Recent Advances in Global Optimization

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"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**

1 Global Optimization Problem

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

References

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2 Complexity Issues

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 general problem is **NP-hard**.

Surprise: Consider the problem:

$$\begin{aligned} \min \quad & f(x) = c^T x + \tfrac{1}{2} x^T Q x \\ \text{s.t.} \quad & Ax \geq b \end{aligned} \tag{1}$$

where Q is an $n \times n$ symmetric matrix, and $c \in R^n$.
If Q has rank one and the only zero eigenvalue is negative, then the problem is **NP-hard** (which is NOT true for network problems).

Another Surprise: Checking if a feasible point is a local optimum is also an **NP-hard** problem.

How far can we go? Consider the following quadratic problem

$$\begin{array}{ll} \min & f(x) = c^T x + \frac{1}{2} x^T Q x \\ \text{s.t.} & x \geq 0 \end{array} \tag{2}$$

where Q is an $n \times n$ symmetric matrix, and $c \in R^n$. The Kuhn-Tucker optimality conditions for this problem become the following so–call ed linear complementarity problem (denoted by LCP(Q, c)): Find $x \in R^n$ (or prove that no such an x exists) such that

$$Qx + c \geq 0, \; x \geq 0 \tag{3}$$

$$x^T (Qx + c) = 0. \tag{4}$$

Hence, the complexity of finding (or proving existence) of Kuhn-Tucker points for the above quadratic problem is reduced to the complexity of solving the corresponding LCP which is **NP-hard**.

Nonconvex problems are very difficult to solve in the worst case. To analyze the average performance of algorithms is a very challenging problem!

Fundamental Problem about Convexity

In most classical optimization algorithms, the underlying theory is based on the assumption that the objective function (or the feasible domain) is convex.

Unless the function has constant Hessian (i.e. is quadratic) or has a very special structure, convexity is not easily recognizable. **Even for multivariable polynomials there is no known computable procedure to decide convexity**.
Therefore, from the practical point of view, a general objective function can be assumed to be neither convex nor concave, having multiple local optima.

3 Continuous Approaches to Discrete Optimization Problems

In 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.

$$\boxed{z \in \{0,1\} \Leftrightarrow z + w = 1, z \geq 0, w \geq 0, zw = 0}$$

Integer constraints are equivalent to continuous nonconvex constraints (complementarity!)

Other approaches:

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

Discrete Optimization $\Longleftrightarrow$ Continuous Optimization

The key issue is:

Convex Optimization $\neq$ Nonconvex Optimization

References

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4 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.

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.**

Maximum Clique Optimization Software Developed

- **C-P.f** is an exact algorithm developed by R. Carraghan and P.M. Pardalos for finding the maximum clique in an arbitrary graph. The FORTRAN code published in OR Letters and many versions in other languages are available.

- The code **P-R.f** is an exact algorithm for the maximum clique problem, based on a quadratic 0-1 formulation (P.M. Pardalos & G.P. Rodgers). This is the first public domain code for the maximum clique problem.

- **Q01SUBS** solves unconstrained quadratic 0-1 problems both for dense and sparse matrices, including concave quadratic minimization problems with box constraints (P.M. Pardalos & G.Rodgers). The code has been used in many industrial and business applications. This is the first public domain code for quadratic zero-one problems.

- **CBHMC** is a Continuous Based Heuristic for the Maximum Clique problem (Panos M. Pardalos, Sara Ericson, Luana. E. Gibbons, Don W. Hearn).

Motzkin-Strauss Formulation:

Consider the continuous **indefinite quadratic programming problem**

$$\begin{aligned} \max \quad & f_G(x) = \sum_{(i,j)\in E} x_i x_j = \tfrac{1}{2} x^T A_G x \\ \text{s.t.} \quad & x \in S = \{x = (x_1, \ldots, x_n)^T : \sum_{i=1}^{n} x_i = 1, \\ & x_i \geq 0 \quad (i = 1, \ldots, n)\}, \end{aligned} \qquad (5)$$

where A_G is the adjacency matric of the graph G.

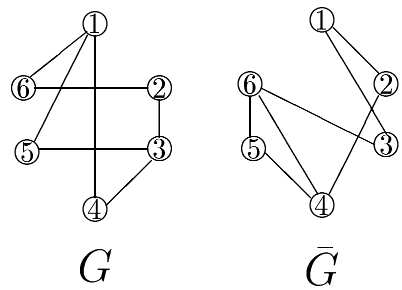
If $\alpha = \max\{f_G(x) : x \in S\}$, then G has a maximum clique C of size $\omega(G) = 1/(1-2\alpha)$. This maximum can be attained by setting $x_i = 1/k$ if $i \in C$ and $x_i = 0$ if $i \notin C$.

Another Continuous Formulation:

If $x*$ is the solution of the following indefinite quadratic programming problem:

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

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



Quadratic 0-1 formulation:

The maximum clique problem is equivalent to the following global quadratic zero-one problem

$$\text{global } \min f(x) = x^T A x, \tag{6}$$

$$\text{s.t. } x \in \{0,1\}^n, \text{ where } A = A_{\overline{G}} - I.$$

Remark: There is a one to one correspondence between maximal cliques of G and discrete local minima of the quadratic 0-1 problem.

Maximum weight independent set problem

$$\text{global } \max f(x) = \sum_{i=1}^{n} w_i x_i, \tag{7}$$
$$\text{s.t. } x_i + x_j \leq 1, \ \forall\, (i,j) \in E, \ x \in \{0,1\}^n.$$

The above formulation is equivalent to the following **continuous** quadratically constrained global optimization problem

$$\text{global } \max f(x) = \sum_{i=1}^{n} w_i x_i, \tag{8}$$
$$\text{s.t. } x_i x_j = 0, \ \forall\, (i,j) \in E,$$
$${x_i}^2 - x_i = 0, \ i = 1, 2, ..., n.$$

Recent Work on Massive Data Sets:

The proliferarion of massive data sets brings with it a series of special computational challenges. Many of these data sets can be modeled as very large multidiagraphs with a special set of edge attibutes that represent special characteristics of the application at hand.
Understanding the structure of the underlying diagraph is essential for storage organization and information retrieval.
In our experiments with data from **telecomunications trafic**, the corresponding mulrigraph has **53,767,087 vertices and over 170 milion of edges**. A **giant connected component with 44,989,297** vertices was computed. The maximum clique (and quasi-clique) problem is considered in this giant component.

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Hamiltonian Cycle Problem (Filar-Pardalos)

Given a directed graph, find a path that enters every node exactly once before returning to the starting node, or determine that no such path exists.

This problem has been formulated as a continuous quadratic optimization problem.

The Steiner Problem in Graphs (Pardalos-Khoury-Du)

Let $G = (\mathcal{N}, \mathcal{A}, \mathcal{C})$ be an undirected graph, where $\mathcal{N} = \{1, \ldots, n\}$ is a set of nodes, $\mathcal{A}$ is a set of undirected arcs (i, j) with each arc incident to two nodes, and $\mathcal{C}$ is a set of nonnegative costs c_{ij} associated with undirected arcs (i, j). Then, the Steiner problem in Graphs (SPG) is defined as follows:

Instance: A graph $G = (\mathcal{N}, \mathcal{A}, \mathcal{C})$, a node subset $\mathcal{R} \in \mathcal{N}$.
Question: Find the minimum cost tree, on G, that would connect all the vertices in $\mathcal{R}$.

New Exact Algorithms and Heuristics have been developed

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

$$\min_{x \in X} \max_{y \in Y} f(x, y) \tag{9}$$

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

References

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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.

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.

Sphere Packing (Pardalos-Maranas-Floudas)

Consider the problems of packing circles in a square. What is the maximum radius of n equal circles that can be packed into a unit square?
Consider the optimization problem:

$$\min_{x_i \in [0,1]\times[0,1]} \max_{1\le i<j\le n} -\|x_i - x_j\|.$$

Let r_n denote the maximum radius in the first problem and d_n the min-max distance in the second problem. It is easy to show that

$$r_n = \frac{d_n}{2(1+d_n)}.$$

Exact solution exist only for n=1-10, 16, 23, 36. We obtained some new results (n=15, 28, 29) using the minimax approach.

5 Nonlinear Assignment Problems

Given a set $\mathcal{N} = \{1, 2, \ldots, n\}$ and $n \times n$ matrices $F = (f_{ij})$ and $D = (d_{kl})$, the **quadratic assignment problem** (QAP) can be stated as follows:

$$\min_{p \in \Pi_{\mathcal{N}}} \sum_{i=1}^{n} \sum_{j=1}^{n} f_{ij} d_{p(i)p(j)},$$

where $\Pi_{\mathcal{N}}$ is the set of all permutations of $\mathcal{N}$.

Generalizations: **Biquadratic** Assignment Problem, **3-dimensional** Assignment, etc.

Applications:

- **Location Theory, VLSI Problems**
- **Statistical Data Analysis**
- **Parallel and Distributing Computing**
- **MultiTarget MultiSensor Tracking Problems**
- **The Turbine Balancing Problem**

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Quadratic Integer Programming

The unconstrained quadratic zero-one programming problem (QP) has the form:

$$global\ min\ f(x) \ = \ c^T x + x^T A x$$

subject to

$$x \in \{0,\ 1\}^n \tag{10}$$

where A is an $n \times n$ rational matrix and c is a rational vector of length n.

A public domain code is available

6 Hierarchical 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.

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:

$$\textbf{(BP)} \quad \min_{y \in Y} \quad \varphi(x(y), y) \tag{11}$$
$$\text{subject to} \quad \psi(x(y), y) \leq 0 \tag{12}$$
$$\text{where} \quad x(y) = \arg\min_{x \in X} f(x, y) \tag{13}$$
$$\text{subject to} \quad g(x, y) \leq 0, \tag{14}$$

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**.

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.

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7 Nonconvex Potential Energy Functions

Problem: Compute the native 3 dimensional conformation (folded state) of a (globular) protein given its amino acid sequence, possibly in the presence of additional agents (e.g., drugs).

Given a cluster of N atoms in $3-$ dimensional space, the potential energy function of the cluster is defined as the summation (over all of the pairs) of the two-body interatomic pair potentials. Let the center of the N atoms be $a_1, \cdots, a_N$. The potential energy function is defined as follows.

$$V_N(a_1, \cdots, a_N) = \sum_{1 \leq i < j \leq N} v(||a_i - a_j||), \tag{15}$$

where $||.||$ is the Euclidean norm and $v(r)$ is the interatomic pair potential.

There are many potential functions that have been considered, e.g.

$v(r) = r^{-12} - 2r^{-6}$ (**Lennard-Jones**)

The global minimization of potential energy functions plays an important role in the determination of ground states or stable states of certain classes of molecular clusters and proteins.

Our approaches:

- **Multispace Search Techniques**
- **Tabu Search**
- **Fast Function Evaluations**
- **Concave Minimization Approaches**

Remark: Nonconvex Energy Functions appear in many areas of engineerings design.

7.1 Global Concave Minimization Approaches

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**).

If $D(x)$ is an objective function in R^n, then the representation $D(x) = p(x) - q(x)$, where p, q are convex functions is said to be a d.c. decomposition of D.

• Every real-valued function on R^n whose second partial derivatives a re continuous is d.c. In that case

$$D(x) = (D(x) + \mu||x||^2) - \mu||x||^2 \tag{16}$$

for some $\mu > 0$. Therefore the d.c. decomposition of D is not unique. It is clear that the function

$$V_N(a_1, \cdots, a_N) = \sum_{1 \leq i < j \leq N} v(||a_i - a_j||), \tag{17}$$

is a d.c. function with many d.c. decompositions.

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

$$\begin{aligned} \min \quad & f(x) - g(x) \\ \text{s.t.} \quad & x \in D \end{aligned} \tag{18}$$

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 (18) can be converted into the equivalent problem

- **Global Concave Minimization**:

$$\begin{aligned} \min \quad & t - g(x) \\ \text{s.t.} \quad & x \in D, f(x) - t \leq 0 \end{aligned} \tag{19}$$

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 (19), then x^* is an optimal solution of (18) and $t^* = f(x^*)$.

Therefore, any d.c. program of type (18) can be solved by an algorithm for minimizing a concave function over a convex set. There are many algorithms for the general problem of minimizing a concave function over a convex set.

Branch and bound type algorithms that exploit the special structure of this problem have deen developed. A new type of branching process is introduced in which every partition set is a *simplicial prism* in R^{n+1}, and the lower bound will be constructed by means of a *piecewise linear approximation* of the convex function $f(x) - t$.

A branch and bound algorithm for the original problem is based on the the above techniques for computing bounds and a prismatic partition of the domain. The efficiency of the branch and bound algorithm is based on the quality of bounds. Moreover, since the original nonconvex energy function does not have a unique d.c. decomposition, experimentation with different decompositions will indicate which one will be best to chose.

7.2 Problem: The Distance Geometry Problem

The **distance geometry problem** is that of determining the coordinates of a set of points in space from a given set of pairwise distance measurements.

We can express the distance geometry problem as the problem of finding three-dimensional coordinates $x_1, \ldots, x_n$ that satisfy:

$$\|x_i - x_j\| = d_{i,j},$$

where i and j are the indexs of the set $1, \ldots, n$ that describes n ranked atoms, and $d_{i,j}$ is the given distance between two atoms i and j.

Generally, we can only know a set of pairwise distances between atoms. This means the distance matrix $D = (d_{i,j})$ is sparse. For any triple of atoms $\{i, j, k\}$, in which all pairwise distances are known, they should satisfy the following triangle inequality:

$$d_{i,j} \leq d_{i,k} + d_{k,j}.$$

Since the distance data available from NMR spectroscopy is necessarily imprecise, we use only upper and lower bounds on the distances $d_{i,j}$. Therefore, we can also express the distance geometry problem as:

$$l_{i,j} \leq \|x_i - x_j\| \leq u_{i,j},$$

where $l_{i,j}$ and $u_{i,j}$ are the lower and upper bounds on the distance constraints, respectively.

We call both $l_{i,j} \leq \|x_i - x_j\| \leq u_{i,j}$ and $\|x_i - x_j\| = d_{i,j}$ the distance constrains.

The distance geometry problem is NP hard even in the one dimensional case.

Many algorithms for the distance geometry problem are based on the minimization of an error function which measures the violations of the distance constraints. One such error function is defined by:

$$f(x) = \sum \left(max \left(0, \frac{\|x_i - x_j\|^2}{u_{i,j}^2} - 1\right) \right)^2 + \left(max \left(0, 1 - \frac{\|x_i - x_j\|^2}{l_{i,j}^2}\right) \right)^2,$$

where the sum Σ ranges over all the given pairwise atoms whose distances are known. Another error function is:

$$f(x) = \frac{1}{2} \sum \left(\|x_i - x_j\|^2 - d_{i,j}^2 \right)^2.$$

The distance geometry problem is defined as the following global optimization problem:

$$\text{M}in \;\; f(x),$$

where the objective function $f(x)$ is the error function defined above.

Algorithmic Approaches:

- Multiquadratic Programming Problem
- Tabu Based Pattern Search Heuristic

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8 Nonconvex Network Problems

- Dynamic Slope Scaling Procedure (DSSP) for Fixed Charge Network Problems.
- Reduction of nonconvex discontinuous network flow problems to fixed charge network flow problems.
- New heuristics based on DSSP and dynamic domain contraction technique for large-scale problems.

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9 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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10 The Road Less Traveled

- **Satisfiability Problem**
- **Feedback Vertex Set Problem**
- **Graph Coloring**
- **Frequency Assignment Problem**
- **Approximate Algorithms**
- **Randomized Algorithms**