

Computational Models and Challenging Optimization Problems

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What are the limits of Computation?

You will not find out the limits of the soul when you go, travelling on every road, so deep a logos does it have.

Whosoever wishes to know about the world must learn about it in its particular details. Knowledge is not intelligence.

In searching for the truth be ready for the unexpected.

Change alone is unchanging.

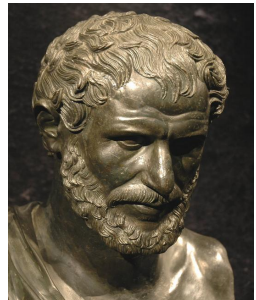
The same road goes both up and down.

The beginning of a circle is also its end.

Not I, but the world says it: all is one.

And yet everything comes in season.

- Heraclitus (c.540 - c.475 BC)



Some Fundamental Questions

- What are the limits of what **humans** can compute?
- What are the limits of what **machines** can compute?
- Are these limits the same?
- What are the physical foundations and limitations of computation?

Charles H. Bennet and Rolf Landauer, *The fundamental physical limits of computation*, *Scientific American* (June 1 2011)

Igor L. Markov, *Limits of fundamental limits to computation*, *Nature* (Aug 1 2014), vol 512, pp. 147-154.

Analog and Digital Computers

The Antikythera mechanism is an ancient analog computer designed to predict astronomical positions and eclipses (recovered from a shipwreck off the Greek island of Antikythera in 1900).

<http://www.antikythera-mechanism.gr/>



- Digital computers
- Mechanical analog computers
- Electronic analog computers
- Turing computability (1936)

Church Theorem

An analog computer with finite resources can be simulated by a digital computer.

Anastasios Vergis, Kenneth Steiglitz, and Bradley Dickinson, *The Complexity of Analog Computation*, Mathematics & Computers in Simulation 28 (1986) 91-113

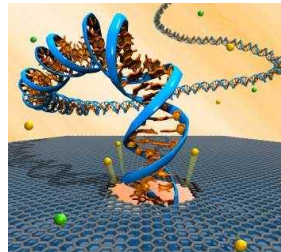
Biocomputers

- Biocomputers perform computational tasks using biologically derived materials. For example, DNA, proteins, peptides etc to perform computational tasks involving storing, retrieving, and processing data.
- Since biological organisms have the ability to self-replicate and self-assemble into functional components, biocomputers could be produced in large quantities from cultures (without machinery needed to assemble them).

DNA Computers

Adleman, L. M. (1994). *"Molecular computation of solutions to combinatorial problems,"* Science 266, pp. 1021-1024.

- This is the first DNA computing paper. It presents a proof-of-concept use of DNA as a form of computation to solve a seven-point Hamiltonian path problem.



Recent Development

- A three-terminal device architecture, termed the transcriptor, that uses bacteriophage serine integrases to control the flow of RNA polymerase along DNA has been developed.

Jerome Bonnet, Peter Yin, Monica E. Ortiz, Pakpoom Subsoontorn, Drew Endy (2013). *Amplifying Genetic Logic Gates*, Science 340, pp. 599-603

- Biochemical, Bioelectronic, and Biochemical computers
- Biochemical and DNA nanocomputers

Ongoing exciting research.

[First conference](#) on DNA Based Computers (DIMACS, Princeton 1995)

[20th International Conference](#) on DNA Computing and Molecular Programming (2014)

<http://link.springer.com/openurl.asp?genre=issue&issn=0302-9743&volume=8727>

Next Information Revolution

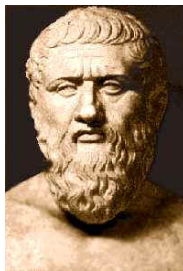
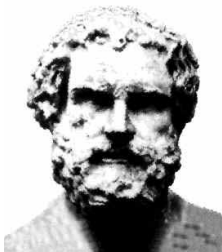
Quantum Computing?

- Quantum computation and quantum information is the study of the information processing tasks that can be accomplished using quantum mechanical systems.

Michael A. Nielsen, Isaac L. Chuang, *Quantum Computation and Quantum Information* (Cambridge Series on Information and the Natural Sciences) 2000.

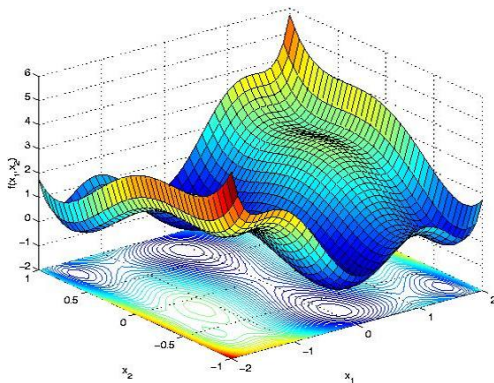
- Quantum computers use quantum-mechanical phenomena (superposition, entanglement) to operate on data.

Very early concepts in Greek philosophers (Democritus, Zeno, etc)



Yuri Mann (1980)
Richard Feynman (1982)
Tommaso Toffoli (1982)
David Deutsch (1985)
Quantum mechanics (early 1920s...)

What is (global) optimization?



Challenging Questions

- Do we find a globally optimal solution?
 - We need a certificate of optimality
- Do we compute “good” locally optimal solutions? (or points that satisfy the optimality conditions?)
- Do we compute “better” solutions than “known” solutions?

When only global optimization matters

- $(\mathcal{P}) \begin{cases} \text{Minimize } f(A) := \text{rank of } A \\ \text{subject to } A \in C. \end{cases}$
 - C is a subset of $\mathcal{M}_{m,n}(\mathbb{R})$
- $(\mathcal{Q}) \begin{cases} \text{Minimize } c(x) \\ \text{subject to } x \in S \end{cases}$
 - $c(x)$ is the number of nonzero components of x .
 - S is a subset of \mathbb{R}^n
- **Every admissible point in (\mathcal{P}) is a local minimizer.**



J.-B. Hiriart-Urruty: *When only global optimization matters.*
J. Global Optimization 56(3): 761-763 2013

References



Abello, J. and Pardalos, P.M. and Resende, M. G. C, *Handbook of Massive Data Sets*. Kluwer Academic Publisher, Holland 1994.



Dixon, L.C.W. and Szegő, G.P., *Towards Global Optimisation* (2 volumes). North Holland, Amsterdam, 1975.



Horst, R. and Pardalos, P. M., *Handbook of Global Optimization*. Kluwer, Dordrecht, 1995.



Horst, R. and Pardalos, P. M. and Thoai, N.V., editors *Introduction to Global Optimization*. volume 3 of Nonconvex Optimization and its Applications. Kluwer Academic Publishers, Dordrecht, Holland 1995.



Horst, R. and Tuy, H., *Global Optimization (Deterministic Approach)*. Springer, Berlin, 1990.



Pardalos, P.M., **On the passage from local to global in optimization**. In J.R, Birge and K.G. Murty, editors, *Mathematical Programming: State of the Art*, pages 220 -247, University of Michigan, Ann Arbor, 1994.



Pardalos, P.M. and Romeijn, E.H., *Handbook of Global Optimization*. Volume 2, Kluwer, Dordrecht, 2002.



Pardalos, P.M. and Rosen, J.B., *Constrained Global Optimization; Algorithms and Applications*. Volume 268, Lecture Notes in Computer Science, Springer, Berlin 1987.

Section 1

Introduction

Some History

Greek mathematicians solved optimally some problems related to their geometrical studies.

- Euclid considered the minimal distance between a point and a line.
- Heron proved that light travels between two points through the path with shortest length when reflecting from a mirror.

Optimality in Nature

- Fermat's principle (principle of least time)
- Hamilton's principle (principle of stationary action)
- Maupertuis' principle (principle of least action)

1951: H.W. Kuhn and A.W. Tucker, Optimality conditions for nonlinear problems.

F. John in 1948 and W. Karush in 1939 had presented similar conditions

Optimality in Biology

- **Optimality principles in biology** (R. Rosen, New York: Plenum Press, 1967).
- **Optimality theory in evolutionary biology** (G. Parker and J. Maynard Smith, Nature 348. 27 - 33, 1990)
- Optimization models help us to test our insight into the biological constraints that influence the outcome of evolution
- Optimization models serve to improve our understanding about adaptations, rather than to demonstrate that natural selection produces optimal solutions.
- Example: What determines the radius of the aorta? The human aortic radius is about 1.5cm (minimize the power dissipated through blood flow)

Section 2

Complexity Issues

Challenging Problems

- Obtain general optimality conditions.
- For large constrained global optimization.
 - feasibility problem.
 - sparsity/structure.

Complexity of Kuhn-Tucker Conditions

Consider the following quadratic problem:

$$\begin{aligned} \min \quad & f(x) = c^T x + \frac{1}{2} x^T Q x \\ \text{st.} \quad & x \geq 0, \end{aligned}$$

where Q is an arbitrary $n \times n$ symmetric matrix, $x \in R^n$. The KKT optimality conditions for this problem become so-called linear complementarity problem ($LCP(Q, c)$)

Complexity of Kuhn-Tucker Conditions

Linear complementarity problem $LCP(Q, c)$ is formulated as follows.

Find $x \in R^n$ (or prove that no such an x exists) such that:

$$Qx + c \geq 0, \quad x \geq 0$$

$$x^T(Qx + c) = 0.$$

Theorem

Theorem (Horst, Pardalos, Thoai, 1994 - [2])

The problem $LCP(Q, c)$ is NP-hard.

Proof.

Consider the following $LCP(Q, c)$ problem in R^{n+3} defined by

$$Q_{(n+3) \times (n+3)} = \begin{pmatrix} -I_n & e_n & -e_n & 0_n \\ e_n^T & -1 & -1 & -1 \\ -e_n^T & -1 & -1 & -1 \\ 0_n^T & -1 & -1 & -1 \end{pmatrix}, \quad c_{n+3} = (a_1, \dots, a_n, -b, b, 0),$$

where a_i , $i = 1, \dots, n$, and b are positive integers, I_n is the $n \times n$ -unit matrix and the vectors $e_n \in R^n$, $0_n \in R^n$ are defined by

$$e_n^T = (1, 1, \dots, 1), \quad 0_n^T = (0, 0, \dots, 0).$$

Theorem (Continue)

Proof.

Consider the following knapsack problem. Find a feasible solution to the system

$$\sum_{i=1}^n a_i x_i = b, \quad x_i \in \{0, 1\} \quad (i = 1, \dots, n).$$

This problem is known to be NP-complete. We will show that $LCP(Q, c)$ is solvable iff the associated knapsack problem is solvable.

If x solves the knapsack problem, then $y = (a_1 x_1, \dots, a_n x_n, 0, 0, 0)^T$ solves $LCP(Q, c)$.

Conversely, assume y solves the considered $LCP(Q, c)$. This implies that $\sum_{i=1}^n y_i = b$ and $0 \leq y_i \leq a_i$. Finally, if $y_i < a_i$, then $y^T(Qy + c) = 0$ enforces $y_i = 0$. Hence, $x = (\frac{y_1}{a_1}, \dots, \frac{y_n}{a_n})$ solves the knapsack problem. □

Complexity of local minimization

Consider following quadratic problem:

$$\begin{array}{ll}\min & f(x) \\ \text{s.t.} & Ax \geq b, x \geq 0\end{array}$$

where $f(x)$ is an indefinite quadratic function. We showed, that the problem of checking local optimality for a feasible point and the problem of checking whether a local minimum is strict are NP-hard.

3-satisfiability problem

Consider the 3-satisfiability (3-SAT) problem: given a set of Boolean variables x_1, \dots, x_n and given a Boolean expression S (in conjunctive normal form) with exactly 3 literals per clause,

$$S = \bigwedge_{i=1}^m \left(\bigvee_{j=1}^3 l_{ij} \right), \quad l_{ij} \in \{x_i, \bar{x}_i \mid i = 1, \dots, n\}$$

is there a truth assignment for the variables x_i which makes S true?

The 3-SAT problem is known to be NP-complete.

A Global Optimization Approach

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

$$\min_{y \in E^m} f(y) \quad (1)$$

where

$$f(y) = \sum_{i=1}^n c_i(y) \quad (2)$$

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

$$c_i = \prod_{j=1}^m q_{ij}(y_{ij}) \quad (3)$$

A Global Optimization Approach

where

$$q_{ij}(y_i) = \begin{cases} |y_i - 1|, & \text{if literal } x_j \text{ is in clause } C_i \\ |y_i + 1|, & \text{if literal } \bar{x}_j \text{ is in clause } C_i \\ 1, & \text{if neither } x_j \text{ nor } \bar{x}_j \text{ is in } C_i \end{cases} \quad (4)$$

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

$$x_i = \begin{cases} 1, & \text{if } y_i = 1 \\ 0, & \text{if } y_i = -1 \\ \text{undefined}, & \text{otherwise} \end{cases} \quad (5)$$

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

A Global Optimization Approach

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

$$\min_{y \in E^m} f(y) \quad (6)$$

where

$$f(y) = \sum_{i=1}^n c_i(y). \quad (7)$$

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

$$c_i = \prod_{j=1}^m q_{ij}(y_j) \quad (8)$$

A Global Optimization Approach

where

$$q_{ij}(y_j) = \begin{cases} |y_j - 1|^{2p}, & \text{if } x_j \text{ is in clause } C_i \\ |y_j + 1|^{2p}, & \text{if } \bar{x}_j \text{ is in clause } C_i \\ 1, & \text{if neither } x_j \text{ nor } \bar{x}_j \text{ is in } C_i \end{cases} \quad (9)$$

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

$$\mathbf{x}_i = \begin{cases} 1, & \text{if } y_i = 1 \\ 0, & \text{if } y_i = -1 \\ \text{undefined}, & \text{otherwise} \end{cases} \quad (10)$$

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

A Global Optimization Approach

- 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* $F(x)$ is true if and only if f takes the global minimum value 0 on the corresponding y

Complexity and Phase Transitions

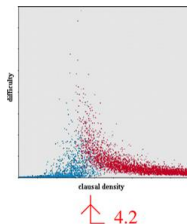
- **Random 3-SAT problem:**

- Three variables per clause are chosen randomly from $\{x_1, \dots, x_N\}$ and negated randomly with probability $\frac{1}{2}$
 - Example: $(x_1 \vee x_{20} \vee \bar{x}_{13}) \wedge (\bar{x}_{21} \vee x_1 \vee x_9) \wedge \dots (x_{95} \vee \bar{x}_8 \vee \bar{x}_{15})$
- Define the threshold: $\alpha = \frac{\text{Number of Clauses}}{\text{Number of Variables}}$

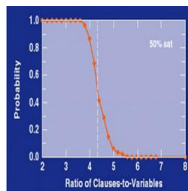
Phase transition threshold: $\alpha_C \approx 4.26$

- Research in the intersection of Computer Science, Information Theory and Statistical Physics

Complexity and Phase Transition



(a)



(b)

Turing's algorithmic lens: From computability to complexity theory

(J. Diza and C. Torras) Arbor - Ciencia, Pensamiento y Cultura, Vol. 189

No. 764(2013). <http://dx.doi.org/10.3989/arbor.2013.764n6003>

Phase Transitions References



Felderhof, B.U., *Do phase transition exist?*. Nature, volume 225, 1970.



Monasson, M. and Zechina, R. and Kirkpatrick, S. and Selman, B. and Troyansky, L., *Determining computational complexity from characteristic 'phase transitions'*. Nature, volume 400, 1999.



Achlioptas, D. and Naor, A. and Peres, Y., *Rigorous location of phase transitions in hard optimization problems*. Nature, volume 435, 2005.



Barbosa, V.C. and Ferreira, R.G., *On the phase transitions of graph coloring and independent sets*. Physica A, volume 343, pages 401 -423, 2004.



Malyshev, D.S., *Analysis pf the impact of the number of edges in connected graphs on the time complexity of an independent set problem*. Journal of Applied and Industrial Mathematics, volume 1, number 1, pages 1 -4, 2012.

Challenging Problems

- Phase transition in continuous optimization.
- What is the boundary between polynomially solvable and NP-hard problems in global optimization?

Construction of indefinite quadratic problem instances

For each instance of a 3-SAT problem we construct an instance of an optimization problem in the real variables x_0, \dots, x_n . For each clause in S we associate a linear inequality in a following way:

If $l_{ij} = x_k$, we retain x_k

If $l_{ij} = \bar{x}_k$ we use $1 - x_k$

We add an additional variable x_0 and require that the corresponding sum is greater than or equal to $\frac{3}{2}$. Thus, we associate to S a system of linear inequalities $A_S x \geq (3/2 + c)$. Let $D(S) \subset R^{n+1}$ be a feasible set of points satisfying these constraints.

With a given instance of the 3-SAT problem we associate the following indefinite quadratic problem:

$$\min_{x \in D(S)} f(x) = - \sum_{i=1}^n (x_i - (1/2 - x_0))(x_i - (1/2 + x_0)).$$

Complexity of local minimization

Theorem (Pardalos, Schnitger, 1988 - [3])

S is satisfiable iff $x^ = (0, 1/2, \dots, 1/2)^T$ is not a strict minimum*

S is satisfiable iff $x^ = (0, 1/2, \dots, 1/2)^T$ is not a local minimum*

Corollary

For a quadratic indefinite problem the problem of checking local optimality for a feasible point and the problem of checking whether a local minimum is strict are NP-hard.



Challenging Problems I

- Average-case complexity
- Parameterized complexity
- For large-scale problems, we need a measure of complexity that considers **sparsity**



Pardalos, P.M. and Rebennack, S., *Computational Challenges with Cliques, Quasi-cliques and Clique Partitions in Graphs*. Experimental Algorithms (SEA 2010), Lecture Notes in Computer Science Vol. 6049 Springer-Verlag, (Editor Paola Festa), pp. 13-22, 2010.

Challenging Problems II

-  Pardalos, P.M. and Vavasis, S.A., *Open questions in complexity theory for numerical optimization*. Mathematical Programming, Volume 57, Issue 1-3, pp 337-339, 1992.
-  Cao, F., Du, D.-Z., Gao, B., Wan, P.-J. and Pardalos P.M., *Minimax Problems in Combinatorial Optimization*. In Minimax and Applications (Edited by D.-Z. Du and P.M. Pardalos), Kluwer Academic Publishers, pp. 262-285 1995.

Complexity of checking convexity of a function

- The role of convexity in modern day mathematical programming has proven to be fundamental
- The great watershed in optimization is not between linearity and nonlinearity, but convexity and nonconvexity (R. Rockafellar)
- The tractability of a problem is often assessed by whether the problem has some sort of underlying convexity.
- Can we decide in an efficient manner if a given optimization problem is convex?

Complexity of checking convexity of a function

One of seven open problems in complexity theory for numerical optimization (Pardalos, Vavasis, 1992):

Given a degree-4 polynomial in n variables, what is the complexity of determining whether this polynomial describes a convex function?

Theorem

Theorem

Deciding convexity of degree four polynomials is strongly NP-hard. This is true even when the polynomials are restricted to be homogeneous (all terms with nonzero coefficients have the same total degree).

Corollary

It is NP-hard to check convexity of polynomials of any fixed even degree $d \geq 4$.

Theorem

Theorem

It is NP-hard to decide strong convexity of polynomials of any fixed even degree $d = 4$.

Theorem

It is NP-hard to decide strict convexity of polynomials of any fixed even degree $d = 4$.

Theorem

Theorem

For any fixed odd degree d , the quasi-convexity of polynomials of degree d can be checked in polynomial time.

Corollary

For any fixed odd degree d , the pseudoconvexity of polynomials of degree d can be checked in polynomial time.

Theorem

Theorem

It is NP-hard to check quasiconvexity/pseudoconvexity of degree four polynomials. This is true even when the polynomials are restricted to be homogeneous.

Corollary

It is NP-hard to decide quasiconvexity of polynomials of any fixed even degree $d \geq 4$.

Amir Ali Ahmadi, Alex Olshevsky, Pablo A. Parrilo, John N. Tsitsiklis, *NP-hardness of deciding convexity of quartic polynomials and related problems* (Mathematical Programming February 2013, Volume 137, Issue 1-2, pp 453-476)

The complexity results described above can be summarized in the following table [1]:

Property versus degree	1	2	Odd ≥ 3	Even ≥ 4
Strong convexity	No	P	No	Strongly NP-hard
Strict convexity	No	P	No	Strongly NP-hard
Convexity	Yes	P	No	Strongly NP-hard
Pseudoconvexity	Yes	P	P	Strongly NP-hard
Quasiconvexity	Yes	P	P	Strongly NP-hard

A yes (no) entry means that the question is trivial for that particular entry because the answer is always yes (no) independent of the input. By P, we mean that the problem can be solved in polynomial time

Challenging Problems

- Is convexity a “**decidable problem**” for a general function?
- DC optimization? In general can we characterize the “best” DC decomposition of a function $f = f_1 - f_2$, where f_1, f_2 are convex?

Computational Approaches

- **Exact Algorithms**

- Exact algorithms are of limited use for global optimization problems
- However, exact algorithms can be very useful for “special cases” of global optimization problems

- **Approximate Algorithms**

- For many problems (e.g. max clique), finding an ϵ -approximate solution is also intractable

Section 3

Heuristics

Heuristics

- *heuristic* (adj.), “serving to discover or find out,” irregular formation from Gk. *heuretikos* “inventive,” related to *heuriskein* “to find”
- The word “Eureka” comes from ancient Greek *eurika*, “I have found (it)”.



General Global Minimization Problems

Consider a general problem of the form:

$$\mathit{global} \min_{x \in S} f(x),$$

where the objective function f is nonconvex and the feasible domain S is a nonempty bounded polyhedron in R^n .

- Problems of this general form are very difficult to solve
- Heuristics based on local search techniques can be used

Frank-Wolfe method

- Consider problem (1) where the objective $f(x)$ is concave
- Suppose we have a set D , a subset of S , of 'starting points' $\alpha_1, \dots, \alpha_M$.
- For each $y = \alpha_i$, $i = 1, \dots, M$, we have the following algorithm:
 - Initial point $x_0 = y \in D$
 - Given x_k compute the gradient $g_k = \nabla f(x_k)$
 - Solve the linear program

$$\min_{x \in S} g_k^T x$$

- Denote the solution of the linear program by x_{k+1} . If $x_{k+1} = x_k$ stop (x_{k+1} is a local minimum). If not, $x_k \leftarrow x_{k+1}$ and go to step 2

Space Covering Techniques

Theorem

Consider the spheres $S_{v_i}(r_i)$ with center v_i and radius $r_i = (f(v_i) - f(v))/L, i = 1, \dots, N$, and suppose that $\cup_{i=1}^N S_{v_i} \supseteq S$. Then v is the global minimum.

Proof.

If $x \in S$ then $x \in S_{v_j}$ for some $j \in \{1, \dots, N\}$ and therefore

$$|f(x) - f(v_j)| \leq L|x - v_j| \leq Lr_i = f(v_j) - f(v)$$

Then $f(x) - f(v_j) \geq -f(v_j) + f(v)$ and so $f(x) \geq f(v)$ for all $x \in S$. □

Space Covering Techniques

Corollary

Suppose that $\cup_{i=1}^N S_{v_i}$ does not necessarily contain S . Let $r_i \leftarrow r_i + \epsilon/L$, and call the new spheres $S_{v_i}^\epsilon$. Assume that $\cup_{i=1}^N S_{v_i}^\epsilon \supseteq S$ for some $\epsilon \geq 0$. Then $f(v)$ is an ϵ -approximate solution in the sense that $f(v) - f^ \leq \epsilon$, where f^* is the global minimum.*

Section 4

Black-Box Optimization

Continuous GRASP

- Continuous GRASP (C-GRASP) is a metaheuristic to finding optimal or near-optimal solutions to
- Min $f(x)$ subject to $:L \leq x \leq U$
 - where $x, L, U \in R^n$
 - and $f(x)$ is continuous but can, for example, have discontinuities, be non-differentiable, be the output of a simulation, etc

C-GRASP

C-GRASP is a multi-start procedure, i.e. a major loop is repeated until some stopping criterion is satisfied.

In each major iteration

- x is initialized with a solution randomly selected from the box defined by vectors L and U
- a number of minor iterations are carried out, where each minor iteration consists of a construction phase and a local improvement phase.
- Minor iterations are done on a dynamic grid and stops when the grid has a pre-specified density.

C-GRASP Reference

C-GRASP is based on the discrete optimization metaheuristic GRASP



M.J. Hirsch, C.N. Meneses, P.M. Pardalos, and M.G.C. Resende, *Global optimization by continuous GRASP*. Optimization Letters, vol. 1, pp. 201-212, 2007.



M.J. Hirsch, P.M. Pardalos, and M.G.C. Resende, *Speeding up continuous GRASP*. European J. of Operational Research, vol. 205, pp. 507-521, 2010.



R.M.A. Silva, M.G.C. Resende, P.M. Pardalos, M.J. Hirsch, *A Python/C library for bound-constrained global optimization with continuous GRASP*. Optimization Letters: 967-984, 2013.



M.J. Hirsch, P.M. Pardalos, M.G.C. Resende, *Solving Systems of Nonlinear Equations with Continuous GRASP*. Nonlinear Analysis Series B: Real World Applications, Vol. 10, No. 4, pp. 2000-2006, 2009.

Black-Box Optimization

- Related problem in machine learning:
 - Given $f(x_1), \dots, f(x_N)$ (f is not known), predict $f(x_{N+1})$



Serafino, L., *Optimizing Without Derivatives: What Does the No Free Lunch Theorem Actually Say?*. Volume 61, Number 7, Notice of the AMS 2014.

Section 5

Software for Global Optimization

1. Mixed Integer Linear Optimization

$$\min c^T x \quad (11)$$

$$s.t. Ax \leq 0 \quad (12)$$

$$x \in X \subset \mathbb{Z}^m \times \mathbb{R}^{n-m} \quad (13)$$

- Excellent software exist for such problems.
- Useful for separable global optimization.

2. Mixed Integer Nonlinear Optimization

$$\min f(x) \tag{14}$$

$$\text{s.t. } g(x) \leq 0 \tag{15}$$

$$x \in X \subset \mathbb{Z}^m \times \mathbb{R}^{n-m} \tag{16}$$

- Several software package exist but this model is very general.

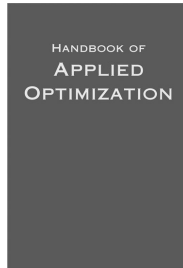
3. Special Software

- Quadratic Optimization
- Quadratic Assignment
- Location Problems
- Graph Problems

Specialized algorithm have been implemented (exact and heuristic)

4. Software for Heuristics

- Genetic Algorithms
- Simulated Annealing
- Global Equilibrium Search
- Tabu Search
- GRASP
- Variable Neighborhood Search



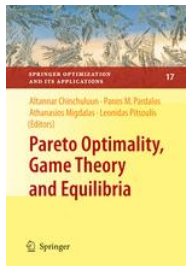
Challenging Problems

- Evaluation of heuristics
 - Experimental testing
 - Automatic parameter identification
 - Good lower/upper bound techniques
 - Test problems with known optimal solution
 - Space covering related techniques

Section 6

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