A New Introduction to Global Optimization over Polyhedrons

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Abstract: - For some kinds of linearly constrained optimization problems with unique optimal solution, such as linear and convex problems, the single local optimum is also global. However, there are a broad variety of problems in which the property of unique solution cannot be simply postulated or verified. The paper presents an effective approach for the global linearly constrained optimization problem with continuous objective function. With the help of a parametric representation of the feasible region an equivalent unconstrained problem is constructed which is much easier to solve. Our aim is to propose a new introduction to global optimization, the design of a general solution algorithm that always finds the solution and provides useful information such as bounding of the objective function. The algorithm and its applications are presented in the context of a numerical example.

Key-Words: - Global optimization, Linearly constrained optimization, Tight bounding, Nonlinear programming, Polyhedrons, Mathematical programming

1 Introduction

Optimization has been of significant interest and relevance in many areas. While the efficient computer packages of local solvers have become widespread, a major limitation is that there is often no guarantee that the generated solutions correspond to the global optima [14].

Global optimization is concerned with the characterization and computation of global minima or maxima of nonlinear functions. Such problems are widespread in mathematical modeling of real world systems for a very broad range of applications [23].

Standard nonlinear programming techniques have not been successful for solving these problems because they use only local information and hence cannot be expected to provide global optimality criteria [18]. Such algorithms usually obtain a local minimum that is global only when certain conditions are satisfied (such as objective function and feasible region being convex). Moreover, the problem of checking local optimality for a feasible point and the problem of checking if a local minimum is strict, are NP-hard problems [24]. Another problem regarding global optimization is that optimum is often attained at the boundary of feasible region and that more than one optimum can exist.

Active research during the past decades has produced a variety of methods for solving global optimization problems. The main classes of problems for which many algorithms exist are [18] concave minimization, reverse convex programming, d.c. programming (global optimization of functions that can be expressed as a difference of two convex functions) and Lipschitzian optimization. Some typical approaches for solving global optimization problems use techniques such as branch and bound, relaxation, outer approximation and valid cutting planes.

Although there are many different algorithms for certain classes of problems are known, their deficiency is also that sometimes it is difficult to classify a problem in the correct class [23].

One of the methods that cover most general problems is d.c. programming, since every continuous function on a compact (convex) set can be approximated by d.c. functions. But in practice it is difficult to construct such approximations. However, in many special cases of interest, the exact d.c. decomposition is already given or easily found, see for example [16]. Another general approach is Lipschitzian optimization [17], [25]. However, the deficiency of this approach is that all methods for solving such problems require knowledge of a Lipschitzian constant for some of all of the functions involved.

It this paper we wish to present an alternative approach for solving linearly constrained global optimization problems that are the subset of general global optimization problems. Although the structure of this problem is simple, finding a global solution - and even detecting a local solution is known to be difficult.

There are well over 400 different solution algorithms for solving different kinds of linearly constrained optimization problems. Some of them were published recently, for example [7], [9], [20]. However, there is not one algorithm superior to others in all cases. Moreover, the optimum (local or global) may not be unique [3]. Therefore the question of finding global solutions to general optimization problems is an important one but as yet unanswered by general optimization theory in a practical way [22, page 34].

The paper develops an effective alternative approach to solve general continous optimization problems with linear constraints. The unified approach is accomplished by converting the constrained optimization problem to an unconstrained optimization problem through a parametric representation of its feasible region.

As a by-product of the proposed solution algorithm, it enables us to compute the tight numerical bounds for a continuous objective function with the linear constraints.

The remainder of this paper is organized as follows: In section 2 the problem is formulated and section 3 explains the algorithm. To illustrate the steps of the algorithm an application is presented in section 4 in the context of published numerical problem solved by other method, which serves also for comparative study purposes. The last section contains the conclusions with some useful remarks.

2 Problem Formulation

We want to solve the following problem with linear feasible region:

Problem P: Maximize $f(\mathbf{x})$

subject to: $\mathbf{Ax} \le \mathbf{b}$

where some variables x_i have explicit upper and/or lower bounds and some are unrestricted in sign, where **A** is $m \times n$ matrix, **b** is m-vector and f is a continuous function. Problem **P** is a subset of a larger set of problems known as Continuous Global Optimization Problems [25].

The feasible region of the problem **P** is the set of points that defines the polyhedron [10], [26]. In the proposed solution we need to find all the critical points of objective function f inside and at the boundaries of the polyhedron.

A *polyhedron* with finite number of vertices can be represented in two equivalent ways [4]: H-representation and V-representation.

An *H-representation* of the polyhedron is given by an $m \times n$ matrix **A** and m-vector **b**:

$$\mathbf{S} = \left\{ \mathbf{x} \in \Re^{\mathbf{n}}; \mathbf{Ax} \le \mathbf{b} \right\}$$

An *V-representation* of the polyhedron is given by a minimal set of M vertices $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_M}$ and N extreme rays $\mathbf{w_1}, \mathbf{w_2}, \ldots, \mathbf{w_N}$:

$$\mathbf{S} = \left\{ \mathbf{x}; \mathbf{x} = \sum_{i=1}^{M} \lambda_i \mathbf{v_i} + \sum_{j=1}^{N} \mu_j \mathbf{w_j}, \lambda_i, \mu_j \ge 0, \sum_{i=1}^{M} \lambda_i = 1 \right\}.$$

A *face* of polyhedron **S** is a boundary set of **S** containing points on a line or plane (or hyper-plane).

A *vertex* of this polyhedron is any of its points that can be specified as an intersection of faces. This is a point $\mathbf{v} \in \Re^{\mathbf{n}}$ of **S** that satisfies an affinely independent set of n inequalities as equations.

An *edge* of the polyhedron is the line segment between any two adjacent vertices.

An *extreme ray* $\mathbf{w} \in \Re^{\mathbf{n}}$ is a direction such that for some vertex **v** and any positive scalar μ, $\mathbf{v} + \mu\mathbf{w}$ is in **S** and satisfies some set of (n-1) affinely independent inequalities as equations.

If a feasible region is bounded then a corresponding polyhedron is called a *polytope*, which has no extreme rays. Its V-representation is given by the convex combination of the vertices.

The *parametric representation* of the objective function f is given by $f(\mathbf{x}) = f(\mathbf{x}(\lambda, \mu)) = f(\lambda, \mu)$.

Critical point of a continuous function is a point where the first partial derivatives are zero or undefined.

3 The algorithm

In the proposed solution algorithm we need to find critical points. It is necessary for the domain to be an open set for the definition of derivative. Therefore, we solve unconstrained problems over some relevant open sub-domains of the feasible region. First, we find critical points on the interior points of the feasible region. Next, we evaluate the objective function at the vertices of the feasible region. Finally, we find critical points on interior points of the faces and edges (i.e., line segments) of the feasible region. The global optimal solution is found by comparing the functional values at the critical points and at the vertices. Therefore, in solving an n dimensional problem, we solve some unconstrained optimization problems in n, n-1,…, 1 dimensions. Thus, removing the constraints by the proposed algorithm reduces the constrained optimization to unconstrained problems, which can be more easily dealt with.

The following provides an overview of the algorithm's process strategy:

Phase 1: *Find the critical points of the objective function and select those, which are feasible by checking the constraints.*

Phase 2: *Find the V-representation of the feasible region, its edges and faces. Evaluate the objective function at the vertices.*

Phase 3: *Find the critical points of the objective function over the open domains: faces, edges,… Then evaluate the objective function at these points.*

Phase 4: *Pick the global solution and construct the numerically tight bounds for the problem.*

The second phase of the algorithm can be implemented by one of the algorithms for finding the vertices, extreme rays, edges and faces of the polyhedron.

There are essentially two main approaches to the problem of generating all the vertices of the polyhedron, both with the origins in the 1950s. The double description method [21] involves building the polyhedron sequentially by adding the defining inequalities one at a time. Recent algorithms and practical implementations of this method have been developed by Fukuda and the others [8], [12], [13].

The second method for finding all the vertices and extreme rays of the polyhedron involves pivoting around the skeleton of the polyhedron. An efficient method using this approach is the reverse search method by Avis and Fukuda [5] and the revisited version [4]. Some other methods are described in [6], [10], [19], [26].

In the third phase of the algorithm we have to find the critical points over the open domains. We can construct the parametric version of the objective function over each domain and look for its critical points. But since there may be many such domains it is more efficient to use the following result.

Suppose that the feasible region is defined by M vertices and N extreme rays. We will need partial derivatives of the objective function **f** over each λ_i, $1 \le i \le M$ and each μ_j, $1 \le j \le N$. We can find them by using the chain-rule:

$$\frac{\partial f}{\partial \lambda_i} = \sum_{k=1}^{n} \frac{\partial f}{\partial x_k} \cdot \frac{\partial x_k}{\partial \lambda_i}$$

$$\frac{\partial f}{\partial \mu_j} = \sum_{k=1}^{n} \frac{\partial f}{\partial x_k} \cdot \frac{\partial x_k}{\partial \lambda_j}$$

Then, suppose the open domain is defined by a subset of the vertices $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_s}$ and a subset of extreme rays $\mathbf{w_1}, \mathbf{w_2}, \dots, \mathbf{w_t}$. To find the critical points in this domain we have to find the critical points of the parametric objective function over the domain

$$\begin{aligned} &\lambda_1 + \cdots + \lambda_s = 1 \\ &\lambda_{s+1} = \cdots = \lambda_M = \mu_{t+1} = \cdots = \mu_N = 0 \\ &\mu_1, \cdots, \lambda_t > 0 \end{aligned}$$

We can construct the Lagrangian

$$\begin{aligned} &L(\lambda_1, \cdots, \lambda_s, \mu_1, \cdots, \lambda_t, c) = f(\lambda_1, \cdots, \lambda_s, \mu_1, \cdots, \lambda_t) + \\ &+ c(1 - \lambda_1 - \cdots - \lambda_s) \end{aligned}$$

In order to find the critical points we have to solve the following system:

$$\begin{aligned} &\frac{\partial L}{\partial \lambda_1} = \frac{\partial f}{\partial \lambda_1} - c = 0 \\ &\vdots \\ &\frac{\partial L}{\partial \lambda_s} = \frac{\partial f}{\partial \lambda_s} - c = 0 \end{aligned}$$

$$\frac{\partial L}{\partial \mu_1} = \frac{\partial f}{\partial \mu_1} = 0$$
$$\vdots$$
$$\frac{\partial L}{\partial \mu_t} = \frac{\partial f}{\partial \mu_t} = 0$$
$$\frac{\partial L}{\partial c} = 1 - \lambda_1 - \cdots - \lambda_s = 0$$

By eliminating c from the system we get

$$\frac{\partial f}{\partial \lambda_1} = \frac{\partial f}{\partial \lambda_2} = \cdots = \frac{\partial f}{\partial \lambda_s}$$
$$\frac{\partial f}{\partial \mu_1} = \frac{\partial f}{\partial \mu_2} = \cdots = \frac{\partial f}{\partial \mu_t} = 0$$
$$\lambda_1 + \lambda_2 + \cdots + \lambda_s = 1$$

It means that if we are looking for the critical points in the open domain defined by a subset of the vertices $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_s}$ and a subset of extreme rays $\mathbf{w_1}, \mathbf{w_2}, \ldots, \mathbf{w_t}$, then we have to solve the above system over the domain $\lambda_i, \mu_j \geq 0$, $1 \leq i \leq M$, $1 \leq j \leq N$.

In order to find the critical points is some open domain we can use the partial derivatives that were found once for all the domains.

In the last phase of the algorithm we have to compare the functional values at the critical points and the vertices. We pick the global solution.

The proposed algorithm also enables us to compute the tight numerical bounds for a continuous objective function with the linear constraints, because it discovers all critical points and vertices that are candidates for global minimums and maximums.

Not all problems go through all three steps. For example, if we are looking for a maximum, the objective function is concave and the interior critical point has been found, then we know that this is the optimal point.

4 Numerical example

In the following example we demonstrate the usefulness of proposed method. It always finds the right solution, while it was not find by the other methods in many cases, although the problems are rather simple. The following quadratic optimization with inequality constraint is attempted to solve in [11, pages 70-82] using the Wolf Method.

Max $f(x_1, x_2) = 2x_1 + x_2 + 3x_1x_2 - x_1^2 - 2x_2^2$

subject to: $x_1 + 2x_2 \leq 10$

$x_1 + 3x_2 \geq 3$

$x_1, x_2 \geq 0$

The partial derivatives of the objective function are

$$\frac{\partial f}{\partial x_1} = 2 - 2x_1 + 3x_2$$
$$\frac{\partial f}{\partial x_2} = 1 + 3x_1 - 4x_2$$

The gradient vanishes at $x_1 = -11$, $x_2 = -8$ which is not feasible. It means that there are no feasible interior critical points.

The vertices of the feasible region and the corresponding objective function values are listed in Table 1.

vertex	its coordinates	f(x)
$\mathbf{v_1}$	(3,0)	-3
$\mathbf{v_2}$	(10,0)	-80
$\mathbf{v_3}$	(0,5)	-45
$\mathbf{v_4}$	(0,1)	-1

Table1: Vertices and function values for numerical example

The edges of the polyhedron are $\mathbf{e_1} = (\mathbf{v_1}, \mathbf{v_2})$, $\mathbf{e_2} = (\mathbf{v_2}, \mathbf{v_3})$, $\mathbf{e_3} = (\mathbf{v_3}, \mathbf{v_4})$, $\mathbf{e_4} = (\mathbf{v_1}, \mathbf{v_4})$. The parametric representation of the feasible region is given by:

$$(x_1, x_2) = (3\lambda_1 + 10\lambda_2, 5\lambda_3 + \lambda_4)$$

where $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 1$, $0 \leq \lambda_1, \lambda_2, \lambda_3, \lambda_4 \leq 1$.

For finding the critical points on the edges we will need partial derivatives of **f** over each λ. By using the chain-rule we get:

$$\frac{\partial f}{\partial \lambda_1} = 3\frac{\partial f}{\partial x_1} = 6 - 6x_1 + 9x_2$$
$$\frac{\partial f}{\partial \lambda_2} = 10\frac{\partial f}{\partial x_1} = 20 - 20x_1 + 30x_2$$
$$\frac{\partial f}{\partial \lambda_3} = 5\frac{\partial f}{\partial x_2} = 5 + 15x_1 - 20x_2$$
$$\frac{\partial f}{\partial \lambda_4} = \frac{\partial f}{\partial x_2} = 1 + 3x_1 - 4x_2$$

To find the critical points on the interior of the edge $\mathbf{e_2} = (\mathbf{v_2}, \mathbf{v_3})$ we have to solve the system

$$\frac{\partial f}{\partial \lambda_2} = \frac{\partial f}{\partial \lambda_3}$$

over the domain $\lambda_2 + \lambda_3 = 1$, $0 < \lambda_2, \lambda_3 < 1$, $\lambda_1 = \lambda_4 = 0$. We get

$$20 - 20x_1 + 30x_2 = 5 + 15x_1 - 20x_2$$

Since $x_1 = 10\lambda_2$ and $x_2 = -5\lambda_2 + 5$, the critical point is $x_1 = 53/12$, $x_2 = 67/24$ with the objective function value 13.52.

There is one more critical point on the edge $\mathbf{e_4} = (\mathbf{v_1}, \mathbf{v_4})$ with objective function value 3.05. On the remaining edges there are no critical points.

Therefore, the optimal solution occurs at $x_1 = 53/12$, and $x_2 = 67/24$ with an optimal value of 13.52. The solution given in the above reference is $x_1 = 9/8$, and $x_2 = 5/8$ with objective function value of 47/16 = 2.94 which is inferior compared with the global solution obtained by the proposed approach.

Tight bounds of the objective function over the feasible region are:

$$-80 \le f(x_1, x_2) \le 13.52 .$$

5 Conclusion

We have presented a new solution algorithm for the general linearly constrained optimization problems with continuous objective function. For a polyhedron specified by a set of linear equalities and/or inequalities, the proposed solution algorithm utilizes its parametric representation. The key to this generalized solution algorithm is that the constrained optimization problem is converted to an unconstrained optimization problem through a parametric representation of the feasible region. This representation of the feasible region enables us to solve a large class of optimization problems.

The proposed algorithm favorably compares with other methods for this type of problems. Unlike other general-purpose solution methods, it guarantees globally optimal solutions, it has simplicity, potential for wide adaptation, and deals with all cases. However, this does not imply that all distinction among problems should be ignored. One can incorporate the special characteristic of the problem to modify the proposed algorithm in solving them.

The main drawback for the proposed algorithm is that all the vertices of the feasible region have to be found. The vertex enumeration problem is a hard problem even with the recent progress.

The main advantages of the presented algorithm are that it covers all linearly constrained optimization problems and that it always finds the optimal solution. There are many problems in the literature for which the proposed algorithm finds optimal solution and others do not. Some additional examples can be found in [2].

Some areas for future research include development of possible refinements. An immediate work is development of an efficient computer code to implement the approach, and performing a comparative computational study.

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