Computational Models and Hard 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)
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.

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


- 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.


- Biochemical, Bioelectronic, and Biochemical computers
- Biochemical and DNA nanocomputers
First conference on DNA Based Computers (DIMACS, Princeton 1995)

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

Quantum Computing?

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


- 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)
Tomasso Toffoli (1982)
David Deutsch (1985) ....
Quantum mechanics (early 1920s...)
What is (global) optimization?

Computational Models and Hard Optimization Problems
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

\[(P) \begin{cases} 
\text{Minimize } f(A) := \text{rank of } A \\
\text{subject to } A \in C.
\end{cases} \\
C \text{ is a subset of } M_{m,n}(\mathbb{R})
\]

\[(Q) \begin{cases} 
\text{Minimize } c(x) \\
\text{subject to } x \in S
\end{cases} \\
c(x) \text{ is the number of nonzero components of } x. \\
S \text{ is a subset of } \mathbb{R}^n
\]

Every admissible point in \((P)\) is a local minimizer.

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


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)

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

- **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.
Consider the following quadratic problem:

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

where $Q$ is an arbitrary $n \times n$ symmetric matrix, $x \in \mathbb{R}^n$. 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:

$$Qx + c \geq 0, \ x \geq 0$$
$$x^T(Qx + c) = 0.$$
Theorem (Horst, Pardalos, Thoai, 1994 - [2])

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

Proof.

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

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

where \( a_i, \ i = 1, \ldots, n, \) and \( b \) are positive integers, \( I_n \) is the \( n \times n \)-unit matrix and the vectors \( e_n \in \mathbb{R}^n, \ 0_n \in \mathbb{R}^n \) are defined by

\[
e_n^T = (1, 1, \ldots, 1), \quad 0_n^T = (0, 0, \ldots, 0).
\]
Proof.

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

\[ \sum_{i=1}^{n} a_i x_i = b, \quad x_i \in \{0, 1\} \quad (i = 1, \ldots, n). \]

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 \( y = (a_1 x_1, \ldots, a_n x_n, 0, 0, 0)^T \) 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, \( x = (\frac{y_1}{a_1}, \ldots, \frac{y_n}{a_n}) \) solves the knapsack problem.
Consider the following quadratic problem:

\[
\begin{align*}
\text{min} & \quad f(x) \\
\text{s.t.} & \quad Ax \geq b, \quad x \geq 0
\end{align*}
\]

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

$$S = \bigwedge_{i=1}^{m} \bigvee_{j=1}^{3} l_{ij}, \quad l_{ij} \in \{x_i, \bar{x}_i | i = 1, \ldots, n\}$$

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 $C_1, \ldots, C_n$, 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 \( y \in \{-1, 1\}^m \).
Next consider a polynomial unconstrained \textbf{global optimization} formulation:

\[ \min_{y \in E^m} f(y) \]  
\[ (6) \]

where

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

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

\[ c_i = \prod_{j=1}^{m} q_{ij}(y_j) \]  
\[ (8) \]
A Global Optimization Approach

where

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

(9)

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

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

(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 $y$. 
Random 3-SAT problem:

- Three variables per clause are chosen randomly from \( \{x_1, \ldots, x_N\} \) and negated randomly with probability \( \frac{1}{2} \).
- Example: \( (x_1 \lor x_{20} \lor \overline{x}_{13}) \land (\overline{x}_{21} \lor x_1 \lor x_9) \land \ldots (x_{95} \lor \overline{x}_8 \lor \overline{x}_{15}) \).
- 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

Phase Transitions References

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 $x_0, \ldots, x_n$. 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 $3/2$. 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])

\[ S \text{ is satisfiable iff } x^* = (0, 1/2, \ldots, 1/2)^T \text{ is not a strict minimum} \]

\[ S \text{ is satisfiable iff } x^* = (0, 1/2, \ldots, 1/2)^T \text{ is not a local minimum} \]

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

Challenging Problems II


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?
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 (Ahmadi et al., 2011)

*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 (Ahmadi et al., 2011)

*It is NP-hard to check convexity of polynomials of any fixed even degree* \( d \geq 4 \).
Theorem (Ahmadi et al., 2011)

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

Theorem (Ahmadi et al., 2011)

It is NP-hard to decide strict convexity of polynomials of any fixed even degree $d = 4$. 
Theorem (Ahmadi et al., 2011)

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

Corollary (Ahmadi et al., 2011)

For any fixed odd degree $d$, the pseudoconvexity of polynomials of degree $d$ can be checked in polynomial time.
Theorem (Ahmadi et al., 2011)

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 (Ahmadi et al., 2011)

It is NP-hard to decide quasiconvexity of polynomials of any fixed even degree \( d \geq 4 \).
The complexity results described above can be summarized in the following table [1]:

<table>
<thead>
<tr>
<th>Property versus degree</th>
<th>1</th>
<th>2</th>
<th>Odd ≥ 3</th>
<th>Even ≥ 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong convexity</td>
<td>No</td>
<td>P</td>
<td>No</td>
<td>Strongly NP-hard</td>
</tr>
<tr>
<td>Strict convexity</td>
<td>No</td>
<td>P</td>
<td>No</td>
<td>Strongly NP-hard</td>
</tr>
<tr>
<td>Convexity</td>
<td>Yes</td>
<td>P</td>
<td>No</td>
<td>Strongly NP-hard</td>
</tr>
<tr>
<td>Pseudoconvexity</td>
<td>Yes</td>
<td>P</td>
<td>P</td>
<td>Strongly NP-hard</td>
</tr>
<tr>
<td>Quasiconvexity</td>
<td>Yes</td>
<td>P</td>
<td>P</td>
<td>Strongly NP-hard</td>
</tr>
</tbody>
</table>

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 $\epsilon$-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)”.

![Image of Eureka moment with a cartoon and a Nobel Prize in Economics]
Consider a general problem of the form:

\[ \text{global \ min } f(x), \quad x \in S \]

where the objective function \( f \) is nonconvex and the feasible domain \( S \) is a nonempty bounded polyhedron in \( \mathbb{R}^n \).

- Problems of this general form are very difficult to solve
- Heuristics based on local search techniques can be used
Consider problem (1) where the objective $f(x)$ is concave.

Suppose we have a set $D$, a subset of $S$, of 'starting points' $\alpha_1, \ldots, \alpha_M$.

For each $y = a_i, i = 1, \ldots, M$, 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
Theorem

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

Proof.

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

Computational Models and Hard Optimization Problems
Corollary

Suppose that $\bigcup_{i=1}^{N} S_{v_i}$ does not necessarily contain $S$. Let $r_i \leftarrow r_i + \epsilon / L$, and call the new spheres $S_{v_i}^\epsilon$. Assume that $\bigcup_{i=1}^{N} S_{v_i}^\epsilon \supseteq S$ for some $\epsilon \geq 0$. Then $f(v)$ is an $\epsilon$-approximate solution in the sense that $f(v) - f^* \leq \epsilon$, where $f^*$ is the global minimum.
Section 4

Black-Box Optimization
Continuous GRASP (C-GRASP) is a metaheuristic to finding optimal or near-optimal solutions to

\[ \text{Min } f(x) \text{ subject to: } L \leq x \leq U \]

- where \( x, L, U \in \mathbb{R}^n \)
- and \( f(x) \) is continuous but can, for example, have discontinuities, be non-differentiable, be the output of a simulation, etc
C-GRASP 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 is based on the discrete optimization metaheuristic GRASP


Black-Box Optimization

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

Section 5

Software for Global Optimization
1. Mixed Integer Linear Optimization

\[
\min c^T x \\
\text{s.t. } Ax \leq 0 \\
x \in X \subset \mathbb{Z}^m \times \mathbb{R}^{n-m}
\]  

- Excellent software exist for such problems.
- Useful for separable global optimization.
2. Mixed Integer Nonlinear Optimization

\[ \begin{align}
\text{min } & f(x) \\
\text{s.t. } & g(x) \leq 0 \\
& x \in X \subset \mathbb{Z}^m \times \mathbb{R}^{n-m}
\end{align} \]  

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

References

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February 22-25, 2015 Gainesville, FL
http://www.caopt.com/WCGO/