Duality and Complexity Issues in Global Optimization

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Duality in Nonlinear Programming (NLP)

Duality in NLP

- Duality theory plays a central role in mathematical programming. This theory is closely related to the theory of so–called minimax problems and saddlepoints.
- Let f, g, F be real–valued functions defined on $X \subseteq \mathbb{R}^m$, $Y \subseteq \mathbb{R}^n$ and $X \times Y \subseteq \mathbb{R}^m \times \mathbb{R}^n$, respectively.
- Assume that the global minima and maxima which we address below do exist in all cases.

Duality in NLP

- Suppose that $f(x) \leq g(y)$ for all $(x, y) \in X \times Y$. Then it is clear that

$$\max_{x \in X} f(x) \leq \min_{y \in Y} g(y).$$

- Under certain conditions the above inequality can be satisfied as an equality

$$\max_{x \in X} f(x) = \min_{y \in Y} g(y).$$

- Each result of this kind is called a **duality theorem**.

Duality in NLP

- It is easy to prove that the following inequality holds:

$$\max_{y \in Y} \min_{x \in X} F(x, y) \leq \min_{x \in X} \max_{y \in Y} F(x, y).$$

- Under certain conditions we can prove that

$$\max_{y \in Y} \min_{x \in X} F(x, y) = \min_{x \in X} \max_{y \in Y} F(x, y).$$

- Each result of this type is called a **minimax theorem**.

Duality in NLP

- The point $(x^*, y^*) \in X \times Y$ is a **saddlepoint** of F (with respect to maximizing in Y and minimizing in X) if

$F(x^*, y) \le F(x^*, y^*) \le F(x, y^*)$ for every $(x, y) \in X \times Y$.

- **Theorem.** The point $(x^*, y^*) \in X \times Y$ is a saddlepoint of F iff

$$F(x^*, y^*) = \max_{y \in Y} \min_{x \in X} F(x, y) = \min_{x \in X} \max_{y \in Y} F(x, y).$$

Duality in NLP

Proof.

- Let (x^*, y^*) be a saddlepoint of F.

$$\begin{aligned} F(x^*, y^*) &\leq \min_{x\in X} F(x, y^*) &&\leq \max_{y\in Y} \min_{x\in X} F(x, y) \\ &\leq \min_{x\in X} \max_{y\in Y} F(x, y) &&\leq \max_{y\in Y} F(x^*, y) \\ &\leq F(x^*, y^*). \end{aligned}$$

Duality in NLP

- If

$$F(x^*, y^*) = \max_{y \in Y} \min_{x \in X} F(x, y) = \min_{x \in X} \max_{y \in Y} F(x, y),$$

then we have

$$\min_{x \in X} F(x, y^*) = F(x^*, y^*) = \max_{y \in Y} F(x^*, y),$$

i.e. (x^*, y^*) is a saddlepoint. $\square$

Duality in NLP

- Consider now the optimization problem (**primal**)

$$\begin{aligned} \min\ & f(x) \\ \text{s.t.}\ & g(x) \le 0,\ x \in X \end{aligned} \qquad \text{(P)}$$

  where $g : \mathbb{R}^n \to \mathbb{R}^p$ and $X \subseteq \mathbb{R}^n$.

- The Lagrangian of (P) is

$$L(x, \lambda) = f(x) + \lambda^T g(x), \lambda \in \mathbb{R}^p_+.$$

Duality in NLP

- Note that

$$\sup_{\lambda \geq 0}\{f(x) + \lambda^T g(x)\} = \begin{cases} f(x) \text{ if } g(x) \leq 0 \\ +\infty \text{ otherwise,} \end{cases}$$

and Problem (P) can be restated in the form

$$\min_{x \in X} \max_{\lambda \geq 0} L(x, \lambda).$$

Duality in NLP

- For $\lambda \geq 0$ define the function

$$d(\lambda) = \min_{x \in X} L(x, \lambda)$$

which is concave (independently of the convexity of f or g). Then the **dual** problem of (P) is defined to be the following optimization problem:

$$\max_{\lambda \geq 0} d(\lambda) = \max_{\lambda \geq 0} \min_{x \in X} L(x, \lambda). \tag{D}$$

- The objective function $d(\lambda)$ of (D) is often called dual function.

Duality in NLP

- **Theorem. (Weak Duality Theorem)** Let x^* be a global minimum point of the primal problem. Then for every $\lambda \geq 0$

$$d(\lambda) \leq d\left(\lambda^*\right) \leq f\left(x^*\right)$$

  where λ^* is a global maximum point of the dual.

- **Proof.** Since $\lambda \geq 0$ and $g(x^*) \leq 0$ it follows that $\lambda^T g(x^*) \leq 0$. On the other hand, for any $\lambda \geq 0$ and $x^* \in X,\ d(\lambda) \leq f(x^*) + \lambda^T g(x^*)$, and hence $d(\lambda) \leq \max_{\lambda \geq 0} d(\lambda) = d(\lambda^*) \leq f(x^*)$.

Duality in NLP

- If $d\,(\lambda^*) < f\,(x^*)$, then the difference $f\,(x^*) - d(\lambda^*)$ is called the **"duality gap"**.
- The following result is then an immediate consequence of last theorem.
- **Theorem.** A point $(x^*, \lambda^*) \in X \times \mathbb{R}^p_+$ is a saddlepoint of the Lagrangian $L(x, \lambda)$ iff x^* is a global minimum point of the primal Problem (P), λ^* is a global maximum point of the dual (D), and the optimal values $f\,(x^*)$ of (P) and $d(\lambda^*)$ of (D) coincide.

Duality in NLP

- The next theorems provide a set of necessary and sufficient conditions for (x^*, λ^*) to be a saddlepoint of $L(x, \lambda)$ and hence for the equivalent duality theorem above.
- **Theorem.** A point $(x^*, \lambda^*) \in X \times \mathbb{R}^p_+$ is a saddlepoint of the Lagrangian $L(x, \lambda)$ iff the following conditions hold:

(i) $L(x^*, \lambda^*) = \min\{L(x, \lambda^*) : x \in X\}$.

(ii) $g(x^*) \leq 0$.

(iii) $\lambda^{*T} g(x^*) = 0$.

Duality in NLP

- **Example.** Consider the quadratic programming problem

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

where the $(n \times n)$–matrix Q is symmetric positive definite, $c \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^n$.

The corresponding Lagrangian function is

$$L(x, \lambda) = c^T x + \tfrac{1}{2} x^T Q x + \lambda^T (Ax - b) =$$

$$= (c + A^T \lambda)^T x + \tfrac{1}{2} x^T Q x - b^T \lambda.$$

Duality in NLP

The minimum of $L(x, \lambda)$ with respect to x occurs at the point x^* where $\nabla L(x^*, \lambda) = 0$, i.e.,

$$x^* = -Q^{-1}(c + A^T \lambda).$$

Substituting in L we obtain the dual function

$$d(\lambda) = -\frac{1}{2}\lambda^T A Q^{-1} A^T \lambda - \lambda^T (b + A Q^{-1} c) - \frac{1}{2} c^T Q^{-1} c.$$

Duality in NLP

Hence the dual problem is given by

$$\max_{\lambda \geq 0} d(\lambda) = -\frac{1}{2}\lambda^T M \lambda + d^T \lambda,$$

where $M = AQ^{-1}A^T$ and $d = -(b + AQ^{-1}c)$.

If λ^* is the solution of the dual problem, then $x^* = -Q^{-1}(c + A^T\lambda^*)$ is the solution of the original primal problem.

So, we see that in the convex quadratic case the duality gap is zero.

Complexity Issues

- The worst case time complexity.
- We call an algorithm for a problem π polynomial if its running time on a computer in terms of the number of required elementary operations (such as arithmetic operations, comparisons, branching instructions, ...) is, in the worst case, bounded from above by a polynomial of degree p in the size L of the input data.
- We say that the algorithm runs in $O(L^p)$ time.

Complexity Issues

Example:

- The standard simplex algorithm for LP requires, in the worst case, a number of steps which is exponential in the size of the input data (e.g., Klee–Minty example).
- Kachiyan's ellipsoid algorithm (or Karmarkar's interior point algorithm) requires only a polynomial number of steps, and each step in these algorithms consists of a polynomial number of elementary operations.

Complexity Issues

- In complexity theory, the collection of problems that can be solved in polynomial time (i.e., by a polynomial algorithm) is denoted by **P**.
- Another important complexity class is **NP**, the set of all problems solvable by a "nondeterministic algorithm" in polynomial time. That is, **NP** is the class of problems for which the correctness of a claimed solution (that may have been computed by a tedious procedure) can be verified in polynomial time.

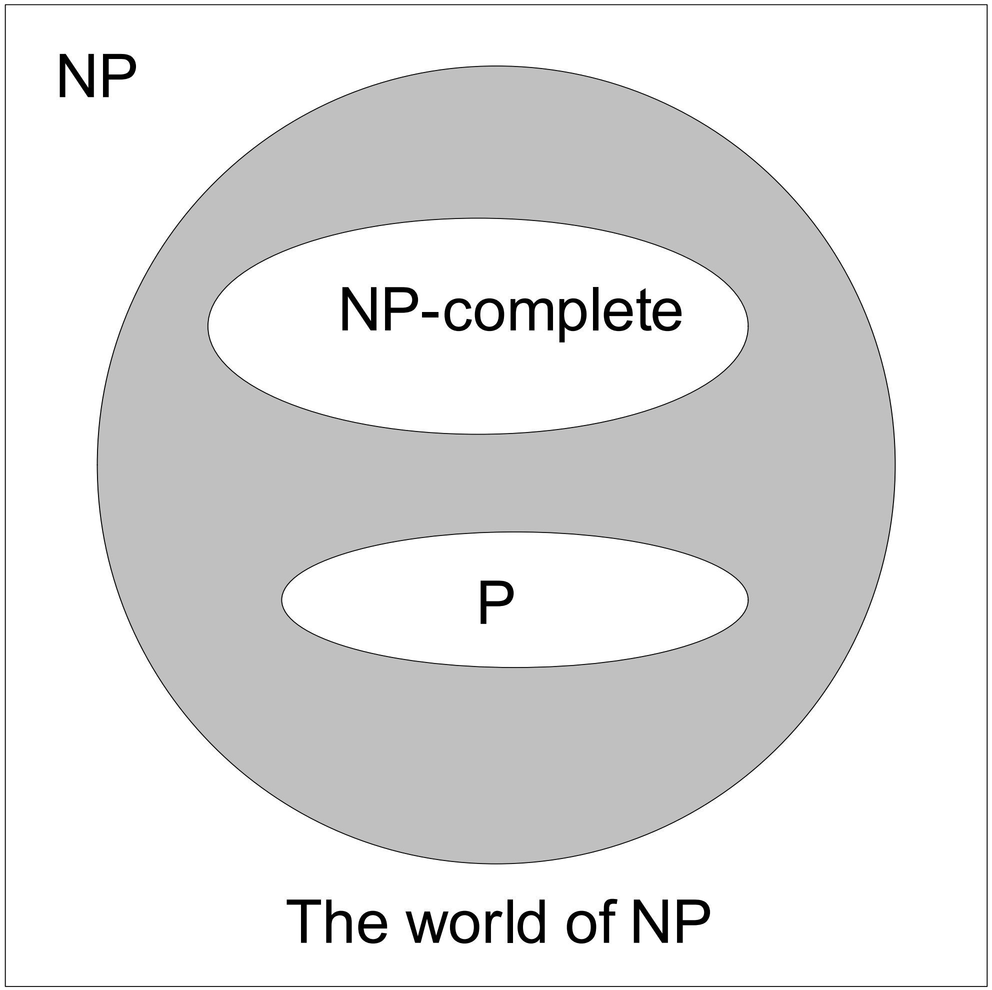
Complexity Issues

- Clearly **P** is a subset of **NP**, and it appears natural that **P** $\neq$ **NP**.
- However, despite enormous research efforts, it remains one of the most famous unsolved problems in theoretical computer science whether the two classes **P** and **NP** are different or not.

Complexity Issues

- We say that a problem π_1 is polynomially transformable to a problem π_2 if a polynomial algorithm for π_2 would imply a polynomial algorithm for π_1.
- A problem π is **NP–complete** if $\pi \in$ **NP** and if every other problem in **NP** can be polynomially transformed to it.
- Every **NP–complete** problem has the following property: if it can be solved in polynomial time, then all problems in **NP** can be solved in polynomial time. In other words, if π is **NP–complete** and if $\pi \in$ **P** then **P**=**NP**.

Complexity Issues



Complexity Issues

- Let $x_1, \ldots, x_n$ be a set of Boolean variables whose value is either true or false, and let $\overline{x}_i$ denote the negation of x_i.
- A literal is either a variable or its negation.
- A Boolean formula is an expression that can be constructed using literals, and the operations "and" ($\wedge$ or $\bullet$) and "or" ($\vee$ or $+$).
- A Boolean formula which can be made true by assigning some values to its variables is said to be **satisfiable**.

Complexity Issues

- The **SATISFIABILITY** problem is to check whether a Boolean formula of the (conjunctive normal) form $F = \bigwedge_{i=1}^{k}(\bigvee_{j=1}^{n_i} \ell_{ij})$, where ℓ_{ij} denotes a literal, is **satisfiable**.
- **Cook's Theorem** (1971). **SATISFIABILITY** is **NP**–complete.

Complexity Issues

- Soon after the appearance of Cook's proof, the list of **NP**–complete problems was substantially enriched. Another "classical" **NP**–complete problem is, for example, to check whether a single linear constraint $\sum_{i=1}^{n} a_i x_i = b$, a_i, b integers, has a solution in $x_i \in \{0, 1\}$ $(i = 1, \ldots, n)$ (knapsack problem).
- Other well–known examples include the traveling salesman problem, the maximum clique problem, and many classes of nonconvex quadratic optimization problems.

Complexity Issues

- How can we prove that some problem is **NP**–complete?
- The following obvious consequence of the definition of **NP**–completeness is often used:

  If a problem π_1 is **NP**–complete and π_1 is polynomially transformable to a problem $\pi_2 \in$ **NP**, then π_2 is **NP**–complete.
- Note, however, that one cannot conclude **NP**–completeness of π_2 by transforming it polynomially to another **NP**–complete problem π_1.

Complexity Issues

- A problem π is called **NP**–hard if there is an **NP**–complete problem which can be polynomially transformed to π.
- Thus, an **NP**–hard problem shares with **NP**–complete problems the basic property of being at least as difficult as any other problem in **NP**-complete, but it may not belong to **NP**.

Complexity: KKT Points in QP

- Consider the following quadratic problem

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

where Q is an $n \times n$ symmetric matrix, and $c \in \mathbb{R}^n$.

Complexity: KKT Points in QP

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

- The KKT conditions for this problem become the following so–called linear complementarity problem (denoted by LCP(Q, c)): Find $x \in \mathbb{R}^n$ (or prove that no such an x exists) such that

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

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

Complexity: KKT Points in QP

- Hence, the complexity of finding (or proving existence of) KKT points for the above quadratic problem is reduced to the complexity of solving the corresponding (symmetric) LCP.
- **Theorem.** The Problem LCP (Q, c) is **NP**–hard.

Complexity: KKT Points in QP

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

$$Q_{(n+3)\times(n+3)} = \begin{bmatrix} -I_n & e_n & -e_n & 0_n \\ e_n^T & -1 & -1 & -1 \\ -e_n^T & -1 & -1 & -1 \\ 0_n^T & -1 & -1 & -1 \end{bmatrix},$$

$$c_{n+3}^T = (a_1, \ldots, a_n, -b, b, 0),$$

where a_i, $i = 1, \ldots, n$, and b are positive integers, I_n is the $(n \times n)$–unit matrix and $e_n \in \mathbb{R}^n$, $0_n \in \mathbb{R}^n$ are the vectors of all ones and zeros, respectively.

Complexity: KKT Points in QP

- Define the following knapsack problem. Find a feasible solution to the system

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

- This problem is known to be NP–complete. Next we show that the 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).

Complexity: KKT Points in QP

- Conversely, assume the point y solves the LCP(Q, c) given above.
- Since $Qy + c \geq 0$, $y \geq 0$ we obtain $y_{n+1} = y_{n+2} = y_{n+3} = 0$. This in turn 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, $x = \left(\frac{y_1}{a_1}, \ldots, \frac{y_n}{a_n}\right)$ solves the knapsack problem.

$\square$

Complexity: KKT Points in QP

- Therefore, in quadratic programming, the problem of deciding whether a Kuhn–Tucker point exists is **NP**–hard.
- Next we investigate the complexity of finding locally optimal solutions to nonlinear optimization problems.

Complexity of Local Minimization

- Computing locally optimal solutions is presumably easier than finding globally optimal solutions.
- However, from the complexity point of view we will show 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 even for problems with a simple structure in the constraints and the objective.

Complexity of Local Minimization

- We focus our investigation on problems that have nonconvex quadratic objective and linear constraints, that is, problems of the form:

$$\min \ f(x)$$
$$\text{s.t.} \quad Ax \geq b, \ x \geq 0$$

where $f(x)$ is an indefinite quadratic function.

Complexity of Local Minimization

- Consider now 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,

$$S = (\ell_{11} + \ell_{12} + \ell_{13})(\ell_{21} + \ell_{22} + \ell_{23}) \ldots (\ell_{m1} + \ell_{m2} + \ell_{m3})$$

  where each literal ℓ_{ij} is either some variable x_k or its negations $\bar{x}_k$, is there a truth assignment for the variables x_i which makes S true?
- Cook: 3–SAT is **NP**–complete.

Complexity of Local Minimization

- For each instance of 3–satisfiability we construct an instance of an optimization problem in the real variables $x_0, x_1, \ldots, x_n$.

Clause in S	$\longleftrightarrow$	a linear inequality
$\ell_{ij} = x_k$		x_k
$\ell_{ij} = \overline{x}_k$		$1 - x_k$
		$\ldots + x_0 \geq \frac{3}{2}$.

- Example: for the clause $x_1 + x_2 + \bar{x}_3$ we have $x_1 + x_2 + (1 - x_3) + x_0 \geq \frac{3}{2}$.

Complexity of Local Minimization

- Thus, we associate to S a system of linear inequalities

$$A_S x \geq (\frac{3}{2} + c)$$

where A_s is a (sparse) matrix with entries in $\{0, 1, -1\}$ and $x^T = (x_0, \ldots, x_n)$.

- Let us consider the set $D(S) \subset \mathbb{R}^{n+1}$ of feasible points satisfying the following linear constraints

$$A_S x \geq (\tfrac{3}{2} + c)$$

$$1/2 - x_0 \leq x_i \leq 1/2 + x_0, \; x_i \geq 0 \;, \; i = 1, \ldots, n$$

Complexity of Local Minimization

- With a given instance S of the 3–satisfiability problem we associate the following indefinite quadratic problem:

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

- Note that $f(x) = -\sum_{i=1}^{n} (x_i - 1/2)^2 + n x_0^2$, i.e., the objective function is a separable indefinite quadratic function with one convex and n concave terms.

Complexity of Local Minimization

- In addition, we have the following:

  a) $f(x) \geq 0$ for all feasible points x. Therefore, the feasible point $x^* = (0, 1/2, \ldots, 1/2)^T$ is a local (global) minimum of $f(x)$ since $f(x^*) = 0$.

  b) $f(x) = 0$ if and only if $x_i \in \{1/2 - x_0,\ 1/2 + x_0\}$, for $i = 1, \ldots, n$.

- Recall that a strict local minimum for the above quadratic problem is a feasible point x^* for which there exists an $\epsilon > 0$ such that

$$f(x^*) < f(x) \text{ for all } x \in D(S) \cap \{x : 0 < \|x - x^*\| \leq \epsilon\}\,.$$

Complexity of Local Minimization

- The following theorem implies that checking strict local optimality is **NP**–hard. Therefore, we cannot expect to find a polynomial time algorithm for this problem (assuming **P** $\neq$ **NP**).
- **Theorem.** S is satisfiable iff $x^* = (0, 1/2, \ldots, 1/2)^T$ is not a strict minimum.
- **Proof:** Let $x_1, \ldots, x_n$ be a truth assignment satisfying S. For any x_0 and $i = 1, \ldots, n$ consider

$$x_i^0 = \begin{cases} 1/2 - x_0 \text{ if } x_i = 0 \\ 1/2 + x_0 \text{ if } x_i = 1. \end{cases}$$

Complexity of Local Minimization

For $x^0 = (x_0, x_1^0, \ldots, x_n^0)^T$ we have $f(x^0) = 0$. Since x_0 can be chosen to be arbitrarily close to zero, x^* is not a strict local minimum.

Suppose now that $x^* = (0, 1/2, \ldots, 1/2)^T$ is not a strict local minimum, that is, there exists $y \neq x^*$ such that $f(y) = f(x^*) = 0$; therefore, $y_i \in \{1/2 - y_0, 1/2 + y_0\}$, $i = 1, \ldots, n$. Then the variables x_i, $i = 1, \ldots, n$ defined by

$$x_i(y) = \begin{cases} 0 \text{ if } y_i = 1/2 - y_0 \\ 1 \text{ if } y_i = 1/2 + y_0 \end{cases}$$

satisfy S.

Complexity of Local Minimization

- If we fix $x_0 = 1/2$ in the above indefinite quadratic problem, then the objective function $f(x)$ is concave with x^* as the global minimum. Therefore, the problem of checking if a given point is a strict global minimum of a concave minimization problem is **NP**–hard.
- Consider now the problem of checking local optimality. We prove that this problem is **NP**–hard.

Complexity of Local Minimization

- Given the 3–satisfiability problem, consider the following indefinite quadratic program:

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

$$-\frac{1}{2n} \sum_{i=1}^{n} (x_i - 1/2)^2.$$

- **Theorem.** S is satisfiable iff $x^* = (0, 1/2, \ldots, 1/2)$ is not a local minimum.

Complexity of Local Minimization

- **Proof:** Let $x_1, \ldots, x_n$ be a truth assignment satisfying S. Given any x_0 arbitrary close to zero, define for $i = 1, \ldots, n$

$$x_i^0 = \begin{cases} 1/2 - x_0 \text{ if } x_i = 0 \\ 1/2 + x_0 \text{ if } x_i = 1. \end{cases}$$

Then we can easily see that $x^0 = (x_0, x_1^0, \ldots, x_n^0)$ is feasible and

$$\phi(x^0) = -\frac{x_0^2}{2} < 0 = \phi(x^*).$$

Hence, x^* is not a local minimum.

Complexity of Local Minimization

Suppose now that x^* is not a local minimum. Then there exists a point $x = (x_0, \ldots, x_n)^T$ such that $\phi(x) < 0$. We will now show, by contradiction, that we can find in each clause of S one literal of value $> 1/2$. This would imply that S is satisfiable with

$$\bar{x}_i = \begin{cases} 0 \text{ if } x_i \leq 1/2 \\ 1 \text{ if } x_i > 1/2. \end{cases}$$

Complexity of Local Minimization

For contradiction, assume that the value of each literal in some clause is $\leq 1/2$. For instance, consider a constraint (clause) of the form

$$x_1 + x_2 + \bar{x}_3 + x_0 \geq 3/2.$$

For this inequality to hold, we must have a value $\geq \frac{1}{2} - \frac{x_0}{3}$ for at least one literal l. Consider the case $l = x_1$ (the other cases follow by an analogous argument).

Complexity of Local Minimization

By assumption we have that $x_1 \leq 1/2$, so

$$\frac{1}{2} - \frac{x_0}{3} \leq x_1 \leq \frac{1}{2} \;\Rightarrow\; -\frac{x_0}{3} \leq x_1 - \frac{1}{2} \leq 0.$$

Hence,

$$(x_1 - 1/2)^2 \leq \frac{x_0^2}{9}.$$

Let

$$\begin{aligned} p(x) &= -\sum_{i=1}^{n} (x_i - (1/2 - x_0))(x_i - (1/2 + x_0)) \\ &= -\sum_{i=1}^{n} ((x_i - 1/2)^2 - x_0^2) \end{aligned}$$

be the "penalty term" in the objective function.

Complexity of Local Minimization

Then, since $(x_1 - 1/2)^2 \leq \frac{x_0^2}{9}$,

$$p(x) \geq -(x_1 - 1/2)^2 + x_0^2 \geq \frac{8}{9} x_0^2.$$

On the other hand, for the "payoff term"

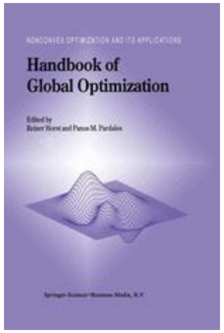
$q(x) = -\frac{1}{2n} \sum_{i=1}^{n} (x_i - 1/2)^2$ we obtain $q(x) \geq -x_0^2/2$.

Hence $\phi(x) \geq \frac{8}{9} x_0^2 - \frac{1}{2} x_0^2 > 0$, a contradiction. $\square$

Complexity of Local Minimization

- Complexity analysis is fundamental in order to understand the inherent difficulty of nonconvex problems and has been a motivation to develop new algorithms.
- It is not clear whether nonconvexity is the only source of complexity, since some classes of nonconvex problems can be solved by polynomial time algorithms.
- Furthermore, there is no easy way to check if a given complicated function is convex or not (even in the case of multivariable polynomials).

Basic References



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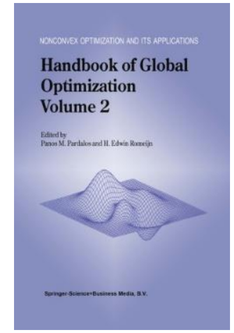

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