Recent advances and trends in global optimization

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Book Series:

- **Nonconvex Optimization and Applications**
- **Applied Optimization**
- **Combinatorial Optimization**
- **Massive Computing**

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- **C.A. Floudas and P. M. Pardalos (Editors), "Encyclopedia of Optimization", Kluwer Academic Publishers (6 Volumes), (2001).**

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CAO Conferences

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  November 19-21, 2003. Destin, Florida, USA.

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2 Global Continuous (or Discrete) Optimization Problem

$$f^* = f(x^*) = global\ min_{x \in D} f(x)\ (or\ max_{x \in D} f(x))$$

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[1] R. HORST AND P. M. PARDALOS (Editors), *Handbook of Global Optimization*, Kluwer Academic Publishers, 1995.

[2] P. M. PARDALOS AND H. E. ROMEIJN (Editors), *Handbook of Global Optimization Vol. 2*, Kluwer Academic Publishers, 2002.

[3] R. HORST, P. M. PARDALOS AND N.V. THOAI, *Introduction to Global Optimization*, Kluwer Academic Publishers, 1995 (**Second Edition** (2000)).

3 Why these problems are difficult?

The main focus of computational complexity is to analyze the **intrinsic difficulty** of optimization problems and to decide which of these problems are likely to be tractable. The pursuit for developing efficient algorithms also leads to **elegant general approaches** for solving optimization problems, and reveals **surprising connections** among problems and their solutions.

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The main focus of computational complexity is to analyze the **intrinsic difficulty** of optimization problems and to decide which of these problems are likely to be tractable. The pursuit for developing efficient algorithms also leads to **elegant general approaches** for solving optimization problems, and reveals **surprising connections** among problems and their solutions.

- The general problem is **NP-hard**. Furthermore, checking existence of a feasible point that satisfies the optimality conditions is also an **NP-hard** problem.

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- The general problem is **NP-hard**. Furthermore, checking existence of a feasible point that satisfies the optimality conditions is also an **NP-hard** problem.
- Fundamental problem:
  How to check convexity!

3 Why these problems are difficult?

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[1] P.M. PARDALOS, *Complexity in Numerical Optimization*, World Scientific, (1993).

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4 DC Optimization Problems

- Many powerful techniques in global optimization are based on the fact that many objective functions can be expressed as the **difference of two convex functions** (so called **d.c. functions**).

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- The space of d.c. functions is **closed** under many operations frequently encountered in optimization (i.e., sum, product, max, min, etc).
- **Hartman 1959**: Every locally d.c. function is d.c.

4 DC Optimization Problems

- For simplicity of notation, consider the d.c. program:

$$\begin{aligned} \min \quad & f(x) - g(x) \\ \text{s.t.} \quad & x \in D \end{aligned} \tag{1}$$

  where D is a *polytope* in R^n with nonempty interior, and f and g are *convex functions* on R^n.
- By introducing an additional variable t, Problem (1) can be converted into the equivalent problem:

4 DC Optimization Problems

- **Global Concave Minimization**:

$$\begin{aligned} \min \quad & t - g(x) \\ \text{s.t.} \quad & x \in D, f(x) - t \leq 0 \end{aligned} \tag{2}$$

with **concave objective function** $t - g(x)$ and **convex feasible set** $\{(x,t) \in R^{n+1} : x \in D, f(x) - t \leq 0\}$. If (x^*, t^*) is an optimal solution of (2), then x^* is an optimal solution of (1) and $t^* = f(x^*)$.

  - **Therefore, any d.c. program of type (1) can be solved by an algorithm for minimizing a concave function over a convex set.**

5 DI Optimization Problems

Monotonicity with respect to some variables (partial monotonicity) or to all variables (total monotonicity) is a natural property exhibited by many problems encountered in applications. The most general problem of **d.i. monotonic optimization** is:

$$\begin{aligned} \min \quad & f(x) - g(x) \\ \text{s.t.} \quad & f_i(x) - g_i(x) \leq 0, i = 1, \ldots, m \end{aligned} \tag{3}$$

where are all functions are increasing on R^n_+.

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- $\Leftrightarrow F(x) - G(x) \leq 0$, where

$$F(x) = \max_i \{f_i(x) + \sum_{i \neq j} g_j(x)\},$$

$$G(x) = \sum_i g_i(x)$$

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$$F(x) = \max_i \{f_i(x) + \sum_{i\neq j} g_j(x)\},$$

$$G(x) = \sum_i g_i(x)$$

- $F(x)$ and $G(x)$ are both increasing functions.

5 DI Optimization Problems

- Problem reduces to:

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & F(x) + t \le F(b), \\ & G(x) + t \ge F(b), \\ & 0 \le t \le F(b) - F(0), \\ & x \in [0, b] \subset R^n_+. \end{array}$$

- A set $G \subseteq R^n_+$ **normal** if for any two points x, x' such that $x' \le x$, if $x \in G$, then $x' \in G$.

5 DI Optimization Problems

Numerous global optimization problems can be reformulated as monotonic optimization problems. Such problems include multiplicative programming, nonconvex quadratic programming, polynomial programming, and Lipschitz optimization problems.

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[1] H. TUY, *Monotonic Optimization*, SIAM Journal of Optimization Vol. 11, No. 2 (2000), pp. 464-494.

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6 Is Continuous Optimization different than Discrete Optimization?

In combinatorial optimization and graph theory many approaches have been developed that link the discrete universe to the continuous universe through **geometric, analytic, and algebraic** techniques. Such techniques include global optimization formulations, semidefinite programming, and spectral theory.

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Examples:

- **Interior Point and Semidefinite Programming Algorithms**
- **Lovász number**
- **Goemans-Williamson Relaxation of the maximum cut problem**
- **Solution of Gilbert-Pollak's Conjecture (Du-Hwang)**

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Examples:

- $$\boxed{z \in \{0,1\} \Leftrightarrow z - z^2 = z(1-z) = 0}$$

  or

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- **Discrete Optimization $\Longleftrightarrow$ Continuous Optimization**
- **The key issue is:**

  Convex Optimization $\neq$ Nonconvex Optimization
- **The Linear complementarity problem (LCP) is equivalent to the linear mixed integer feasibility problem (Pardalos-Rosen)**

7 Continuous Approaches to Discrete Optimization Problems

References

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7 Continuous Approaches to Discrete Optimization Problems

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7.1 Satisfiability Problems

The satisfiability problem (SAT) is central in mathematical logic, computing theory, and many industrial application problems. Problems in computer vision, VLSI design, databases, automated reasoning, computer-aided design and manufacturing, involve the solution of instances of the satisfiability problem. Furthermore, SAT is the basic problem in computational complexity. Developing efficient exact algorithms and heuristics for satisfiability problems can lead to general approaches for solving combinatorial optimization problems.

7.1 Satisfiability Problems

Let $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_n$ be n clauses, involving m Boolean variables $x_1, x_2, \ldots, x_m$, which can take on only the values `true` or `false` (1 or 0). Define clause i to be

$$\mathcal{C}_i = \bigvee_{j=1}^{m_i} l_{ij},$$

where the literals $l_{ij} \in \{x_i, \bar{x}_i \mid i = 1, \ldots, m\}$.

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In the **Satisfiability Problem** (CNF)

$$\bigwedge_{i=1}^{n} \mathcal{C}_i = \bigwedge_{i=1}^{n} (\bigvee_{j=1}^{m_i} l_{ij})$$

one is to determine the assignment of truth values to the m variables that satisfy all n clauses.

7.1 Satisfiability Problems

Given a CNF formula $F(\mathbf{x})$ from $\{0,1\}^m$ to $\{0,1\}$ with n clauses $C_1, \ldots, C_n$, we define a real function $f(\mathbf{y})$ from E^m to E that transforms the SAT problem into an unconstrained **global optimization problem**:

$$\min_{\mathbf{y} \in \mathbf{E}^m} f(\mathbf{y}) \tag{4}$$

where

$$f(\mathbf{y}) = \sum_{i=1}^{n} c_i(\mathbf{y}). \tag{5}$$

A clause function $c_i(\mathbf{y})$ is a product of m *literal functions* $q_{ij}(y_j)$ $(1 \leq j \leq m)$:

$$c_i = \prod_{j=1}^{m} q_{ij}(y_j), \tag{6}$$

7.1 Satisfiability Problems

where

$$q_{ij}(y_j) = \begin{cases} |y_j - 1| & \text{if literal } x_j \text{ is in clause } C_i \\ |y_j + 1| & \text{if literal } \bar{x}_j \text{ is in clause } C_i \\ 1 & \text{if neither } x_j \text{ nor } \bar{x}_j \text{ is in } C_i \end{cases} \quad (7)$$

The correspondence between **x** and **y** is defined as follows (for $1 \leq i \leq m$):

$$x_i = \begin{cases} 1 & \text{if } y_i = 1 \\ 0 & \text{if } y_i = -1 \\ undefined & \text{otherwise} \end{cases}$$

F(**x**) is true iff f(**y**)=0 on the corresponding **y**$\in \{-1, 1\}^m$.

7.1 Satisfiability Problems

Next consider a polynomial unconstrained **global optimization** formulation:

$$\min_{\mathbf{y}\in\mathbf{E}^m} f(\mathbf{y}), \tag{8}$$

where

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$$q_{ij}(y_j) = \begin{cases} (y_j - 1)^{2p} & \text{if } x_j \text{ is in clause } C_i \\ (y_j + 1)^{2p} & \text{if } \bar{x_j} \text{ is in clause } C_i \\ 1 & \text{if neither } x_j \text{ nor } \bar{x_j} \text{ is in } C_i \end{cases} \quad (11)$$

where p is a positive integer.

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- **These models transform the SAT problem from a discrete, constrained decision problem into an unconstrained global optimization problem.**
- A good property of the transformation is that **these models establish a correspondence between the global minimum points of the objective function and the solutions of the original SAT problem.**
- A *CNF* $F(\mathbf{x})$ is true *if and only if* f takes the global minimum value 0 on the corresponding $\mathbf{y}$.

7.1 Satisfiability Problems

References

[1] D.-Z. Du, J. Gu, and P. M. Pardalos (Editors), *Satisfiability Problem: Theory and Applications, DIMACS Series Vol. 35, American Mathematical Society, (1997).*

7.2 The Maximum Clique Problem

Consider a graph $G = G(V, E)$, where $V = \{1, \ldots, n\}$ denotes the set of vertices (nodes), and E denotes the set of edges. Denote by (i, j) an edge joining vertex i and vertex j. A clique of G is a subset C of vertices with the property that every pair of vertices in C is joined by an edge. In other words, C is a clique if the subgraph $G(C)$ induced by C is complete. The maximum clique problem is the problem of finding a clique set C of maximal cardinality.

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Applications:

• project selection, classification theory, fault tolerance, coding theory, computer vision, economics, information retrieval, signal transmission theory, aligning DNA and protein sequences, and other specific problems.

Multivariable polynomial formulations

- If $x*$ is the solution of the following (**continuous**) quadratic program

$$\max f(x) = \sum_{i=1}^{n} x_i - \sum_{(i,j)\in E} x_i x_j = e^T x - 1/2 x^T A_G x$$
$$\text{subject to } 0 \leq x_i \leq 1 \text{ for all } 1 \leq i \leq n$$

then, $f(x*)$ equals the size of the maximum independent set.

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- If $x*$ is the solution of the following (**continuous**) polynomial program

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- **In both cases a polynomial time algorithm has been developed that finds independent sets of large size.**

Multivariable polynomial formulations

References

[1] J. Abello, S. Butenko, P. M. Pardalos and M. G. C. Resende, "Finding Independent Sets in a Graph Using Continuous Multivariable Polynomial Formulations", *Journal of Global Optimization 21* (2001), pp. 111-137.

Motzkin-Strauss type approaches

Consider the continuous **indefinite quadratic programming problem**

$$\begin{aligned} \max \quad & f_G(x) = \sum_{(i,j)\in E} x_i x_j = \frac{1}{2} x^T A_G x \\ \text{s.t.} \quad & x \in S = \{x = (x_1, \ldots, x_n)^T : \sum_{i=1}^n x_i = 1, \\ & x_i \geq 0 \quad (i = 1, \ldots, n)\}, \end{aligned} \tag{12}$$

where A_G is the adjacency matric of the graph G.

Motzkin-Strauss type approaches

- If $\alpha = \max\{f_G(x) : x \in S\}$, then G has a maximum clique C of size $\omega(G) = 1/(1-2\alpha)$. This maximum can be attained by setting $x_i = 1/k$ if $i \in C$ and $x_i = 0$ if $i \notin C$.

Motzkin-Strauss type approaches

- If $\alpha = \max\{f_G(x) : x \in S\}$, then G has a maximum clique C of size $\omega(G) = 1/(1-2\alpha)$. This maximum can be attained by setting $x_i = 1/k$ if $i \in C$ and $x_i = 0$ if $i \notin C$.
- (Pardalos and Phillips 1990) If A_G has r negative eigenvalues, then at least $n-r$ constraints are active at any global maximum x^* of $f(x)$. Therefore, if A_G has r negative eigenvalues, then the size $|C|$ of the maximum clique is bounded by $|C| \leq r+1$.

The Call Graph

The **“call graph”** comes from telecommunications traffic. The vertices of this graph are telephone numbers, and the edges are calls made from one number to another (including additional billing data, such as, the time of the call and its duration). The challenge in studying call graphs is that they are massive. Every day AT & T handles approximately 300 million long-distance calls.

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How can we visualize such massive graphs? To flash a terabyte of data on a 1000x1000 screen, you need to cram a megabyte of data into each pixel!

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A **giant connected component with 44,989,297** vertices was computed. The **maximum (quasi)-clique problem** is considered in this giant component.

References

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Optimization on Massive Graphs

Several other graphs have been considered:

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J. Abello, P. M. Pardalos and M.G.C. Resende (Editors), “Handbook of Massive Data Sets ”, Kluwer Academic Publishers, Dordrecht, 2002.

7.3 Minimax Problems

Techniques and principles of minimax theory play a key role in many areas of research, including game theory, optimization, scheduling, location, allocation, packing, and computational complexity.
In general, a minimax problem can be formulated as

$$\min_{x \in X} \max_{y \in Y} f(x, y) \tag{13}$$

where $f(x, y)$ is a function defined on the product of X and Y spaces.

7.3 Minimax Problems

References

[1] D.-Z. Du and P. M. Pardalos (Editors), *Minimax and Applications*, Kluwer Academic Publishers (1995).

[2] P. M. Pardalos and D.-Z. Du (Editors), *Network Design: Connectivity and Facilities Location, DIMACS Series Vol. 40, American Mathematical Society, (1998).*

7.3 Minimax Problems

Du and Hwang: Let $g(x) = \max_{i \in I} f_i(x)$ where the f_i's are continuous and pseudo-concave functions in a convex region X and $I(x)$ is a finite index set defined on a compact subset X' of P. Denote $M(x) = \{i \in I(x) \mid f_i(x) = g(x)\}$. Suppose that for any $x \in X$, there exists a neighborhood of x such that for any point y in the neighborhood, $M(y) \subseteq M(x)$. If the minimum value of $g(x)$ over X is achieved at an interior point of X', then **this minimum value is achieved at a DH-point,** i.e., a point with maximal $M(x)$ over X'. Moreover, if x is an interior minimum point in X' and $M(x) \subseteq M(y)$ for some $y \in X'$, then y is a minimum point.

7.3 Minimax Problems

Solution of Gilbert-Pollak's Conjecture

D.Z. DU AND F.K. HWANG, *An approach for proving lower bounds: solution of Gilbert-Pollak's conjecture on Steiner ratio*, *Proceedings 31th FOCS* (1990), 76-85.

7.3 Minimax Problems

The finite index set I in above can be replaced by a compact set. The result can be stated as follows:

Du and Pardalos: Let $f(x, y)$ be a continuous function on $X \times I$ where X is a polytope in $\mathbf{R}^m$ and I is a compact set in $\mathbf{R}^n$. Let $g(x) = \max_{y \in Y} f(x, y)$. If $f(x, y)$ is concave with respect to x, then the minimum value of $g(x)$ over X is achieved at some DH-point.

The proof of this result is also the same as the proof the previous theorem except that the existence of the neighborhood V needs to be derived from the compactness of I and the existence of $\hat{x}$ needs to be derived by Zorn's lemma.

7.3 Minimax Problems

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7.4 Multi-Quadratic 0–1

$P:$ min $f(x) = x^T Ax$, s.t.
$Bx \geq b,\ x^T Cx \geq \alpha,\ x \in \{0,1\}^n,\ \alpha$ is a constant.

$\bar{P}:$ min $g(s,x) = e^T s - Me^T x$, s.t.
$Ax - y - s + Me = 0,\ Bx \geq b,\ \ y \leq 2M(e - x),\ Cx - z + M'e \geq 0,\ e^T z - M'e^T x \geq \alpha,\ z \leq 2M'x,\ x \in \{0,1\}^n,\ y_i,\ s_i,\ z_i \geq 0$, where $M' = \|C\|_\infty$ and $M = \|A\|_\infty$.

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$Ax - y - s + Me = 0,\ Bx \geq b,\ \ y \leq 2M(e-x),\ Cx - z + M'e \geq 0,\ e^T z - M'e^T x \geq \alpha,\ z \leq 2M'x,\ x \in \{0,1\}^n,\ y_i,\ s_i,\ z_i \geq 0$, where $M' = \|C\|_\infty$ and $M = \|A\|_\infty$.

- **Theorem:** P has an optimal solution x^0 *iff* there exist $y^0,\ s^0,\ z^0$ such that (x^0, y^0, s^0, z^0) is an optimal solution of $\bar{P}$.

7.4 Multi-Quadratic 0–1

- Multi-Quadratic 0–1 programming can be reduced to linear mixed 0–1 programming problems. The number of new additional continuous variables needed for the reduction is only $O(n)$ and the number of initial 0–1 variables remains the same.

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- This technique allows us to solve Quadratic and Multi-Quadratic 0–1 Programming problems by applying any commercial package used for solving Linear Mixed Integer Programming problems, such as CPLEX, and XPRESS-MP by Dash Optimization.
- We used this technique in medical applications (epilepsy seizure prediction algorithms).

7.4 Multi-Quadratic 0–1

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8 Hierarchical (Multilevel) Optimization

The word *hierarchy* comes from the Greek word "$\iota\epsilon\rho\alpha\rho\chi\iota\alpha$", a system of graded (religious) authority.

8 Hierarchical (Multilevel) Optimization

The word *hierarchy* comes from the Greek word "$\iota\epsilon\rho\alpha\rho\chi\iota\alpha$", a system of graded (religious) authority.

The mathematical study of hierarchical structures can be found in diverse scientific disciplines including environment, ecology, biology, chemical engineering, classification theory, databases, network design, transportation, game theory and economics. The study of hierarchy occurring in biological structures reveals interesting properties as well as limitations due to different properties of molecules. To understand the complexity of hierarchical designs requires "**systems methodologies that are amenable to modeling, analyzing and optimizing**" (Haimes Y.Y. 1977) these structures.

8 Hierarchical (Multilevel) Optimization

Hierarchical optimization can be used to study properties of these hierarchical designs. In **hierarchical optimization, the constraint domain is implicitly determined by a series of optimization problems which must be solved in a predetermined sequence**.

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Hierarchical optimization can be used to study properties of these hierarchical designs. In **hierarchical optimization, the constraint domain is implicitly determined by a series of optimization problems which must be solved in a predetermined sequence**.

Hierarchical (or multi-level) optimization is a generalization of mathematical programming. The simplest two-level (or bilevel) programming problem describes a hierarchical system which is composed of two levels of decision makers and is stated as follows:

8 Hierarchical (Multilevel) Optimization

$$\textbf{(BP)} \quad \min_{y \in Y} \quad \varphi(x(y), y) \tag{14}$$

$$\text{subject to} \quad \psi(x(y), y) \leq 0 \tag{15}$$

$$\text{where} \quad x(y) = \arg\min_{x \in X} f(x, y) \tag{16}$$

$$\text{subject to} \quad g(x, y) \leq 0, \tag{17}$$

where $X \subset R^n$ and $Y \subset R^m$ are closed sets, $\psi : X \times Y \to R^p$ and $g : X \times Y \to R^q$ are multifunctions, φ and f are real-valued functions. The set $\mathcal{S} = \{(x, y) : x \in X, y \in Y, \psi(x, y) \leq 0, g(x, y) \leq 0\}$ is the *constraint set* of **BP**.

8 Hierarchical (Multilevel) Optimization

Multi-level programming problems have been studied extensively in their general setting during the last decade. In general, hierarchical optimization problems are nonconvex and therefore is not easy to find globally optimal solutions. Moreover, suboptimal solutions may lead to both theoretical and real-world paradoxes (as for instance in the case of network design problems).

8 Hierarchical (Multilevel) Optimization

Multi-level programming problems have been studied extensively in their general setting during the last decade. In general, hierarchical optimization problems are nonconvex and therefore is not easy to find globally optimal solutions. Moreover, suboptimal solutions may lead to both theoretical and real-world paradoxes (as for instance in the case of network design problems).

Many algorithmic developments are based on the properties of special cases of **BP** (and the more general problem) and reformulations to equivalent or approximating models, presumably more tractable. Most of the exact methods are based on **branch and bound or cutting plane techniques** and can handle only moderately size problems.

8 Hierarchical (Multilevel) Optimization

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9 Multivariate Partition Approach

The basic idea of this approach is to partition all the variables appearing in the optimization problem into several groups, each of which consists of some variables, and regard each group as a set of active variables for solving the original optimization problem.

With this approach we can formulate optimization problems as multi-level optimization problems.

9 Multivariate Partition Approach

- Consider the following problem:

$$\min_{x \in D \subseteq R^n} f(x), \tag{1}$$

  where D is a robust set and $f(x)$ is continuous.

- Let $\{\Delta_i, i = 1, \ldots, p\}$ be a partition of $S = \{x_1, \ldots, x_n\}, p > 1$.

9 Multivariate Partition Approach

- (1) is equivalent to the following multilevel optimization problem:

$$\min_{y_{\sigma_1} \in D_{\sigma_1}} \{ \min_{y_{\sigma_2} \in D_{\sigma_2}} \ldots \{ \min_{y_{\sigma_p} \in D_{\sigma_p}} f(\Delta_1, \ldots, \Delta_p)\} \ldots \}, \quad (2)$$

where $\sigma = (\sigma_1, \ldots, \sigma_n)$ is any permutation of $\{1, 2, \ldots, p\}$. The components of the vector y_{σ_i} coincide with the elements of Δ_i and D_{σ_i} is defined as a feasible domain of y_{σ_i}.

9 Multivariate Partition Approach

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9 Multivariate Partition Approach

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10 Nonconvex Network Problems

Pharmaceutical Industry Supply Chain Management, E-commerce

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10 Nonconvex Network Problems

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- Dynamic Slope Scaling Procedure (DSSP) for Fixed Charge Network Problems.
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- New local search techniques.

10 Nonconvex Network Problems

Computational results in bipartite networks with up to 350350 arcs and 1351 nodes, and layered networks with up to 297000 arcs and 2501 nodes are very promising.

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11 Parallel Algorithms

We discussed a small fraction of research directions in global optimization. Furthermore, the existence of commercial multiprocessing computers has created substantial interest in exploring the uses of **parallel processing** for solving global optimization problems.

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11 **Parallel Algorithms**

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HERACLITUS

“Seekers after gold dig up much earth and find little”

“The lord whose oracle is at Delphi neither speaks nor conceals, but gives signs”

- HERACLITUS