4TE3/6TE3

Algorithms for

Continuous Optimization

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The general NLO problem

$$
\begin{array}{lll}
(NLO) & \min & f(x) \\
& \text{s.t.} & h_i(x) = 0, \quad i \in I = \{1, \cdots, p\} \\
& & g_j(x) \le 0, \quad j \in J = \{1, \cdots, m\} \\
& & x \in \mathcal{C}.
\end{array}
$$

where $x \in \mathbb{R}^n$, $\mathcal{C} \subseteq \mathbb{R}^n$ is a certain set and $f, h_1, \cdots, h_p, g_1, \cdots, g_m$ are functions defined on $\mathcal{C}$.
Set of feasible solutions:

$$\mathcal{F} = \{x \in \mathcal{C} \mid h_i(x) = 0, \forall\, i \text{ and } g_j(x) \le 0, \forall\, j\}.$$

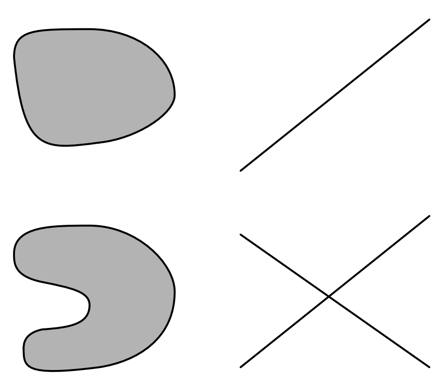
Definition 1 *Let two points $x^1, x^2 \in \mathbb{R}^n$ and $0 \le \lambda \le 1$ be given. Then the point*

$$x = \lambda x^1 + (1 - \lambda) x^2$$

is a convex combination *of the two points x^1, x^2.*

The set $\mathcal{C} \subset \mathbb{R}^n$ is called convex, *if all convex combinations of any two points $x^1, x^2 \in \mathcal{C}$ are again in $\mathcal{C}$.*

Convex and nonconvex sets in the plane.



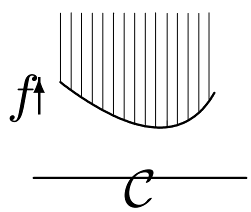
Convex functions

Definition 2 *A function* $f : \mathcal{C} \to R$ *defined on a convex set* $\mathcal{C}$ *is called* convex *if for all* $x^1, x^2 \in \mathcal{C}$ *and* $0 \le \lambda \le 1$ *one has*

$$f(\lambda x^1 + (1-\lambda)x^2) \le \lambda f(x^1) + (1-\lambda) f(x^2).$$

Definition 3 *The epigraph of a function* $f : \mathcal{C} \to R$ *is the* $(n+1)$*-dimensional set*

$$\left\{(x, \tau) \;:\; f(x) \le \tau, x \in \mathcal{C},\ \tau \in \mathbb{R}\right\}.$$



The epigraph of a convex function f.

Lemma 1 *A a function* f *is convex iff epi*(f) *is convex.*

$\mathbb{R}^n_+$ is convex.

$f : \mathbb{R}^n \to \mathbb{R}$ is called a *quadratic* function if there is a square matrix $Q \in \mathbb{R}^{n\times n}$, a vector $c \in \mathbb{R}^n$ and a number $\gamma \in \mathbb{R}$ such that

$$f(x) = \frac{1}{2} x^T Q x + c^T x + \gamma \text{ for all } x \in \mathbb{R}^n;$$

if $Q = 0$ then f is called *affine (linear)*.

Examples

Convex functions:

- $\exp(x)$
- $-\log(x)$
- $x \log(x)$
- $-\sqrt{x}$ when $x \geq 0$
- $(x_1 - 2)^2 + (x_2 + 1)^2 - 2$
- $\cos(x)$ on the interval $[\frac{\pi}{2}, \frac{3\pi}{2}]$

Non-Convex functions:

- $\log(x)$
- $-(x_1 - 2)^2 + (x_2 + 1)^2 - 2$
- $\sin(x)$
- $x \sin(x)$
- $(x - 2)^4 - 10 * (x - 2)^2$

Pre-knowledge:

You are supposed to be familiar with.

- Calculus
- Linear algebra
- Positive semidefinite matrix
- Gradient of n-dimensional functions
- Hessian of n-dimensional functions
- Taylor series of n-dimensional functions
- Lagrange multiplicator rule

Classification of NLO problems

Linear Optimization (LO): $f, h_1, \cdots, h_p, g_1, \cdots, g_m$ are affine (linear) and the set $\mathcal{C}$ either equals to $\mathbb{R}^n$ or to $\mathbb{R}^n_+$.

Unconstrained Optimization: The index sets I and J are empty and $\mathcal{C} = \mathbb{R}^n$.

Convex Optimization (CO): $f, g_1, \cdots, g_m$ are convex, $h_1, \cdots, h_p$ are affine and $\mathcal{C}$ is convex.

Smooth Convex Optimization: It is a CO problem and all the functions are at least twice continuously differentiable (further smoothness requirements later).

Quadratic Optimization (QO): The objective f is quadratic $h_1, \cdots, h_p, g_1, \cdots, g_m$ are affine (linear) and either $\mathcal{C} = \mathbb{R}^n$ or $\mathcal{C} = \mathbb{R}^n_+$.

Quadratically Constrained QO (QCQO): The same as QO, but $g_1, \cdots, g_m$ are quadratic.

Convex Quadratic Optimization (CQO): The same as QO, but the objective f is convex.

Convex Quadratically Constrained QO (CQCQO): As QCQO, but the objective function f and the quadratic functions $g_1, \cdots, g_m$ are convex.

Solve the problems

Solve the following problem:

$$\min \ \exp(x) + \frac{1}{2}x^2$$

Show that the function $\exp(x) + \frac{1}{2}x^2$ is convex.

Consider the following problem:

$$\begin{aligned} \min \quad & \sqrt{(x_1 - x_4)^2 + (x_2 - x_5)^2 + (x_3 - x_6)^2} \\ & x_1^2 + x_2^2 + x_3^2 \le 5 \\ & (x_4 - 3)^2 + x_5^2 \le 1 \\ & 4 \le x_6 \le 8 \end{aligned}$$

Check that this is a convex problem.

Find the optimal solution of this problem.

Generic Algorithm

$$\begin{array}{ll} \text{min} & f(x) \\ \text{s.t.} & x \in \mathcal{C}. \end{array}$$

Input:
$\epsilon > 0$ is the accuracy parameter;
x^0 is a given (relative interior) feasible point;

Step 0: $x := x^0$, $k = 0$;

Step 1: Find **search direction** s^k s.t. $\delta f(x^k, s^k) < 0$
(This should be a descending feasible direction in the constrained case).

Step 1a: If no such direction exists **STOP,** optimum found.

Step 2: **Line search** : find $\lambda^k = \min_{\lambda} f(x^k + \lambda s^k)$;

Step 3: $x^{k+1} = x^k + \lambda^k s^k, \quad k = k + 1$;

Step 4: If **stopping criteria** satisfied **STOP,** else GOTO Step 1.

Optimality

Unconstrained minimization

Consider the problem

$$\text{minimize} \quad f(x),$$

where $x \in \mathcal{F} \subseteq \mathbb{R}^n$ a convex set and $f : \mathbb{R}^n \to \mathbb{R}$ is a differentiable function. First we define local and global minima of the above problem.

Definition 4 *Let a function $f : \mathbb{R}^n \to \mathbb{R}$ be given.*

A point $\bar{x} \in \mathbb{R}^n$ is a local minimum *of the function f if there is an $\epsilon > 0$ such that $f(\bar{x}) \leq f(x)$ for all $x \in \mathbb{R}^n$ when $\|\bar{x} - x\| \leq \epsilon$.*

A point $\bar{x} \in \mathbb{R}^n$ is a strict local minimum *of the function f if there is an $\epsilon > 0$ such that $f(\bar{x}) < f(x)$ for all $x \in \mathbb{R}^n$ when $\bar{x} \neq x$ and $\|\bar{x} - x\| \leq \epsilon$.*

A point $\bar{x} \in \mathbb{R}^n$ is a global minimum *of the function f if $f(\bar{x}) \leq f(x)$ for all $x \in \mathbb{R}^n$.*

A point $\bar{x} \in \mathbb{R}^n$ is a strict global minimum *of the function f if $f(\bar{x}) < f(x)$ for all $x \in \mathbb{R}^n$ when $\bar{x} \neq x$.*

Lemma 2 *Any (strict) local minimum $\bar{x}$ of a convex function f over the set $\mathcal{F}$ is a (strict) global minimum of f as well.*

Examples:

Local and Global minimizers

Find the local/global minimum of the functions if exist

- $\exp(x)$
- $-\log(x)$
- $x\log(x)$
- $-\sqrt{x}$ when $x \geq 0$
- $(x_1-2)^2+(x_2+1)^2-2$
- $\cos(x)$ on the interval $[\frac{\pi}{2}, \frac{3\pi}{2}]$
- $\log(x)$
- $-(x_1-2)^2+(x_2+1)^2-2$
- $\sin(x)$
- $x\sin(x)$
- $(x-2)^4-10*(x-2)^2$

Algorithms

Order and speed of convergence

Definition 5 *Let* $\alpha_1, \alpha_2, \ldots, \alpha_k, \ldots \to \alpha$ *be a convergent sequence. We say that the order of convergence of this sequence is* p^* *if*

$$p^* = \sup \left\{ p \ : \limsup_{k\to\infty} \frac{|\alpha_{k+1} - \alpha|}{|\alpha_k - \alpha|^p} < \infty \right\}.$$

The larger p^* is, the faster the convergence. Let $\beta = \limsup_{k\to\infty} \frac{|\alpha_{k+1} - \alpha|}{|\alpha_k - \alpha|}$. If $p^* = 1$ and $0 < \beta < 1$ we are speaking about *linear (or geometric rate of) convergence*. If $p^* = 1$ and $\beta = 0$ the convergence rate is *super-linear*, while if $\beta = 1$ the convergence rate is *sub-linear*. If $p^* = 2$ then the convergence is *quadratic*.

Example 1: The sequence $\alpha_k = a^k$, where $0 < a < 1$ converges linearly to zero while $\beta = a$.
Example 2: The sequence $\alpha_k = a^{(2^k)}$, where $0 < a < 1$ converges quadratically to zero.
Example 3: The sequence $\alpha_k = \frac{1}{k}$ converges sub-linearly to zero.
Example 4: The sequence $\alpha_k = (\frac{1}{k})^k$ converges super-linearly to zero.

Exercise: Find a sequence that converges to its limit with order 4.

Algorithms

Speed of convergence in n-dimension

A sequence of candidate solutions converge to an optimal point :

$$x^0, x^1, x^2, \cdots, x^k, \cdots \longrightarrow \bar{x} \in R^n$$

We can define α_k in various ways:

- $\alpha_k = \|x^k - \bar{x}\|$
  Problem: depends on scaling.
  Do normalize!
- $\alpha_k = \frac{\|x^k - \bar{x}\|}{\|x^k\|}$
  Problem: x^k might be zero.
  Never divide by zero!
- $\alpha_k = \frac{\|x^k - \bar{x}\|}{1+\|x^k\|}$
  Problem: $\|x^k - \bar{x}\|$ might be small while $|f(x^k - f(x)|$ big.
  Use objective or combined merit function.
- $\alpha_k = \frac{|f(x^k) - f(\bar{x})|}{1+|f(x^k)|}$, or $\alpha_k = \frac{\|x^k - \bar{x}\|}{1+\|x^k\|} + \frac{|f(x^k) - f(\bar{x})|}{1+|f(x^k)|}$
  Problem: $\bar{x}$ is not known!
  Monitor progress of the algorithm.
- $\alpha_k = \frac{|f(x^{k+1}) - f(x^k)|}{1+|f(x^k)|}$, or
  $\alpha_k = \frac{\|x^{k+1} - x^k\|}{1+\|x^k\|} + \frac{|f(x^{k+1}) - f(x^k)|}{1+|f(x^k)|}$.

Optimization versus feasibility

Solving nonlinear equations/inequalities

$$\min \{f(x) \mid x \in \mathcal{F}\}$$
$$\mathcal{F} = \{x \in \mathcal{C} \mid h_i(x) = 0, \forall\, i \text{ and } g_j(x) \le 0, \forall\, j\}.$$

- Feasibility (solving nonlinear equations/inequalities) is a part of the optimization problem.
- Solving any nonlinear equations, inequalities can be regarded as an optimization problem.
  - We consider the objective function to be the zero function.
  - Solve: $\{h_i(x) = 0, \forall\, i,\ g_j(x) \le 0, \forall\, j\}$ can be cast as

$$\min \sum_{i=1}^{p} (h_i(x))^2 + \sum_{j=1}^{m} (g_j(x) + z_j^2)^2$$

or

$$\min \sum_{i=1}^{p} |h_i(x)| + \sum_{j=1}^{m} \max\{0, g_j(x)\}$$

- Optimization problem can be cast as solving a series of feasibility problems for various ϑ values:

$$f(x) = \vartheta;\ h_i(x) = 0, \forall\, i,\ g_j(x) \le 0, \forall\, j$$

- We will see later that duality theory will provide a more powerful approach.

Nonlinear equations can be solved by using Newton's method. Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable.

$$\begin{aligned} F(x) &= 0 \\ F(x^k) + JF(x)(x - x^k) &= 0 \\ x^{k+1} &= x^k - (JF(x))^{-1} F(x^k) \end{aligned}$$

Direct search (Black box) methods

Pattern search methods

Cyclic coordinate search (Hooke and Jeeves)

$$\min \{ f(x) \mid x \in \mathbb{R}^n \}$$

Input: $\epsilon > 0$ is the accuracy parameter;
n linearly independent search direction $d^1, d^2, \cdots, d^n$;
$0 < \alpha < 1$ damping factor;
x^0 is a given initial point;

Step 0: $k = 0$; $y^0 = x^0$;
Step 1: $y^0 = x^k$, CALL PS:
Step 2: IF $y^n = y^0$ THEN $d^j = \alpha d^j$; GOTO Step 6.
Step 2a: $z = y^n$
Step 3: Here $f(z) < f(x^k)$;
Let $y^0 := y^n + (y^n - x^k)$; CALL PS;
Step 4: IF $f(y^n) < f(z)$ THEN $z = y^n$;
Step 5: Here $f(z) < f(x^k)$; Let $x^{k+1} = z$; $k = k+1$
Step 6: IF $\|d_1\| < \epsilon$ **STOP,** ELSE GOTO Step 1.

SUBROUTINE (PS): Pattern search:
FOR $j = 1 : n$ DO
IF $f(y^{j-1} + d^j) < f(y^{j-1})$ THEN $y^j = y^{j-1} + d^j$;
ELSEIF $f(y^{j-1} - d^j) < f(y^{j-1})$
THEN $y^j = y^{j-1} - d^j$;
ELSE $y^j = y^{j-1}$;
END

Direct search methods II

Simplex method (Nelder and Mead) I

$$\min \{ f(x) \mid x \in \mathbb{R}^n \}$$

Input: $\epsilon > 0$ is the accuracy parameter;
$n+1$ points $x^0, x^1, \cdots, x^n$ in general position;
$0 < \alpha < 1$ damping factor;
$0 < \beta < 1$ contraction factor;
$1 < \gamma$ extension factor;

Step 1: SORT the points in the order of ascending function value;

$$f(x^0) \le f(x^1) \le \cdots \le f(x^n)$$

Step 2: LET $\bar{x} := \frac{1}{n} \sum_{j=0}^{n-1} x^j$; $x^r := \bar{x} + (\bar{x} - x^n)$;

Step 2a: IF $f(x^r) < f(x^0)$
THEN $x^e := \bar{x} + \gamma(\bar{x} - x^n)$
IF $f(x^e) \le f(x^r)$
THEN DROP x^n ADD x^e GOTO 1.
ELSE DROP x^n ADD x^r GOTO 1.

Direct search methods III

Simplex method (Nelder and Mead)

Step 2b: IF $f(x^0) \leq f(x^r) < f(x^{n-1})$
THEN DROP x^n ADD x^r GOTO 1.

Step 2c: IF $f(x^{n-1}) \leq f(x^r) < f(x^n)$
THEN $x^c := \bar{x} + \beta(\bar{x} - x^n)$
IF $f(x^c) \leq f(x^{n-1})$
THEN DROP x^n ADD x^c GOTO 1.

Step 2d: IF $f(x^r) \geq f(x^n)$
THEN $x^c := \bar{x} - \beta(\bar{x} - x^n)$
IF $f(x^c) \leq f(x^{n-1})$
THEN DROP x^n ADD x^c GOTO 1.

Step 3: IF $\max\{\|x^i - x^j\| : 1 \leq i, j\} < \epsilon$
OR $f(x^n) - f(x^0) < \epsilon$ THEN **STOP**

Step 4: Contract the simplex to x^0;
$x^j := x^0 + \alpha(x^j - x^0), j = 1, 2, \cdots, n$; GOTO 1.