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Constrained Global Optimization: Algorithms and Applications

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Constrained Global Optimization: Algorithms and Applications

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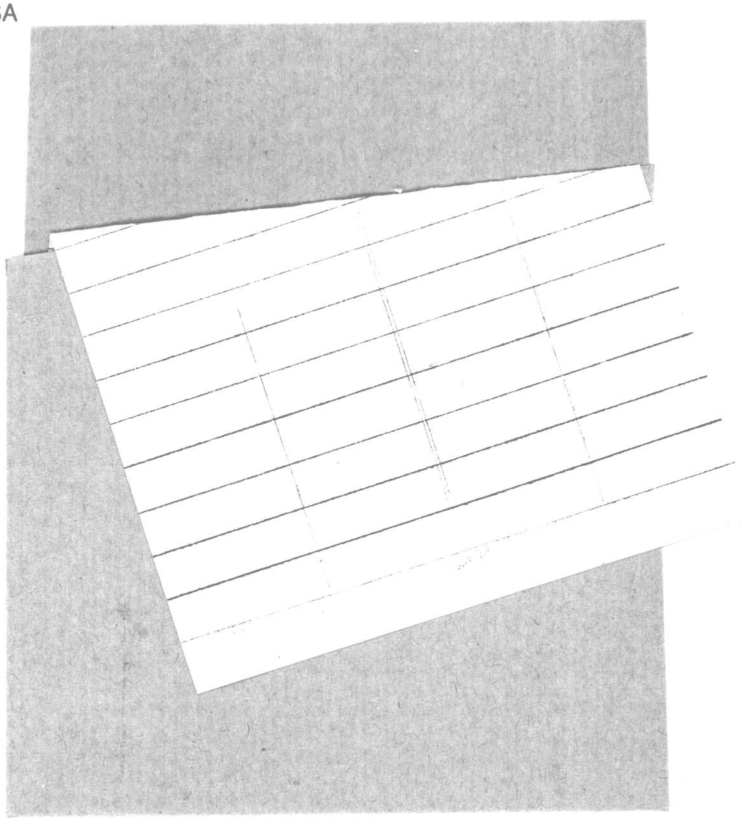
Authors

Panos M. Pardalos
Computer Science Department, The Pennsylvania State University
University Park, PA 16802, USA

J. Ben Rosen
Computer Science Department, University of Minnesota
Minneapolis, MN 55455, USA



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Preface

Global optimization is concerned with the characterization and computation of global minima or maxima of nonlinear functions. The general constrained global minimization problem has the following form:

Given: $K \subseteq R^n$ *compact set,* $f: K \to R$ *continuous function*

Find: $x^* \in K$, $f^* = f(x^*)$ *such that* $f^* \le f(x)$ *for all* $x \in K$

Such problems are widespread in mathematical modeling of real world systems for a very broad range of applications. Such applications include economies of scale, fixed charges, allocation and location problems, quadratic assignment and a number of other combinatorial optimization problems. More recently it has been shown that certain aspects of VLSI chip design and database problems can be formulated as constrained global optimization problems with a quadratic objective function. Although standard nonlinear programming algorithms will usually obtain a local minimum to the problem, such a local minimum will only be global when certain conditions are satisfied (such as f and K being convex). In general several local minima may exist and the corresponding function values may differ substantially. The problem of designing algorithms that obtain global solutions is very difficult, since in general, there is no local criterion for deciding whether a local solution is global.

Active research during the past two decades has produced a variety of methods for finding constrained global solutions to nonlinear optimization problems. In this monograph we consider deterministic methods which include those concerned with enumerative techniques, cutting planes, branch and bound, bilinear programming, general approximate algorithms and large-scale approaches.

There has been a significant recent increase in research activity on the subject of constrained global optimization and related computational algorithms. This monograph summarizes much of this recent work and contains an extensive list of references to papers on constrained global optimization, deterministic solution methods, and applications. We hope that this work will be valuable for other researchers in global optimization.

We wish to express our appreciation and thanks to Andrew T. Phillips and Nainan Kovoor who carefully read an earlier version of this monograph and suggested a number of valuable improvements. The authors' research described in this monograph was supported in part by the National Science Foundation Grant DCR8405489.

June 1987 P.M. Pardalos, J.B. Rosen

Table of Contents

Chapter 1 Convex sets and functions

Convex sets and functions play a dominant role in optimization and some of their properties are essential in the study of several algorithms. In this introductory chapter we start with summary of some of the most important properties that we are going to use.

1.1 Convex sets

A subset C of the Euclidean space R^n is said to be convex if for every $x_1, x_2 \in C$ and λ real, $0 \le \lambda \le 1$, the point $\lambda x_1 + (1-\lambda) x_2 \in C$.

The geometric interpretation of this definition is clear. For any two points of C, the line segment joining these two points lies entirely in C.

Given the vectors $x_1, \ldots, x_m$ in R^n and real numbers $\lambda_i \ge 0$ with $\sum_{i=1}^{m} \lambda_i = 1$, the vector sum $\lambda_1 x_1 + \cdots + \lambda_m x_m$ is called a convex combination of these points. Some properties of convex sets are summarized in the next theorems.

Theorem 1.1.1: A subset of R^n is convex iff it contains all the convex combinations of its elements.

Proof: Let C be a convex set in R^n. If $x_i \in C$ and $\lambda_i \ge 0$, $i=1, \ldots, k$, such that $\sum_{i=1}^{k} \lambda_i = 1$, prove by induction on k that the convex combination $\sum_{i=1}^{k} \lambda_i x_i \in C$.

Theorem 1.1.2: Let F be a family of convex sets. Then the intersection $\bigcap_{C \in F} C$ is also a convex set.

However, it is easy to see that the union of convex sets need not be convex. Some other algebraic set operations that preserve convexity are defined below.

Theorem 1.1.3: 1) Let C be a convex set in R^n and a a real number. Then the set $aC = \{x: x = ay, y \in C\}$ is also convex.
2) Let C_1, C_2 be convex sets in R^n. Then the set

$$C_1 + C_2 = \{x: x = x_1+x_2, x_1 \in C_1, x_2 \in C_2\}$$

is also convex.

1.2 Linear and affine spaces

For any $x, y \in R^n$ the inner product $x^T y$ is the real number $\sum_{i=1}^{n} x_i y_i$. The Euclidean norm is defined to be $\|x\| = (\sum_{i=1}^{n} x_i^2)^{1/2}$. Other notations and terminology not defined here are the standard ones used in the literature.

A hyperplane H in R^n is a set of the form

$$H = \{x \in R^n : c^T x = b\}.$$

for some vector $c \in R^n$ and $b \in R$. Similarly we define the closed half spaces

$$H_1 = \{x \in R^n : c^T x \geq b\}, \quad H_2 = \{x \in R^n : c^T x \leq b\}.$$

It is very easy to see that H, H_1, H_2 are all convex sets.

A nonempty subset V of R^n is called a (linear) subspace if the following conditions are true:
i) if $x, y \in V$ then $x+y \in V$,
ii) if $x \in V$ and $r \in R$ then $rx \in V$.

Next we define the structure of linear subspaces. Let $S=\{v_1, \ldots, v_m\}$ be a set of vectors in V. We say that S spans V if for every vector $v \in V$, $v = \sum_{i=1}^{m} c_i v_i$, where the c_i's are real numbers. The set S is said to be linearly independent if we cannot find constants $c_1, \ldots, c_m$ not all zero such that $c_1 v_1 + \cdots + c_m v_m = 0$ (otherwise S is called linearly dependent).

If the set S spans V and is linearly independent we call it a basis of V. The dimension of the subspace V, $dim(V)$, is defined to be the number of vectors in some basis S.

To get more insight into the geometric and algebraic nature of a subspace we equivalently define a linear subspace to be the set

$$V = \{x \in R^n : c_{i1}x_1 + \cdots + c_{in}x_n = 0, \ i = 1, \ldots, m\},$$

that is, V is the solution set of the homogeneous system of linear equations $Cx = 0$ where C is the $m \times n$ matrix of the coefficients c_{ij}. Here the dimension of V is equal to $n - rank(C)$ where the $rank$ of the matrix is the maximum number of linearly independent columns (or rows) of the matrix.

An affine subspace A of R^n is a linear subspace V translated by some vector u, that is $A = \{x \in R^n : x = u + v, \ v \in V\}$. Also $dim(A) = dim(V)$. Equivalently we can define

$$A = \{x \in R^n : c_{i1}x_1 + \cdots + c_{in}x_n = b, \ i = 1, \ldots, m\},$$

that is, A is the solution set of the (nonhomogeneous) linear system $Cx = b$.

From the above discussion it is clear that a hyperplane in R^n is an affine subspace of dimension $n-1$.

1.3 Convex hull

Another important concept in convexity is that of forming the smallest convex set containing a given subset S in R^n. The convex hull of S is the set

$$Co(S) = \cap\{C : C \text{ convex in } R^n \text{ and } C \supseteq S\}.$$

The convex hull of a finite set of points is called a convex polytope.

It is clear that a convex polytope is always bounded. A convex polytope that contains all its boundary points is closed. A point x on the boundary of S is called an extreme point (or vertex) if there are no distinct points $x_1, x_2 \in S$ such that $x = \lambda x_1 + (1-\lambda)x_2$, $0 < \lambda < 1$. For example in the plane a triangle has 3 extreme points, and the sphere has all its boundary points as extreme points. The following theorem gives a very important characterization of a certain kind of convex set.

Theorem (Krein-Milman) 1.3.1: A closed, bounded convex set in R^n is the convex hull of its extreme points.

A (convex) polyhedron is the intersection of finitely many half spaces. Using matrix notation we can define a polyhedron to be the set of points $P=\{x \in R^n : Ax \leq b\}$ where A is an $m \times n$ matrix and $b \in R^m$. Polyhedral sets of this form are of central importance in mathematical programming.

1.4 Convex and concave functions

If $c \in R^n$, the linear function $f : R^n \to R$ defined by $f(x) = c^T x$ is known as a linear function on R^n.

Theorem 1.4.1: Let C be a convex polyhedron in R^n. Consider the linear programming problem

$$\min_{x \in C} f(x) = c^T x. \qquad \text{(LP)}$$

If (LP) has a solution then it occurs at some vertex of C.

Proof: Let $v_1, \ldots, v_k$ be the vertices of C, and let v be the vertex such that $f(v) = \min_{1 \leq i \leq k} \{f(v_i)\}$. Since for any $x \in C$, $x = \sum_{i=1}^{k} \lambda_i v_i$, $\lambda_i \geq 0$, and $\sum_{i=1}^{k} \lambda_i = 1$, we have that $f(x) = \sum_{i=1}^{k} \lambda_i f(v_i) \geq \sum_{i=1}^{k} \lambda_i f(v) = f(v)$.

A function $f : C \subseteq R^n \to R$, where C is a convex set, is called convex if

$$f(\lambda x_1 + (1-\lambda) x_2) \leq \lambda f(x_1) + (1-\lambda) f(x_2)$$

for any $x_1, x_2 \in C$ and $0 \leq \lambda \leq 1$. The function f is called concave iff $-f$ is convex.

If the function $f(x)$ has continuous second derivatives, then the following conditions give necessary and sufficient conditions for convexity:

a) $f(y) \geq f(x) + \nabla f(x)(y-x)$ for all $x, y \in C$, or

b) The Hessian is positive semidefinite for all $x \in C$.

Theorem 1.4.2: Let $f_i : S \subseteq R^n \rightarrow R$ be convex functions. Then

1) $\sum_{i=1}^{k} \alpha_i f_i(x)$, $\alpha_i \geq 0$, is also convex

2) $\max_{1 \leq i \leq k} (f_i(x))$ is convex

3) $\max_{1 \leq i \leq k} (0, f_i(x))$ is convex.

We are concerned here with the constrained nonlinear minimization problem of the general form

$$\min_{x \in P} f(x) \qquad \text{(NP)}$$

where P is a compact convex set in R^n and $f(x)$ is a continuous function defined on P.

A point $x^* \in P$ is said to be a relative or local minimum point if $f(x^*) \leq f(x)$ for all $\| x - x^* \| \leq \varepsilon$ for some $\varepsilon > 0$. We say that x^* is a global minimum point if $f(x^*) \leq f(x)$ for all $x \in P$.

When $f(x)$ is convex the problem (NP) is referred to as a convex programming problem, and when $f(x)$ is nonconvex we are talking about nonconvex programming. When the objective function $f(x)$ is convex (or more generally quasiconvex) then every local minimum is also global. This is no longer true for nonconvex functions.

Theorem 1.4.3: Suppose P is a convex compact set and $f : P \subseteq R^n \rightarrow R$ is a convex function. Then every local minimum of f over P is also global.

Proof: Let x^* be a local minimum and suppose that there exists another point y such that $f(y) < f(x^*)$. Then on the line $\lambda y + (1-\lambda)x^*$ $(0 < \lambda < 1)$ we have

$$f(\lambda y + (1-\lambda)x^*) \leq \lambda f(y) + (1-\lambda) f(x^*) < f(x^*)$$

contradicting the fact that x^* is a local minimum.

The above theorem makes convex programming a much easier problem to solve than the general nonlinear programming problem. Consider now the case where $f(x)$ is a concave function. In this case we may have many local minima which are not global. However, this problem has the following important property that also characterizes linear programming.

Theorem 1.4.4: Consider the problem

$$\text{global} \min_{x \in P} f(x)$$

where $f(x)$ is a continuous concave function defined on the bounded polyhedron P. Then every global (and local) minimum is attained at some vertex of P.

Proof: Similar to that of Theorem 1.4.1.

Note that since $\min f(x) = -\max(-f(x))$ minimization of a convex function is equivalent to maximization of a concave function(and vice versa). For continuously differentiable functions convexity and local optima are characterized using the gradient and the Hessian matrix of the function (e.g. [LUEN84], [STOE70]). For additional details regarding different convexity results see [MANG69], [GRUN67] and [ROCK70].

1.5 Convex envelopes

An important concept in nonconvex optimization is that of the convex envelope of a function.

Definition 1.5.1: Let $f : S \to R$ be a lower semi-continuous function, where S is a nonempty subset (of its domain) in R^n. Then the convex envelope of $f(x)$ taken over S is a function $F_S(x)$ such that

i) $F_S(x)$ is convex on the convex hull $Co(S)$

ii) $F_S(x) \leq f(x)$ for all $x \in S$

iii) If $h(x)$ is any convex function defined on $Co(S)$ such that $h(x) \le f(x)$ for all $x \in S$, then $h(x) \le F_S(x)$ for all $x \in Co(S)$.

From this definition, the convex envelope of a function is actually the best convex underestimator over S. Convex envelopes were first introduced by Kleibohm [KLEI67], who proved that with each nonconvex optimization problem is associated a convex one whose global solution is the same as that of the original problem. More precisely we have the following:

Theorem 1.5.1: Consider the problem

$$\text{global} \min_{x \in P} f(x)$$

where P is a convex set in R^n, and assume that the global minimum occurs at $x^* \in P$. Let $F(x)$ be the convex envelope of $f(x)$ over P. Then we have

$$\min_{x \in P} f(x) = \min_{x \in P} F(x)$$

and

$$\{y \in P : f(y) = \min_{x \in P} f(x)\} \subseteq \{y \in P : F(y) = \min_{x \in P} F(x)\}.$$

Proof: By definition $F(x) \le f(x)$ for all $x \in P$. Therefore

$$\min_{x \in P} F(x) \le \min_{x \in P} f(x) = f(x^*).$$

The constant function $G(x) = f(x^*) \le f(x)$ is a convex underestimating function. Again by the definition of the convex envelope we have that $F(x) \ge f(x^*)$ for all x and so

$$\min_{x \in P} F(x) \ge f(x^*) = \min_{x \in P} f(x).$$

We prove the second part by contradiction. Let x^* be a global minimum of $f(x)$ over P, and suppose that x^* is not a minimum of $F(x)$ over P. Let y^* be the minimum. Then

$$F(y^*) < F(x^*) \le f(x^*) = f^*.$$

Consider now the function $H(x) = \max(f^*, F(x))$. Then $H(x)$ is convex since the maximum of two convex functions is convex. Now $H(x) \ge F(x)$ for all $x \in P$ and