strategy will be examined. The convergence concept, which we use in Chapter 4 in connection with the examination of the ω-subdivision, is – from a theoretical point of view – weaker than the one used in Chapter 3. We will not prove that each accumulation point of a sequence generated by the variant of our approach using ω-subdivisions is optimal. We will only show that this method determines in finite time either an approximate solution or the emptiness of the feasible region of the considered problem. As we will see in Chapter 4 – from a practical point of view – this convergence concept has non the less the same quality as the stronger concept mentioned above.

We conclude the more theoretically oriented Chapter 4 with a finiteness result. We prove that a simplicial branch-and-bound algorithm, which employs only ω-subdivisions and which is applied to the minimization of a concave function with respect to linear constraints, is even finite, if two additional assumptions are fulfilled.

In Chapter 5 we close our consideration of Problem (QP) by examining an application of this class of global optimization problems. This chapter deals with the problem of packing n equal circles of maximal radius into the unit square, which we will call *packing problem*. Unfortunately, the solution methods, which we developed for general problems of type (QP), are not able to solve the optimization problem resulting from this application. At least they are not able to solve the problem for a high enough number of circles. Therefore, we develop a special global optimization algorithm for solving this problem.

We start in Chapter 5 with a study of the packing problem from a theoretical point of view. Some new properties, which have to be satisfied by at least one solution of this problem, are introduced. These properties state the intuitive fact that as many circles as possible should touch the boundary of the unit square. Subsequently we propose a basic rectangular branch-and-bound algorithm and derive special bounds exploiting the structure of the packing problem. We introduce some tools with respect to the subdivision and the possible refinement of the considered hyperrectangles, which again exploit the special structure of the packing problem. They use in particular the theoretical properties of some solutions mentioned above. Applying these tools in the rectangular branch-and-bound algorithm we obtain an efficient algorithm.

In the literature good solutions of the packing problem with up to 50 circles are known. However, the quality of these solutions with respect to their optimality is mostly not known – at least for the packing problem with more than 20 circles. The new approach developed in this thesis is able to guarantee the ϵ-optimality of determined solutions of this problem. Furthermore, the implementation of our solution method showed a really good numerical performance for the packing problem with up to 27 circles. Moreover, we were also able to solve this problem approximately with up to 31 circles. This means that global optimization problems with a dimension of up to 63 can be solved up to a certain accuracy.

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