Introduction to the course "Optimization Methods and Game Theory"

G. Mastroeni

Department of Computer Science, University of Pisa

Optimization Methods and Game Theory
Master of Science in Artificial Intelligence and Data Engineering
University of Pisa – A.Y. 2023/24

Preliminary informations

Giandomenico Mastroeni

Dipartimento di Informatica

Largo B. Pontecorvo, 3 - Pisa

Building C - 2 floor - room 347DE

tel. 050 2212708

e-mail: giandomenico.mastroeni@unipi.it

Question time: by appointment (send e-mail)

Course schedule

- thursday 15 - 18, Room SI5
- friday 16 - 18 , Room ETR F2

Course material

- Microsoft Teams platform: Team 696AA 23/24 - Optimization Methods and Game Theory [WAI-LM] (Slides of the lectures)
- https://elearn.ing.unipi.it/course/view.php?id=3049

Aim of the course

Study optimization methods for data analysis and decision problems

Main tool

Optimization problems defined by

$$\min \ (max) \ \{f(x): \ x \in X\} \qquad (P)$$

- $f : \mathbb{R}^n \to \mathbb{R}$ is the objective function
- $X \subseteq \mathbb{R}^n$ is the constraints set or feasible region
- If $X \equiv \mathbb{R}^n$ then (P) is said to be unconstrained

(P) can be considered as a decision problem where X is the set of all the admissible (feasible) decisions x and $f(x)$ is the value of the decision x (for example, a cost or a gain).

In general X is defined by constraint functions

- $X = \{x \in \mathbb{R}^n : g(x) \leq 0, h(x) = 0\}$
- $g(x) = (g_1(x), \ldots, g_m(x))$, where $g_i : \mathbb{R}^n \to \mathbb{R}$, $i = 1, \ldots, m$ are the inequality constraints functions
- $h(x) = (h_1(x), \ldots, h_p(x))$, where $h_j : \mathbb{R}^n \to \mathbb{R}$, $j = 1, \ldots, p$ are the equality constraints functions

$$\begin{cases} \min \ f(x) \\ g(x) \leq 0 \\ h(x) = 0 \end{cases}$$

We will generally consider minimization problems since

$$\max\{f(x) : \ x \in X\} = -\min\{-f(x) : \ x \in X\}.$$

It is of fundamental importance to analyze the properties of (P) under suitable assumptions on X and on the involved functions:

- convexity
- differentiability

An application: Economical Power Dispatch

The production, distribution and consume of electricity are global concerns. In recent years, due to the scarcity of energy resources, it was observed an increasing power generation cost and ever-growing demand for electric energy: in this context, optimal economic dispatch has become an extremely important issue in power systems.

- We consider a power system that has a given electricity load demand P_D;
- The electricity is produced by n different units that can work with different loads. The production is based on a suitable fuel (petroleum, coal, gas, nuclear) and a given fuel cost function is associated with each unit.
- The Economical Power Dispatch (EPD) is modeled as a constrained optimization problem and consists in determining, the load of electricity to be produced by each unit, in a given interval of time T, in order to minimize the total fuel cost and supplying the total load demand and some technical requirements of the system.

The model

- We consider n generating units and we define the variable p_i the (unknown) power supply generated by unit $i = 1, .., n$;
- $f_i(p_i)$ is the fuel cost function, in (Euro/T), for the i-th unit, e.g.,

$$f_i(p_i) = a_i p_i^2 + b_i p + c_i,$$

  with a_i, b_i, c_i the fuel cost coefficients of unit i, $\quad i = 1, .., n$.
- p_{min_i} and p_{max_i} are the minimum and the maximum output limit of the i-th generating unit, for $i = 1, .., n$;
- P_D is the total load demand of the power system in MW;
- P_L is the amount of the system losses.

EPD problem formulation

$$
\begin{cases}
\min F(p) := \sum_{i=1}^n f_i(p_i) \\
p_1 + p_2 + ... + p_n = P_D + P_L \\
p_{min_i} \le p_i \le p_{max_i}, \ i = 1, .., n
\end{cases}
$$

An extension: Environmental/Economical Power Dispatch

It is of interest to consider the problem of simultaneously minimizing the total fuel cost of meeting the energy requirement of the system and the emissions of pollutants (e.g., fine dust emissions) of the units: this is a multiobjective optimization problem and is called the Environmental/Economical Power Dispatch (EEPD).

Besides the assumptions of problem (EPD) define:

- $e_i(p_i)$ the emission function, in (Kg/T), for the i-th unit, e.g.,

$$e_i(p_i) = \alpha_i p_i^2 + \beta_i p + \gamma_i,$$

   with α_i, β_i, γ_i the fuel emission coefficients of unit i, $\quad i = 1, .., n$.
- $E(p) = \sum_{i=1}^{n} e_i(p_i)$ the total quantity of emissions of the n units.

EEPD problem formulation

$$\begin{cases} \min(F(p), E(p)) \\ p_1 + p_2 + ... + p_n = P_D + P_L \\ p_{min_i} \leq p_i \leq p_{max_i}, \ i = 1, .., n \end{cases}$$

Outline of the program of the course

- Preliminaries of convex analysis
- Optimization problems: existence of optima, optimality conditions, duality
- Solution methods for optimization problems:
  - gradient and conjugate gradient method
  - Newton and quasi-Newton methods
  - active-set, penalty, logarithmic barrier methods
- Applications to machine learning:
  - Supervised machine learning: optimization models for classification and regression problems
  - Unsupervised machine learning: clustering problems
- Multiobjective (or vector) optimization problems:
  - Pareto and weak Pareto optimal solutions
  - existence, optimality conditions, scalarization approach, goal method
- Non-cooperative game theory:
  - zero-sum finite games: Nash Equilibrium (NE), existence, min–max theorem
  - non zero-sum finite games: existence, optimality conditions, algorithms
  - convex games: existence of NE, optimality conditions, merit functions
- Exercise sessions with MATLAB software

MATLAB

You can download and install MATLAB on your laptop using the Campus License paid by University of Pisa, see:

Link for Matlab installation

- https://unipi.it/matlab
- "Accedi per iniziare"
- Recall that in order to install Matlab it is necessary to use your istitutional mail, namely, ...@studenti.unipi.it, and not any e-mail address.
- In particular, install the optimization toolbox.

Bibliography

- S. Boyd and L. Vandenberghe, Convex optimization, Cambridge University Press, 2004.

- M.S. Bazaraa, H.D. Sherali, C.M. Shetty, Nonlinear Programming: Theory and Algorithms, Wiley-Interscience, 2006.

- J. Nocedal, S. Wright, Numerical Optimization, Springer Series in Operations Research and Financial Engineering, 2006.

- D.T. Luc, Theory of Vector Optimization, Springer, 1989.

- Y. Sawaragi, H. Nakayama, T. Tanino, Theory of Multiobjective Optimization, Academic Press, 1985.

- M.J. Osborne, A. Rubinstein, A Course in Game Theory, MIT press, 1994.

1 - Preliminary notions of convex analysis

G. Mastroeni

Department of Computer Science, University of Pisa

Optimization Methods and Game Theory
Master of Science in Artificial Intelligence and Data Engineering
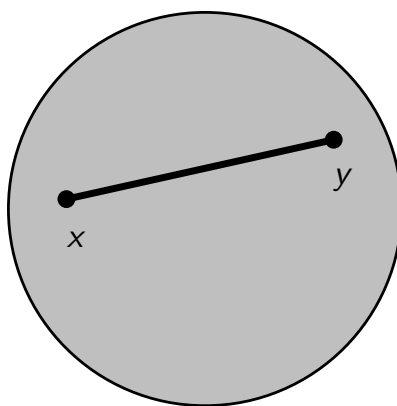University of Pisa – A.Y. 2023/24

Contents of the lessons

- Convex sets

- Cones

- Convex functions

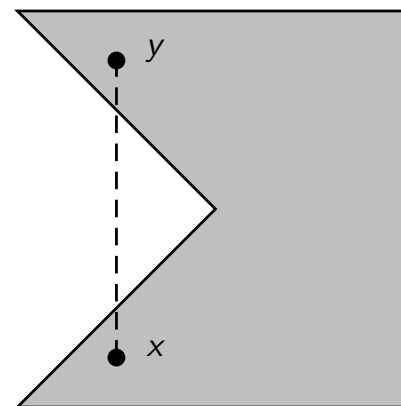- Strictly and strongly convex functions

Convex sets

Definition (Convex set)

A set $C \subseteq \mathbb{R}^n$ is convex if, for every $x, y \in C$ and for every $\alpha \in [0, 1]$,

$$\alpha x + (1 - \alpha) y \in C.$$

convex set

non-convex set

Definition (Affine set)

A set $C \subseteq \mathbb{R}^n$ is affine if, for every $x, y \in C$ and every $\alpha \in \mathbb{R}$,

$$\alpha x + (1 - \alpha)y \in C.$$

Examples of affine sets:

- any single point $\{x\}$
- any line
- the solution set of a system of linear equations

$$C = \{x \in \mathbb{R}^n : Ax = b\},$$

  where A is a $m \times n$ matrix and $b \in \mathbb{R}^m$

- any subspace

Examples of convex sets: subspaces

Note that a subspace is a particular affine set.

In fact, a set $S \subseteq \mathbb{R}^n$ is a subspace if, for every $x, y \in S$ and every $\alpha, \beta \in \mathbb{R}$,

$$\alpha x + \beta y \in S$$

Examples of subspaces:

- $\{0\}$
- any line which passes through zero
- the solution set of a homogeneous system of linear equations

$$S = \{x \in \mathbb{R}^n : \ Ax = 0\},$$

where A is a $m \times n$ matrix.

Definition

A convex combination of the points $x^1, x^2, ..., x^k$ is a point

$$y = \sum_{i=1}^{k} \alpha_i x^i \text{ where } \alpha_1, \ldots, \alpha_k \in [0, 1] \text{ and } \sum_{i=1}^{k} \alpha_i = 1.$$
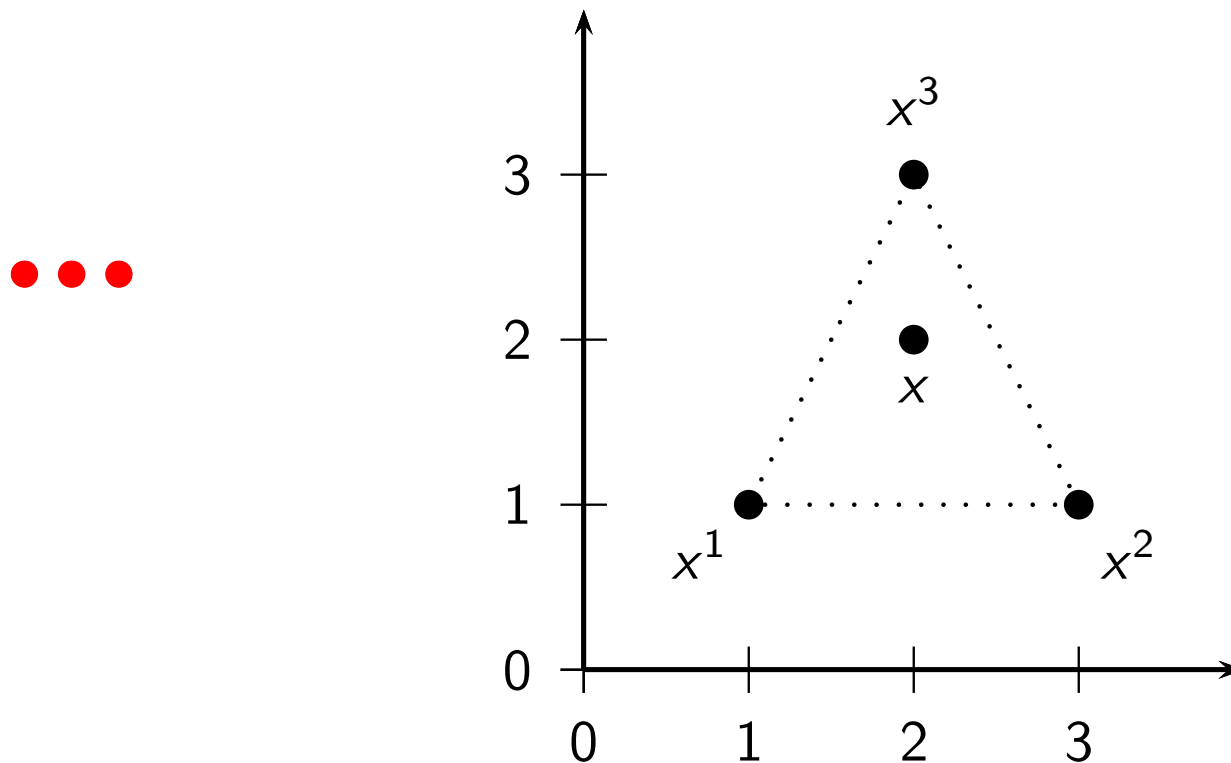
Remark

By definition, a set $C \subseteq \mathbb{R}^n$ is convex if it contains all the convex combinations of any two points in C.

Example. Consider the following 3 points in the plane:

$$x^1 = (1,1), \qquad x^2 = (3,1), \qquad x^3 = (2,3).$$

$x = (2,2)$ is a convex combination of x^1, x^2 e x^3, in fact:

$$x = \frac{1}{4}\,x^1 + \frac{1}{4}\,x^2 + \frac{1}{2}\,x^3.$$

A convex set contains any convex combination of its points.

Lemma 1

If C is convex, then for any $x^1, \ldots, x^k \in C$ and $\alpha_1, \ldots, \alpha_k \in [0,1]$ s.t. $\sum_{i=1}^{k} \alpha_i = 1$,

$$\sum_{i=1}^{k} \alpha_i x^i \in C.$$

Proof. By induction on k. For $k = 2$, the thesis holds, by definition of convexity. Assume that the thesis holds for a given k and let us prove it holds for $k + 1$.

Let $x^1, \ldots, x^{k+1} \in C$ and $\alpha_1, \ldots, \alpha_{k+1} \in [0, 1]$ s.t. $\sum_{i=1}^{k+1} \alpha_i = 1$. With no loss of generality, we assume that $\alpha_1 \neq 0$.

$$\sum_{i=1}^{k+1} \alpha_i x^i = \alpha_1 x_1 + \sum_{i=2}^{k+1} \alpha_i x^i = \alpha_1 x_1 + (1 - \sum_{i=2}^{k+1} \alpha_i) \sum_{i=2}^{k+1} \frac{\alpha_i}{1 - \sum_{i=2}^{k+1} \alpha_i} x^i$$

Since $\sum_{i=2}^{k+1} \frac{\alpha_i}{1 - \sum_{i=2}^{k+1} \alpha_i} = 1$, by inductive assumption we have:

$$\bar{x} := \sum_{i=2}^{k+1} \frac{\alpha_i}{1 - \sum_{i=2}^{k+1} \alpha_i} x^i \in C$$

and finally, since C is convex,

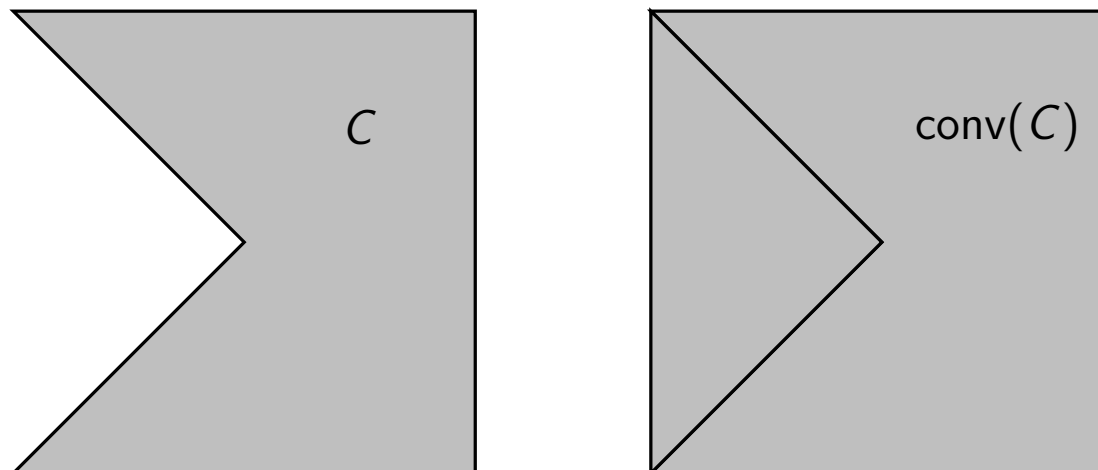$$\alpha_1 x_1 + (1 - \sum_{i=2}^{k+1} \alpha_i) \bar{x} \in C.$$

Proposition

If $\{C_i\}_{i \in I}$ is any (possibly infinite) family of convex sets, then $\bigcap_{i \in I} C_i$ is convex.

Definition (Convex hull)

The convex hull $\mathrm{conv}(C)$ of a set C is the intersection of all the convex sets containing C.
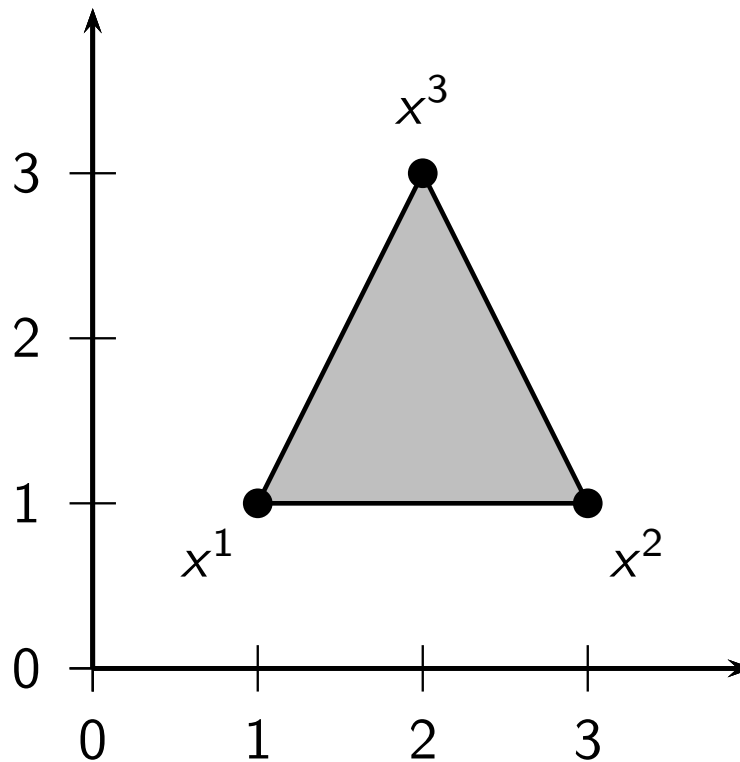
In other words, it is the smallest convex set containing C.

C

$\mathrm{conv}(C)$

The convex hull of the points

$$x^1 = (1,1), \qquad x^2 = (3,1), \qquad x^3 = (2,3).$$

is the grey triangle with vertexes the three points:

Proposition

$$\text{conv}(C) = \{\text{all convex combinations of points in } C\}$$

Proof. It can be proved that the set of convex combinations of points in C is a convex set containing C, so that

$$\text{conv}(C) \subseteq \{\text{all convex combinations of points in } C\}.$$

Since $C \subseteq \text{conv}(C)$ and $\text{conv}(C)$ is convex, by Lemma 1 it contains any convex combination of its points, and therefore

$$\text{conv}(C) \supseteq \{\text{all convex combinations of points in } C\}.$$

Remark

Observe that C is convex if and only if $C = \text{conv}(C)$.

Definition (Polyhedron)

A polyhedron P is the intersection of a finite number of closed halspaces in $\mathbb{R}^n$.

A closed halfspace is the set of solutions of a linear inequality:

$$a^{\mathsf{T}}x \leq \beta, \qquad \text{where } a \in \mathbb{R}^n \text{ e } \beta \in \mathbb{R}.$$

Consequently, a polyhedron

$$P = \{x \in \mathbb{R}^n : \ Ax \leq b\}$$

is the solution set of a system of linear inequalities where A is a $m \times n$ matrix and $b \in \mathbb{R}^m$.

A polyhedron P is convex since any closed halfspace is a convex set and the intersection of convex sets is convex.

- A ball is defined by $B(\bar{x}, r) := \{z \in \mathbb{R}^n : \|z - \bar{x}\| \leq r\}$, where $\|\cdot\|$ is any norm, e.g.

$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2} \text{ (Euclidean norm)}$$

$$\|x\|_1 = \sum_{i=1}^{n} |x_i| \text{ (Manhattan distance)}$$

$$\|x\|_\infty = \max_{i=1,\ldots,n} |x_i| \text{ (Chebyshev norm)}$$

$$\|x\|_p = \sqrt[p]{\sum_{i=1}^{n} |x_i|^p}, \text{ with } 1 \leq p < +\infty$$

$\|x\|_A = \sqrt{x^\mathsf{T} A x}$, where A is a symmetric and positive definite matrix, i.e.,

$$x^\mathsf{T} A x > 0 \qquad \forall \, x \neq 0.$$

Norms

Recall that a norm on a real vector space X is a function $p : X \to \mathbb{R}$ such that:

1 $p(x + y) \leq p(x) + p(y), \quad \forall x, y \in X$;

2 $p(\alpha x) = |\alpha| p(x), \quad \forall x \in X, \ \forall \alpha \in \mathbb{R}$;

3 $p(x) = 0 \quad \Leftrightarrow \quad x = 0$.

By the previous conditions it follows that $p(x) \geq 0, \ \forall x \in X$.

Exercise 1.1 Find the unit ball $B(0,1)$ w.r.t. $\| \cdot \|_1$, $\| \cdot \|_\infty$ and $\| \cdot \|_A$, where $A = \begin{pmatrix} 4 & 0 \\ 0 & 1 \end{pmatrix}$.

Algebraic operations

Sum and product by a constant

If C_1 and C_2 are convex, then $C_1 + C_2 := \{x + y : x \in C_1, y \in C_2\}$ is convex.

If C is convex and $\alpha \in \mathbb{R}$, then $\alpha C := \{\alpha x : x \in C, \}$ is convex.

Consequently, if C_1 and C_2 are convex, then $C_1 - C_2 := \{x - y : x \in C_1, y \in C_2\}$ is convex.

Topological operations

Closure and interior

If C is convex, then $\mathrm{cl}(C)$ is convex.
If C is convex, then $\mathrm{int}(C)$ is convex, provided that $\mathrm{int}(C) \neq \emptyset$.

Relative interior

Given a set $C \subseteq \mathbb{R}^n$ we denote by $aff(C)$ the smallest affine set containing C.

Definition (relative interior)

Let $C \subseteq \mathbb{R}^n$ be a convex set.
The relative interior of C is defined by

$$ri(C) = \{x \in C : \exists \epsilon > 0 \text{ s.t. } aff(C) \cap B(x, \epsilon) \subseteq C\}$$

.

Examples

- Let $C := \{(x_1, x_2) \in \mathbb{R}^2 : 1 \leq x_1 \leq 3, x_2 = 0\}$. Then

$$ri(C) := \{(x_1, x_2) \in \mathbb{R}^2 : 1 < x_1 < 3, x_2 = 0\}.$$

- Let $C = \{\bar{x}\}$, then $ri(C) = C$.

Theorem

Let C be a nonempty convex set in $\mathbb{R}^n$. Then the relative interior of C is a nonempty convex set.

Separation of convex sets

The sets A and B in $\mathbb{R}^n$ are said to be linearly separable if there exists $a \in \mathbb{R}^n$, $a \neq 0$, $\beta \in \mathbb{R}$, such that

$$a^T x \geq \beta \quad \forall x \in A, \qquad a^T x \leq \beta \quad \forall x \in B,$$

The separation is said to be proper if strict inequality holds for at least one $x \in A \cup B$.

Theorem

Let A, B be nonempty convex sets in $\mathbb{R}^n$. Then A and B are properly linearly separable if and only if
$$ri(A) \cap ri(B) = \emptyset.$$

In particular two disjoint convex sets are always properly linearly separable.

Example Let $A := \{(x_1, x_2) \in \mathbb{R}^2 : 1 \leq x_1 \leq 2, x_2 = 0\}$,
$B := \{(x_1, x_2) \in \mathbb{R}^2 : 2 \leq x_1 \leq 4, x_2 = 0\}$.
Then $ri(A) \cap ri(B) = \emptyset$ and the sets are properly separable by the hyperplane of equation $x_1 = 2$.

Affine functions

Let $f : \mathbb{R}^n \to \mathbb{R}^m$ be affine, i.e. $f(x) = Ax + b$, with $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$.

- If $C \subseteq \mathbb{R}^n$ is convex, then $f(C) = \{f(x) : x \in C\}$ is convex
- If $C \subseteq \mathbb{R}^m$ is convex, then $f^{-1}(C) = \{x \in \mathbb{R}^n : f(x) \in C\}$ is convex

Examples:

- $f(x) = \alpha x$, with $\alpha \in \mathbb{R}$
- $f(x) = x + b$, with $b \in \mathbb{R}^n$
- $f(x) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} x$, with $\theta \in (0, 2\pi)$ (rotation)
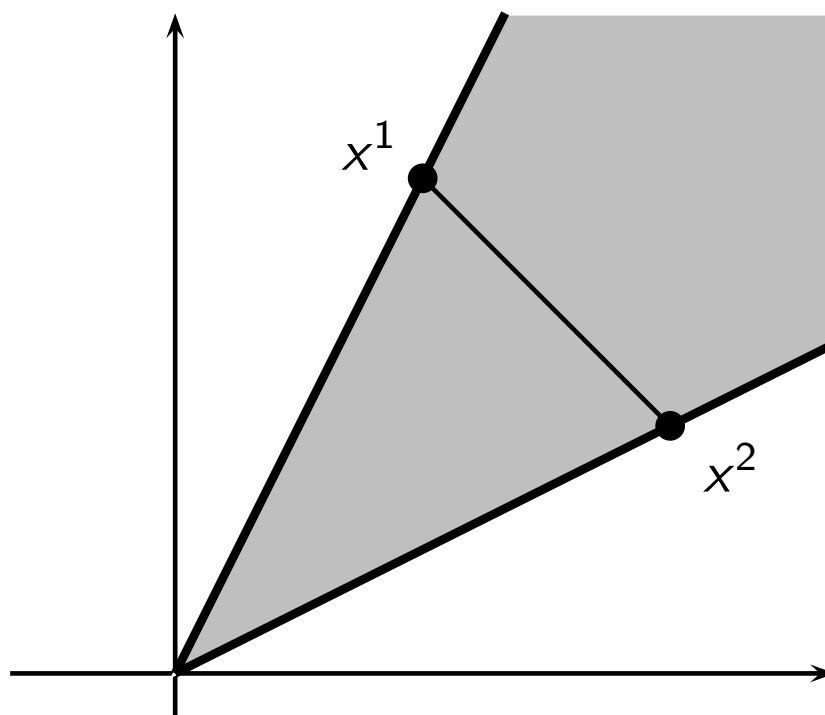
Definition (Cone)

A set $C \subseteq \mathbb{R}^n$ is a cone if, for every $x \in C$ and for every $\lambda \geq 0$, it results
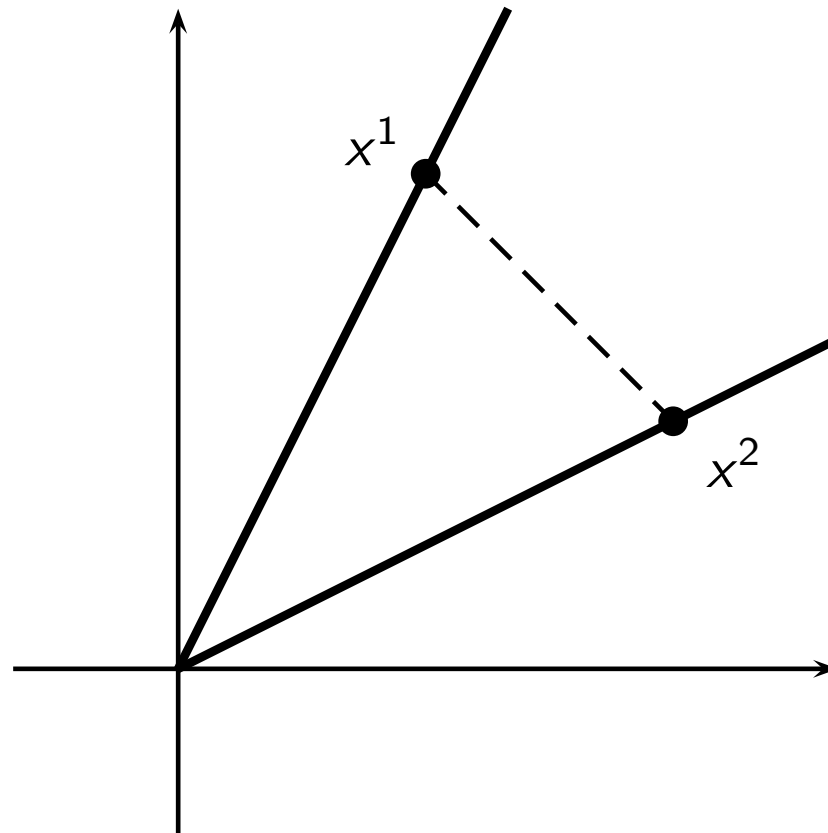
$$\lambda x \in C.$$

In other words, if C contains a point x different from 0 , then it contains the whole halfline starting from 0 and passing through x.

Example. A cone may be convex

or non convex:

Examples of cones

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

- $\{x \in \mathbb{R}^2 : x_1 x_2 = 0\}$ is a non-convex cone.

- Given a polyhedron $P = \{x : Ax \leq b\}$, the recession cone of P is defined as

$$\text{rec}(P) := \{d : x + \alpha d \in P \quad \text{for any } x \in P, \alpha \geq 0\}.$$

  It can be proved that $\text{rec}(P) = \{d : Ad \leq 0\}$, thus it is a polyhedral cone.

- $\left\{x \in \mathbb{R}^3 : x_3 \geq \sqrt{x_1^2 + x_2^2}\right\}$ is a non-polyhedral cone.

- Given $\bar{x} \in cl(C) \subseteq \mathbb{R}^n$, the set

$$T_C(\bar{x}) = \left\{d \in \mathbb{R}^n : \exists \{z_k\} \subset C, \exists \{t_k\} > 0, \ z_k \to \bar{x}, \ t_k \to 0, \lim_{k \to \infty} \frac{z_k - \bar{x}}{t_k} = d\right\}$$

  is called the *tangent cone* to C at $\bar{x}$. ● ● ●

Example

$$P_1 = \{x \in \mathbb{R}^2 : x_2 \leq x_1, \quad x_2 \geq 0\}$$
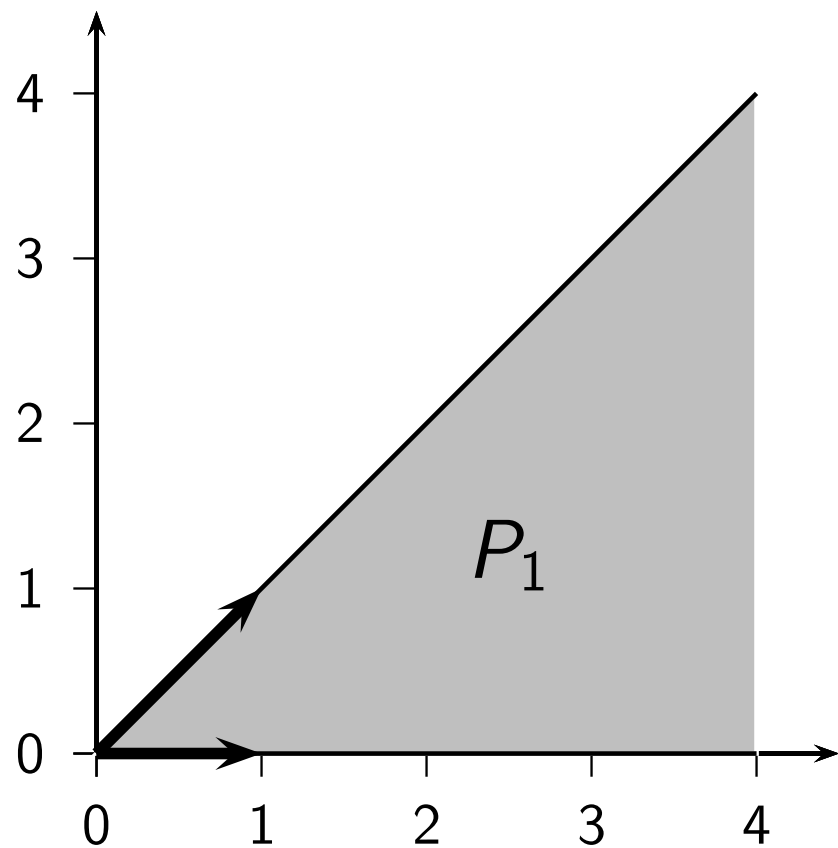
is a polyhedral cone.

$$rec(P_1) = P_1, \quad T_{P_1}((0,0)) = P_1.$$

Example

$$P_2 = \{x \in \mathbb{R}^2 : \ x_1 \geq 1, \quad x_2 \geq 1, \quad x_1 + x_2 \geq 3\}$$
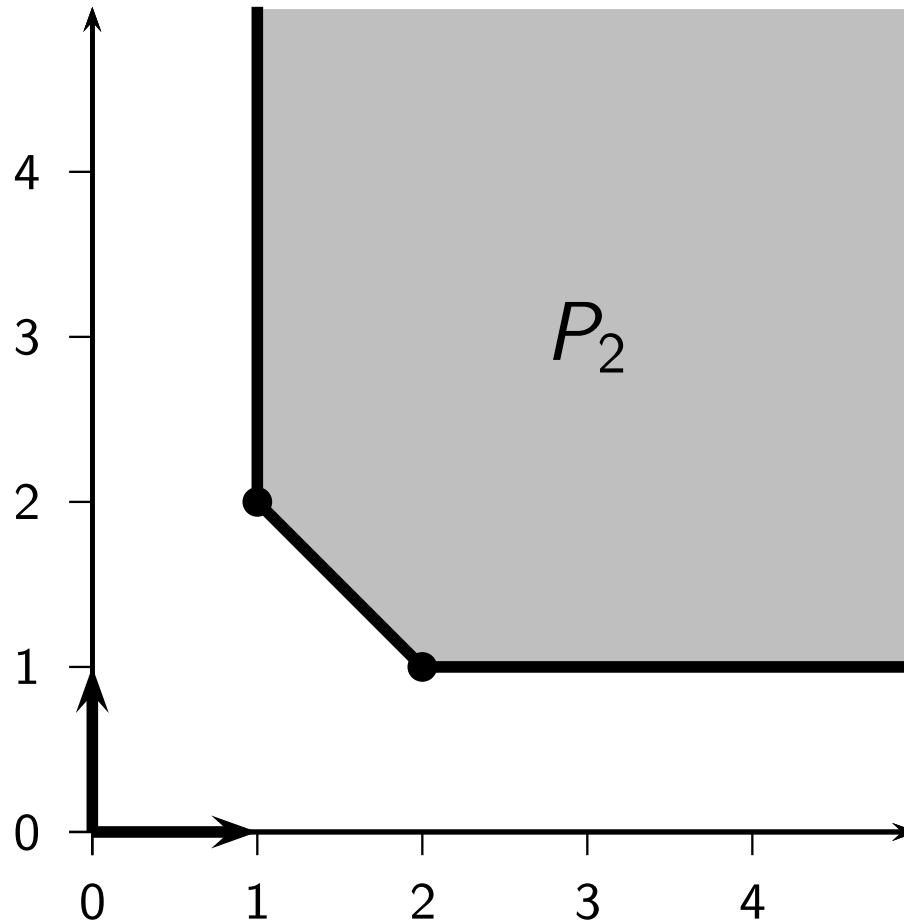
$$rec(P_2) = \{d \in \mathbb{R}^2 : \ d_1 \geq 0, \quad d_2 \geq 0\}$$

$$T_{P_2}((1,2)) = \{d \in \mathbb{R}^2 : \ d_1 \geq 0, \quad d_1 + d_2 \geq 0\}$$

1.2 Let $P = \{x : Ax \leq b\}$ where $A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$. Prove that $rec(P) = \{d \in \mathbb{R}^n : Ad \leq 0\}$.

1.3 If C_1 and C_2 are convex, then is $C_1 \cup C_2$ convex?

1.4 Prove that $B(\bar{x}, r) := \{z \in \mathbb{R}^n : \|z - \bar{x}\| \leq r\}$, is a convex set, whatever the norm $\|\cdot\|$ may be.

1.5 Write the vector $(1,1)$ as a convex combination of the vectors $(0,0), (3,0), (0,2), (3,2)$.

Definition (Convex function)

Let $C \subseteq \mathbb{R}^n$ be convex. A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex on C if

$$f(\alpha y + (1 - \alpha)x) \leq \alpha f(y) + (1 - \alpha)f(x) \qquad \forall \, x, y \in C, \forall \, \alpha \in [0, 1]$$
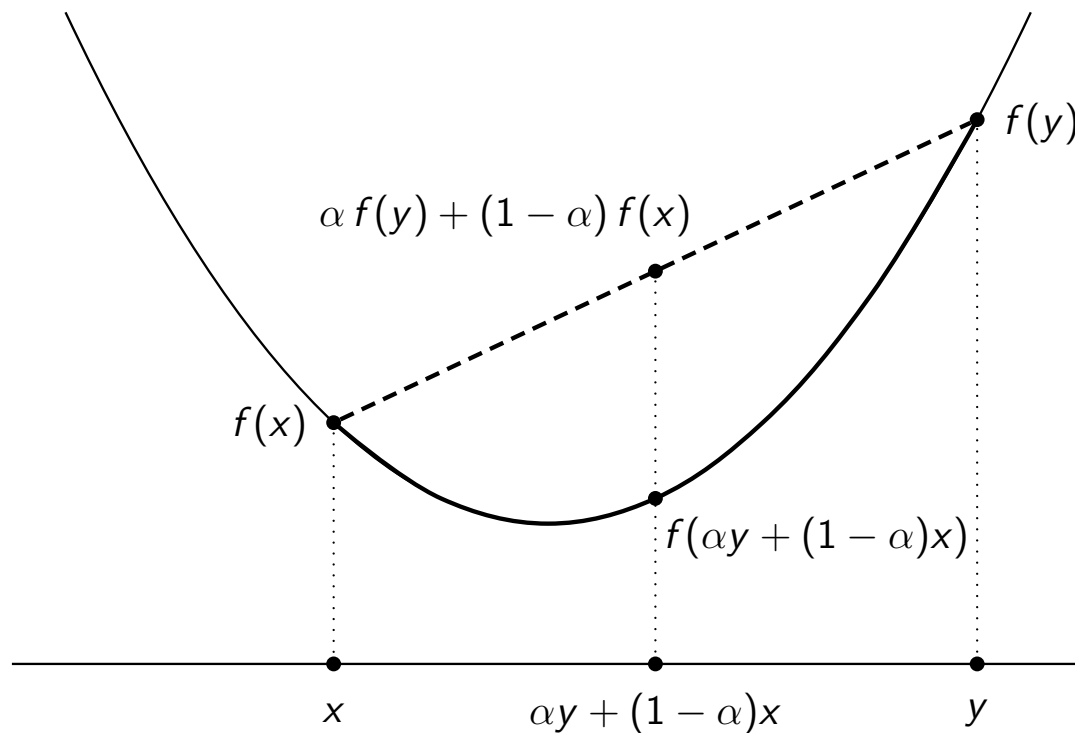
Remark

When $C = \mathbb{R}^n$ we will simply say that f is convex.

Theorem ●

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex on $\mathbb{R}^n$ if and only if the set

$$epi\ f_C := \{(x, y) \in C \times \mathbb{R} : y \geq f(x)\}$$

is convex.

Definition (Concave function)

Given a convex set $C \subseteq \mathbb{R}^n$, a function $f : \mathbb{R}^n \to \mathbb{R}$ is concave on C if $-f$ is convex, i.e.,

$$f(\alpha y + (1-\alpha)x) \geq \alpha f(y) + (1-\alpha)f(x) \qquad \forall\ x, y \in C, \forall\ \alpha \in [0, 1]$$

Examples.
- A linear (affine) function $f(x) = c^{\mathsf{T}}x + b$ is both convex and concave.
- Let $\|\cdot\|$ be any norm, then $f(x) = \|x\|$ is convex.

Theorem (continuity of convex functions)

Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex on the convex set $C \subseteq \mathbb{R}^n$. Then f is continuous on $ri(C)$.

Strictly convex and strongly convex functions

Definition (strictly convex function) 🔴

Given a convex set $C \subseteq \mathbb{R}^n$, a function $f : \mathbb{R}^n \to \mathbb{R}$ is strictly convex on C if

$$f(\alpha y + (1 - \alpha)x) < \alpha f(y) + (1 - \alpha)f(x) \qquad \forall \, x, y \in C, x \neq y, \forall \, \alpha \in (0, 1)$$

Definition (strongly convex function) 🔴

Given a convex set $C \subseteq \mathbb{R}^n$, a function $f : \mathbb{R}^n \to \mathbb{R}$ is strongly convex on C if there exists $\tau > 0$ s.t.

$$f(\alpha y + (1 - \alpha)x) \leq \alpha f(y) + (1 - \alpha)f(x) - \frac{\tau}{2}\alpha(1 - \alpha)\|y - x\|_2^2$$
$$\forall \, x, y \in C, \forall \, \alpha \in [0, 1]$$

Remark

Similarly to convex functions, we say that f is strictly (strongly) concave on C if $-f$ is strictly (strongly) convex on C.

Theorem

f is strongly convex if and only if $\exists\, \tau > 0$ such that $f(x) - \dfrac{\tau}{2}\,\|x\|_2^2$ is convex

Remark

By the previous theorem it follows that f is strongly convex if and only if there exists a convex function ψ and $\tau > 0$ such that $f(x) = \psi(x) + \dfrac{\tau}{2}\,\|x\|_2^2$.

Exercise 1.6

- Prove that: strongly convex $\implies$ strictly convex $\implies$ convex
- convex $\implies$ strictly convex ?
- strictly convex $\implies$ strongly convex ?

First order conditions

Assume that $C \subseteq \mathbb{R}^n$ is open and convex, $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable on C.

Theorem

f is convex on C if and only if

$$f(y) \geq f(x) + (y - x)^\mathsf{T} \nabla f(x) \qquad \forall\ x, y \in C.$$

First-order approximation of f is a global understimator

First order conditions

Theorem ●

- f is strictly convex on C if and only if

$$f(y) > f(x) + (y - x)^\mathsf{T} \nabla f(x) \qquad \forall\, x, y \in C, \text{with } x \neq y.$$

- f is strongly convex on C if and only if there exists $\tau > 0$ such that

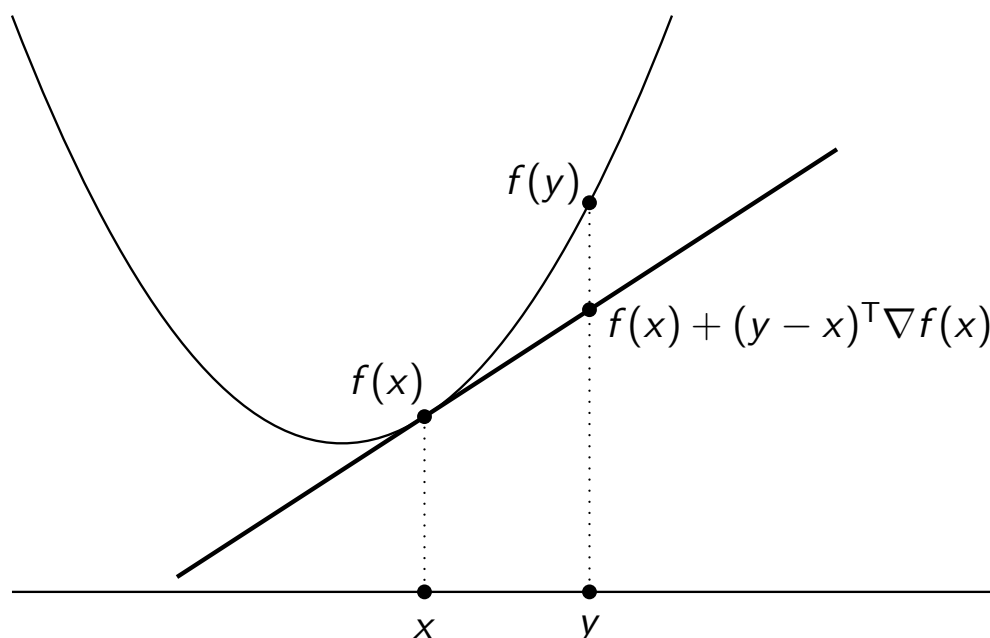$$f(y) \geq f(x) + (y - x)^\mathsf{T} \nabla f(x) + \frac{\tau}{2}\|y - x\|_2^2 \qquad \forall\, x, y \in C.$$

Second order conditions

Assume that $C \subseteq \mathbb{R}^n$ is open and convex, $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable on C.

Theorem ● ● ●

- f is convex on C if and only if for all $x \in C$ the Hessian matrix $\nabla^2 f(x)$ is positive semidefinite, i.e.

$$v^\mathsf{T} \nabla^2 f(x) v \geq 0 \qquad \forall\, v \in \mathbb{R}^n,\; \forall x \in C,$$

  or, equivalently, the eigenvalues of $\nabla^2 f(x)$ are ≥ 0, $\forall x \in C$.

- If $\nabla^2 f(x)$ is positive definite for all $x \in C$, then f is strictly convex on C.

- f is strongly convex on C if and only if there exists $\tau > 0$ such that $\nabla^2 f(x) - \tau I$ is positive semidefinite for all $x \in C$, i.e.

$$v^\mathsf{T} \nabla^2 f(x) v \geq \tau \|v\|_2^2 \qquad \forall\, v \in \mathbb{R}^n, \quad \forall\, x \in C,$$

  or, equivalently, the eigenvalues of $\nabla^2 f(x)$ are $\geq \tau$, $\forall\, x \in C$.

Convexity of quadratic functions

Let $f : \mathbb{R}^n \to \mathbb{R}$ be defined by

$$f(x) = \frac{1}{2}x^{\mathsf{T}}Qx + c^{\mathsf{T}}x$$

where Q is a $n \times n$ symmetric matrix, $c \in \mathbb{R}^n$. It is easy to check that

- $\nabla f = \frac{1}{2}(Qx + (x^{\mathsf{T}}Q)^{\mathsf{T}}) + c = Qx + c$
- Q is the Hessian of f.

Then f is:

- convex iff Q is positive semidefinite
- strongly convex iff Q is positive definite
- concave iff Q is negative semidefinite
- strongly concave iff Q is negative definite

Let $f : \mathbb{R} \to \mathbb{R}$ and $C := \mathbb{R}_+ \setminus \{0\}$.

- $f(x) = e^{px}$ for any $p \in \mathbb{R} \setminus \{0\}$ is strictly convex (on $\mathbb{R}$), but not strongly convex
- $f(x) = x^p$ is strictly convex on C if $p > 1$ or $p < 0$.
  Is it strongly convex?
- $f(x) = x^p$ is strictly concave on C if $0 < p < 1$
- $f(x) = \log(x)$ is strictly concave, but not strongly concave on C

Let $f : \mathbb{R}^n \to \mathbb{R}$.

- $f(x) = \|x\|$ is convex, but not strictly convex
- $f(x) = \max\{x_1, \ldots, x_n\}$ is convex, but not strictly convex

1.7 Prove that $f(x) = \|x\|$ is convex, whatever the norm $\|\cdot\|$ may be.

1.8 Prove that if f is convex, then for any $x^1, \ldots, x^k \in C$ and $\alpha_1, \ldots, \alpha_k \in (0,1)$ s.t. $\sum_{i=1}^{k} \alpha_i = 1$, one has $f\left(\sum_{i=1}^{k} \alpha_i x^i\right) \leq \sum_{i=1}^{k} \alpha_i f(x^i)$.

Hint. Follow the proof given in Lemma 1.

1.9 Prove that $f(x_1, x_2) = \dfrac{1}{x_1 \, x_2}$ is convex on the set $\{x \in \mathbb{R}^2 : \; x_1, x_2 > 0\}$.

1.10 Analyse the convexity properties of the function

$$f(x_1, x_2, x_3) = 2x_1^2 + 2x_2^2 + x_3^2 + 3x_1 x_2 + x_2 x_3 - 6x_1 - 4x_2 - 3x_3$$

1.11 Let f_1 and f_2 be convex, then is the product $f_1 \, f_2$ convex?

Operations that preserve convexity

Theorem ● ● ●

- If f is convex and $\alpha > 0$, then αf is convex
- If f_1 and f_2 are convex, then $f_1 + f_2$ are convex
- If f is convex, then $f(Ax + b)$ is convex

Examples

- Log barrier for linear inequalities:

$$f(x) = -\sum_{i=1}^{m} log(b_i - a_i^\mathsf{T} x) \qquad C = \{x \in \mathbb{R}^n : \ b_i - a_i^\mathsf{T} x > 0 \quad \forall \, i = 1, \dots, m\}$$

- Norm of affine function: $f(x) = \|Ax + b\|$

Pointwise maximum

Theorem

- If $f_1, \ldots, f_m$ are convex, then $f(x) = \max\{f_1(x), \ldots, f_m(x)\}$ is convex.
- If $\{f_i\}_{i \in I}$ is a family of convex functions, then $f(x) = \sup_{i \in I} f_i(x)$ is convex.

Example. If $\psi(x, \lambda) : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ is convex in x and concave in λ, then

$$p(x) = \sup_{\lambda} \psi(x, \lambda) \quad \text{is convex}$$

$$d(\lambda) = \inf_{x} \psi(x, \lambda) \quad \text{is concave}$$

Composition

$f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$.

Theorem ● ● ●

- If f is convex and g is convex and nondecreasing, then $g \circ f$ is convex.
- If f is concave and g is convex and nonincreasing, then $g \circ f$ is convex.

- If f is concave and g is concave and nondecreasing, then $g \circ f$ is concave.
- If f is convex and g is concave and nonincreasing, then $g \circ f$ is concave.

Examples Let $f : \mathbb{R} \to \mathbb{R}$.

- If f is convex, then $e^{f(x)}$ is convex
- If f is concave and positive, then $\log f(x)$ is concave
- If f is convex, then $-\log(-f(x))$ is convex on $\{x : \ f(x) < 0\}$
- If f is concave and positive, then $\dfrac{1}{f(x)}$ is convex
- If f is convex and nonnegative, then $f(x)^p$ is convex for all $p \geq 1$

Sublevel sets

Given $f : \mathbb{R}^n \to \mathbb{R}$ and $k \in \mathbb{R}$, the set

$$S_k(f) = \{x \in \mathbb{R}^n : \ f(x) \le k\}$$

is said the *k*-sublevel set of f.

Exercise 1.12 Prove that if f is convex, then $S_k(f)$ is a convex set for any $k \in \mathbb{R}$.

Is the converse true?

Quasiconvex functions

Definition (Quasiconvex convex function)

Given a convex set $C \subseteq \mathbb{R}^n$, $f : \mathbb{R}^n \to \mathbb{R}$ is said quasiconvex on C if the sets

$$S_k(f) \cap C = \{x \in C : f(x) \leq k\}$$

are convex for all $k \in \mathbb{R}$.

f is said quasiconcave on C if $-f$ is quasiconvex on C.

Examples

- $f(x) = \sqrt{|x|}$ is quasiconvex on $\mathbb{R}$
- $f(x_1, x_2) = x_1 x_2$ is quasiconcave on $\{x \in \mathbb{R}^2 : x_1 > 0, x_2 > 0\}$
- $f(x) = \log x$ is quasiconvex and quasiconcave

2 - Existence of optimal solutions and optimality conditions for unconstrained problems

G. Mastroeni

Department of Computer Science, University of Pisa
giandomenico.mastroeni@unipi.it

Optimization Methods and Game Theory
Master of Science in Artificial Intelligence and Data Engineering
University of Pisa – A.Y. 2023/24

- Existence of optimal solutions for optimization problems
- Existence of optimal solutions in the presence of convexity assumptions
- First and second order optimality conditions for unconstrained optimization problems
- Optimal solutions of unconstrained quadratic programming problems

Optimization problem in standard form

$$f_* = \min\{f(x) : \ x \in X\} \qquad (P)$$

- $f : \mathbb{R}^n \to \mathbb{R}$ is the objective function
- $X \subseteq \mathbb{R}^n$ is the constraints set or feasible region
- If $X \equiv \mathbb{R}^n$ then (P) is said to be unconstrained

From now on, we will only consider minimization problems since

$$\max\{f(x) : \ x \in X\} = -\min\{-f(x) : \ x \in X\}.$$

In general X is defined by the expression:

$$X := \{x \in \mathbb{R}^n : g_i(x) \leq 0, \ i \in \mathcal{I}, \ h_j(x) = 0, \ j \in \mathcal{J}\},$$

where $g_i : \mathbb{R}^n \longrightarrow \mathbb{R}$, $i \in \mathcal{I} := \{1, .., m\}$, $h_j : \mathbb{R}^n \longrightarrow \mathbb{R}$, $j \in \mathcal{J} := \{1, .., p\}$, Using the notation:

$$g(x) := (g_1(x), .., g_m(x))^T, \quad h(x) := (h_1(x), .., h_p(x))^T,$$

then $X = \{x \in \mathbb{R}^n : g(x) \leq 0, \ h(x) = 0\}$, $g : \mathbb{R}^n \longrightarrow \mathbb{R}^m$, $h : \mathbb{R}^n \longrightarrow \mathbb{R}^p$.

g and h are called the "constraint functions".

Remark

In this case (P) is also referred to as a *mathematical programming problem*.

Global and local optima

Optimal value

The optimal value of (P) is defined by: $v(P) = \inf\{f(x) : x \in X\}$
$v(P) \in \mathbb{R}$ if the problem is bounded from below
$v(P) = -\infty$ if the problem is unbounded from below
$v(P) = +\infty$ if the problem is infeasible, i.e., $X = \emptyset$

Global optimal solution

A global optimal solution of (P) is a point $x^* \in X$ s.t. $f(x^*) \leq f(x)$ for all $x \in X$.
$X_* = \arg\min\{f(x) : x \in X\}$ denotes the set of global minima of f on X.

Local optimal solution

A local optimal solution of (P) is a point $x^* \in X$ s.t. $f(x^*) \leq f(x)$ for all $x \in X \cap B(x^*, r)$ for some $r > 0$.

Examples

- $f(x) = x$, $X = \mathbb{R}$, $v(P) = -\infty$, no optimal solution
- $f(x) = e^x$, $X = \mathbb{R}$, $v(P) = 0$, no optimal solution
- $f(x) = x^3 - 3x$, $X = \mathbb{R}$, $v(P) = -\infty$, $x^* = 1$ is a local optimum, no global optimum
- $f(x) = x \log(x)$, $X = \mathbb{R}_{++}$, $v(P) = -1/e$, $x^* = 1/e$ is a global optimum
- $f(x) = 3x^4 - 8x^3 - 6x^2 + 24x + 19$, $X = \mathbb{R}$, $v(P) = 0$, $x^* = -1$ is a global optimum and $\tilde{x} = 2$ is a local optimum

Existence of global optima

Theorem (Weierstrass) ● ● ●

If the objective function f is continuous and the feasible region X is closed and bounded, then (at least) a global optimum exists.

Proof. Let $v(P) = \inf\limits_{x \in X} f(x)$. Define a minimizing sequence $\{x^k\} \subseteq X$ s.t. $f(x^k) \to v(P)$. Since $\{x^k\}$ is bounded, the Bolzano-Weierstrass theorem guarantees that there exists a subsequence $\{x^{k_p}\}$ converging to some point x^*. Since X is closed, we get $x^* \in X$. Finally, $f(x^{k_p}) \to f(x^*)$ since f is continuous. Therefore, $f(x^*) = v(P)$, i.e., x^* is a global optimum. $\qquad \square$

Example

$$\min \ x_1 + x_2 : \quad x \in X := \{(x_1, x_2) : x_1^2 + x_2^2 - 4 \leq 0\}$$

admits a global optimum.

Corollary 2 ● ● ●

If the objective function f is continuous, the feasible region X is closed and there exists $k \in \mathbb{R}$ such that the k-sublevel set

$$S_k(f) = \{x \in X : \ f(x) \leq k\} \tag{1}$$

is nonempty and bounded, then (at least) a global optimum exists.

Proof. Minimizing f on X is equivalent to minimize f on $S_k(f)$ which is bounded and closed since f is continuous and X is closed. □

Example

The function $f(x_1, x_2) = x_1^2 + x_2^2 - 4x_1 - 2x_2$ fulfils the condition (1).

In fact, suitably choosing k, the set

$$x_1^2 + x_2^2 - 4x_1 - 2x_2 \leq k$$

is a circle with center $C = (2, 1)$ and ray $r = \sqrt{2^2 + 1^2 + k}$

Example

$$\begin{cases} \min \ e^{x_1 + x_2} \\ x \in X := \{x_1 - x_2 \le 0, -2x_1 + x_2 \le 0\} \end{cases}$$

f is continuous, X is closed and unbounded. But the sublevel set $S_2(f) = \{x \in X : \ f(x) \le 2\}$ is nonempty and bounded, thus a global optimum exists.

Note that $S_2(f)$ is the solution set of the system:

$$\begin{cases} x_1 + x_2 \le \log 2 \\ x_1 - x_2 \le 0 \\ -2x_1 + x_2 \le 0 \end{cases}$$

Existence of global optima

Corollary 3 ●●●

If the objective function f is continuous and coercive, i.e.,

$$\lim_{\substack{\|x\|\to\infty \\ x\in X}} f(x) = +\infty, \tag{2}$$

and the feasible region $X \neq \emptyset$ is closed, then (at least) a global optimum exists.

Proof. Let $\bar{x} \in X$ and $k := f(\bar{x})$. By (2) the sublevel set $S_k(f)$ is nonempty and bounded, then apply Corollary 2 to show that a global optimum exists. $\square$

Example

$$\begin{cases} \min\ x^4 + 3x^3 - 5x^2 + x - 2 \\ x \in \mathbb{R} \end{cases}$$

Since f is coercive, then there exists a global optimum.

Example

The function $f(x_1, x_2) = x_1^2 + x_2^2 - 4x_1 - 2x_2$ fulfils the condition (2), with $X = \mathbb{R}^2$.

Indeed, $f(x_1, x_2) = x_1^2 + x_2^2 - 4x_1 - 2x_2 = (x_1 - 2)^2 - 4 + (x_2 - 1)^2 - 1$.

If $\|x\| = \|(x_1, x_2)\| \to +\infty$, then at least one of the following conditions holds:

$$|x_1| \to +\infty \quad or \quad |x_2| \to +\infty$$

In the first case we have:

$$\lim_{\|x\| \to +\infty} f(x_1, x_2) \geq \lim_{|x_1| \to +\infty} (x_1 - 2)^2 - 5 = +\infty$$

In the second case:

$$\lim_{\|x\| \to +\infty} f(x_1, x_2) \geq \lim_{|x_2| \to +\infty} (x_2 - 1)^2 - 5 = +\infty$$

Therefore, for any sequence $\{x^n\} = \{(x_1^n, x_2^n)\}$ such that $\|x^n\| \to +\infty$, we get

$$\lim_{n \to +\infty} f(x^n) = +\infty,$$

which guarantees that (2) is fulfilled.

Existence in the presence of convexity assumptions

Theorem 1 ● ● ●

Assume that f is convex on the convex set X. Then any local optimum of (P) is a global optimum.

Proof. Let x^* be a local optimum of (P), i.e., there is $r > 0$ s.t.

$$f(x^*) \leq f(z) \qquad \forall \, z \in X \cap B(x^*, r).$$

By contradiction, assume that x^* is not a global optimum, then there exists $y \in X$ s.t. $f(y) < f(x^*)$. Take $\alpha \in (0, 1)$ s.t. $\alpha x^* + (1 - \alpha)y \in B(x^*, r)$. Then, we have

$$f(x^*) \leq f(\alpha x^* + (1 - \alpha)y) \leq \alpha f(x^*) + (1 - \alpha)f(y) < \alpha f(x^*) + (1 - \alpha)f(x^*) = f(x^*),$$

that is impossible. □

Proposition 1 ● ● ●

Assume that f is strictly convex on the convex set X and that (P) admits a global optimum x^*. Then x^* is the unique optimal solution of (P).

Proof. By contradiction, assume that there exists $\hat{x} \in X$, with $\hat{x} \neq x^*$, such that $f(\hat{x}) = f(x^*)$. Since f is strictly convex, we have

$$f(\alpha x^* + (1 - \alpha)\hat{x}) < \alpha f(x^*) + (1 - \alpha)f(\hat{x}) = f(x^*) \quad \forall \alpha \in (0, 1)$$

which contradicts that x^* is a global optimum of (P). □

Theorem 2 ● ● ●

If $f : \mathbb{R}^n \to \mathbb{R}$ is strongly convex on $\mathbb{R}^n$ and X is closed, then there exists a global optimum.

Proof. It is known that any convex function on $\mathbb{R}^n$ is continuous, moreover, recall that any strongly convex function is the sum of a convex function plus the function $\tau\|x\|_2^2$, for some $\tau > 0$, i.e.,

$$f(x) = \psi(x) + \tau\|x\|_2^2,$$

with ψ convex.

Since ψ is convex then it is bounded from below by linear function:

$$f(x) = \psi(x) + \tau\|x\|_2^2 \geq a^T x + \tau\|x\|_2^2 \geq -\|a\|_2\|x\|_2 + \tau\|x\|_2^2$$

By the previous inequalities it follows that f is coercive, so that the thesis follows from Corollary 3. □

Corollary 1 ● ● ●

If f is strongly convex (on $\mathbb{R}^n$) and X is closed and convex, then there exists a unique global optimum.

Proof. By the previous theorem we know that a global minimum point exists, then the proof follows from Proposition 1. □

Example

Any quadratic programming problem

$$\min \ \frac{1}{2}x^\mathsf{T}Qx + c^\mathsf{T}x, \quad x \in X,$$

where Q is a positive definite matrix and X is closed and convex, has a unique global optimum.

Optimality conditions for unconstrained problems

We now consider the particular case where X is an open set. In particular, this assumption is fulfilled in when $X := \mathbb{R}^n$, i.e., (P) is an unconstrained problem defined by

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

Theorem 3 (Necessary optimality condition)

Assume that X is an open set and let f be differentiable at $x^* \in X$. If x^* is a local optimum of (P), then

$$\nabla f(x^*) = 0.$$

Proof. By contradiction, assume that $\nabla f(x^*) \neq 0$. Choose direction $d = -\nabla f(x^*)$, define $\varphi(t) = f(x^* + td)$,

$$\varphi'(0) = d^{\mathsf{T}} \nabla f(x^*) = -\|\nabla f(x^*)\|^2 < 0,$$

thus $f(x^* + td) < f(x^*)$ for all t small enough, which is impossible because x^* is a local optimum. $\qquad\square$

Second order optimality conditions

Assume that $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ has continuous first and second order partial derivatives for every $x \in X$.

Theorem 4 (Second order necessary optimality condition)

Let X be an open set and let $x^* \in X$ be a local optimum for (P). Then the following conditions hold:

- $\nabla f(x^*) = 0$;
- The Hessian matrix $\nabla^2 f(x^*)$ is positive semidefinite.

Theorem 5 (Second order sufficient optimality condition)

Let X be an open set, $x^* \in X$ and assume that the following conditions hold:

- $\nabla f(x^*) = 0$;
- The Hessian matrix $\nabla^2 f(x^*)$ is positive definite.

Then x^* is a local optimum for (P).

Theorem 6 (Optimality condition for convex problems)

Let f be a differentiable convex function on the open convex set X, then $x^* \in X$ is a global optimum for (P) if and only if $\nabla f(x^*) = 0$.

Proof. The necessity follows from Theorem 3.
Assume that $\nabla f(x^*) = 0$. Recall that, under the given differentiability assumptions f is convex on X if and only if

$$f(x) - f(y) \geq (x - y)^T \nabla f(y) \qquad \forall \; x, y \in X.$$

Setting $y = x^*$ we obtain

$$f(x^*) \leq f(x), \qquad \forall x \in X.$$

□

Similarly we can prove the following uniqueness result.

Theorem 7

Let f be a differentiable strictly convex function on the open convex set X, then $x^* \in X$ is a unique global optimum for (P) if and only if $\nabla f(x^*) = 0$.

Existence of global optima for unconstrained quadratic programming problems

Consider the quadratic problem

$$
\begin{cases}
\min\ f(x) := \dfrac{1}{2}x^{\mathsf{T}}Qx + c^{\mathsf{T}}x \\
x \in \mathbb{R}^n
\end{cases}
\tag{P}
$$

where Q is a $n \times n$ symmetric matrix.

Corollary 2

There exists a global optimum x^* for (P) if and only if the following conditions hold:

(i) $Qx^* + c = 0$,

(ii) Q is positive semidefinite.

Remark

Notice that, from (ii) a quadratic unconstrained problem admits an optimal solution only if f is convex, so that any local solution is also global.

Remark

We already observed that if Q is positive definite then (P) admits a unique global optimum. Indeed, in such a case Q is nonsingular and the system in (i) admits the unique solution $x^* = -Q^{-1}c$.

Let us consider more in details the case where Q is positive semidefinite but not positive definite.

In order to guarantee the existence of a global optimal solution we have to analyze the existence of a solution of the system $Qx + c = 0$.

By the Rouche'-Capelli Theorem the system $Qx = -c$ admits a solution if and only if

$$rank([Q, -c]) = rank(Q) \tag{3}$$

Proposition

If Q is positive semidefinite and (3) is fulfilled then (P) admits global optima given by the set of solutions of the system $Qx = -c$.

Example

Check if the function

$$f(x_1, x_2, x_3) = 2x_1^2 + 2x_2^2 + x_3^2 + 3x_1x_2 + x_2x_3 - 6x_1 - 4x_2 - 3x_3$$

admits a global minimum on $\mathbb{R}^3$.

The Hessian matrix is $Q = \begin{pmatrix} 4 & 3 & 0 \\ 3 & 4 & 1 \\ 0 & 1 & 2 \end{pmatrix}$

By the Matlab command $eig(Q)$ we obtain the eigenvalues of Q

$$eig(Q) \approx [0.61, 2.28, 7.09]$$

Then f is strongly convex and the global minimum point is

$x^* = -Q^{-1}c = -inv(Q) * c$, where $c = [-6, -4, -3]'$

$$x^* = -inv(Q) * c = inv(Q) * [-6, -4, -3]'$$

$x^* =$

    2.7000
   -1.6000
    2.3000

Example

Check if the function

$$f(x_1, x_2, x_3) = x_1^2 + 3x_2^2 + x_3^2 + x_1 x_2 - 2x_1 x_3 - x_2 x_3 + x_1 - x_3$$

admits a global minimum on $\mathbb{R}^3$.

The Hessian matrix is $Q = \begin{pmatrix} 2 & 1 & -2 \\ 1 & 6 & -1 \\ -2 & -1 & 2 \end{pmatrix}$, $\quad c = (1, 0, -1)^T$.

By the Matlab command $eig(Q)$ we obtain the eigenvalues of Q

$$eig(Q) \approx [0, 3.26, 6.73]$$

Then f is convex but not strongly convex and the global minimum points, if any, are given by the solutions of the system $Qx + c = 0$.

Setting $c = [1, 0, -1]'$, by the Matlab command "rank", we check that

$$rank([Q, -c]) = rank(Q) = 2,$$

which proves that the system admits solutions.

We note that the first two rows of Q are linearly independent.
Therefore, we can delete the third equation of system $Qx = -c$, which turns out to be equivalent to

$$\begin{pmatrix} 2 & 1 & -2 \\ 1 & 6 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}. \tag{S}$$

Setting,

$$B = \begin{pmatrix} 2 & 1 \\ 1 & 6 \end{pmatrix}, \quad N = \begin{pmatrix} -2 \\ -1 \end{pmatrix}$$

then (S) can be written as

$$B \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + Nx_3 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$

i.e.,

$$\begin{pmatrix} 2 & 1 \\ 1 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} -2 \\ -1 \end{pmatrix} x_3 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$

Then,

$$B \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} - Nx_3$$

and, provided that $det(B) \neq 0$, we obtain,

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = B^{-1} \left[\begin{pmatrix} -1 \\ 0 \end{pmatrix} - Nx_3 \right] = B^{-1} \begin{pmatrix} -1 \\ 0 \end{pmatrix} - B^{-1} Nx_3$$

Computing by Matlab, $inv(B) * [-1; 0]$ and $inv(B) * N$, we obtain:

$$B^{-1} \begin{pmatrix} -1 \\ 0 \end{pmatrix} = \begin{pmatrix} -0.5455 \\ 0.0909 \end{pmatrix} \qquad B^{-1} N = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$

so that,

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -0.5455 \\ 0.0909 \end{pmatrix} - \begin{pmatrix} -1 \\ 0 \end{pmatrix} x_3 = \begin{pmatrix} -0.5455 + x_3 \\ 0.0909 \end{pmatrix}$$

The set of global minima of the function f is given by

$$X_* = \{(x_1, x_2, x_3) : x_1 = -0.5455 + x_3, x_2 = 0.0909, x_3 \in \mathbb{R}\}$$

An optimization problem $\begin{cases} \min\ f(x) \\ g(x) \leq 0 \\ h(x) = 0 \end{cases}$ is said convex if the following conditions hold:

- objective function f is convex
- inequality constraints $g_1, \ldots, g_m$ are convex functions
- equality constraints $h_1, \ldots, h_p$ are affine functions (i.e., $h_j(x) = c^\top x + d$)

Examples

a) Problem $\begin{cases} \min\ x_1^2 + x_1 x_2 + 3x_2^2 + 4x_1 + 5x_2 \\ x_1^2 + x_2^2 - 4 \leq 0 \\ x_1 + x_2 - 2 = 0 \end{cases}$ is convex

b) Problem $\begin{cases} \min\ x_1^2 + x_2^2 \\ x_1/(1 + x_2^2) \leq 0 \\ (x_1 + x_2)^2 = 0 \end{cases}$ is NOT convex,

but it is equivalent to the problem $\begin{cases} \min\ x_1^2 + x_2^2 \\ x_1 \leq 0 \\ x_1 + x_2 = 0 \end{cases}$ that is convex.

Main properties of convex problems

Proposition

In a convex optimization problem the feasible region X is a convex set.

Proof. The sublevel sets of convex functions are convex and the level sets of affine functions are convex. □

Proposition

In a convex optimization problem any stationary point is a global optimal solution.

Unconstrained optimization methods

G. Mastroeni

Department of Computer Science, University of Pisa

Optimization Methods and Game Theory
Master of Science in Artificial Intelligence and Data Engineering
University of Pisa – A.Y. 2023/24

Contents of the lessons

- Gradient method

- Conjugate gradient method

- Newton methods

Gradient method

Consider an unconstrained problem: $\min\limits_{x\in\mathbb{R}^n} f(x)$.

Current point x^k, search direction $d^k = -\nabla f(x^k)$ (steepest descent direction)

Gradient method ● ● ●

1. Choose $x^0 \in \mathbb{R}^n$, set $k = 0$. Go to Step 2.
2. If $\nabla f(x^k) = 0$, STOP. Otherwise go to Step 3.
3. Let $d^k = -\nabla f(x^k)$ [search direction]
   compute an optimal solution t_k of the problem: $\min\limits_{t>0} f(x^k + t\,d^k)$ [step size];
   Set $x^{k+1} = x^k + t_k\,d^k$, $k = k + 1$;
   Go to Step 2.

Example 3.1 $f(x) = x_1^2 + x_2^2 - x_1 x_2$, starting point $x^0 = (1, 1)$.

$$\nabla f(x^0) = (1, 1), \ d^0 = (-1, -1), \ x^0 + td^0 = (1 - t, 1 - t)$$

,

$$f(x^0 + td^0) = (1 - t)^2 \quad t_0 = 1, \quad x^1 = (0, 0)$$

Gradient method - convergence

Proposition

Let f be continuously differentiable.

- $(d^k)^\mathsf{T} d^{k+1} = 0$ for any iteration k.
- If $\{x^k\}$ converges to x^*, then $\nabla f(x^*) = 0$, i.e. x^* is a stationary point of f.

Theorem

If f is coercive, then for any starting point x^0 the generated sequence $\{x^k\}$ is bounded and any of its cluster points is a stationary point of f.

Corollary

If f is coercive and convex, then for any starting point x^0 the generated sequence $\{x^k\}$ is bounded and any of its cluster points is a global minimum of f.

Corollary

If f is strongly convex, then for any starting point x^0 the generated sequence $\{x^k\}$ converges to the unique global minimum of f.

Gradient method - quadratic case

If $f(x) = \frac{1}{2}x^{\mathsf{T}}Qx + c^{\mathsf{T}}x$, with Q positive definite matrix, then, by the Taylor expansion at x^k, we have

$$f(x^k + td^k) = f(x^k) + (td^k)^{\mathsf{T}}\nabla f(x^k) + \frac{1}{2}(td^k)^{\mathsf{T}}Q\, td^k =$$

$$= \frac{1}{2}(d^k)^{\mathsf{T}}Q\, d^k\, t^2 + (d^k)^{\mathsf{T}}g^k\, t + f(x^k),$$

where $g^k = \nabla f(x^k) = Q\,x^k + c$. Thus the step size is equal to

$$t_k = -\frac{(d^k)^{\mathsf{T}}g^k}{(d^k)^{\mathsf{T}}Q\, d^k}.$$

Gradient method - convergence rate

As already observed, two subsequent directions are orthogonal: $(d^k)^\mathsf{T} d^{k+1} = 0$. This implies that the generated sequence has a zig-zag behaviour.

Theorem (Error bound)

If $f(x) = \frac{1}{2} x^\mathsf{T} Q x + c^\mathsf{T} x$, with Q positive definite matrix, and x^* is the global minimum of f, then the sequence $\{x^k\}$ satisfies the following inequality:

$$\|x^{k+1} - x^*\|_Q \leq \left(\frac{\frac{\lambda_n}{\lambda_1} - 1}{\frac{\lambda_n}{\lambda_1} + 1} \right) \|x^k - x^*\|_Q, \quad \forall \, k \geq 0, \quad \text{(linear convergence)}$$

where $\|x\|_Q = \sqrt{x^\mathsf{T} Q x}$ and $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ are the eigenvalues of Q.

Remark

If λ_n/λ_1 (condition number of Q) is $>> 1$, then the ratio $\left(\frac{\frac{\lambda_n}{\lambda_1} - 1}{\frac{\lambda_n}{\lambda_1} + 1} \right) \simeq 1$ and the convergence may be slow.
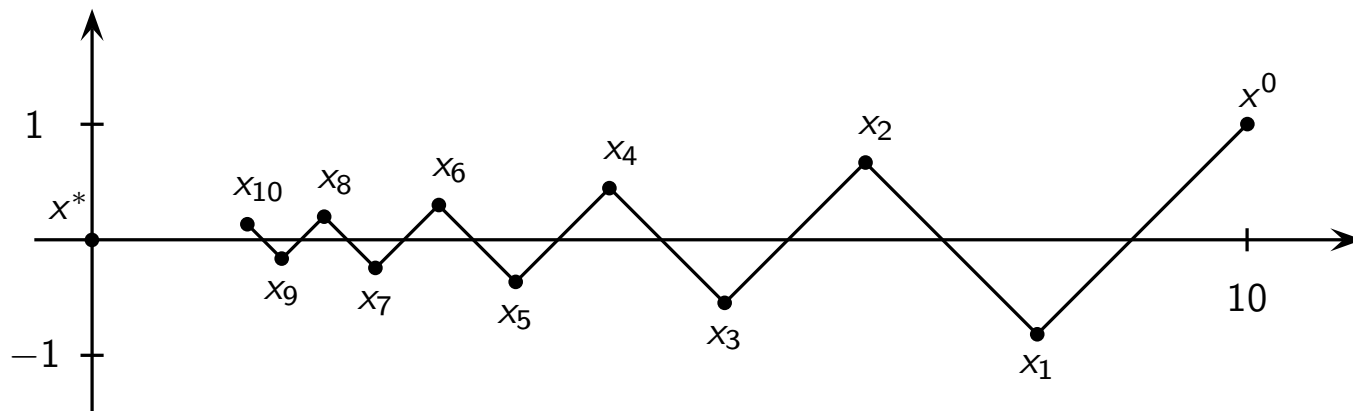
Gradient method - convergence rate

Example 3.2 $f(x) = x_1^2 + 10\, x_2^2$, global minimum is $x^* = (0,0)$.

If the starting point is $x^0 = (10, 1)$, then the generated sequence is:

$$x^k = \left(10 \left(\frac{9}{11}\right)^k, \left(-\frac{9}{11}\right)^k\right), \qquad \forall\ k \geq 0,$$

hence

$$\|x^{k+1} - x^*\| = \frac{9}{11} \|x^k - x^*\| \qquad \forall\ k \geq 0.$$

Gradient method - exercise

Exercise 3.1 Implement in MATLAB the gradient method for solving the problem

$$
\begin{cases}
\min \ \dfrac{1}{2}x^{\mathsf{T}}Qx + c^{\mathsf{T}}x \\
x \in \mathbb{R}^{n}
\end{cases}
$$

where Q is a positive definite matrix. In particular, solve the problem

$$
\begin{cases}
\min \ 3x_1^2 + 3x_2^2 + 3x_3^2 + 3x_4^2 - 4x_1 x_3 - 4x_2 x_4 + x_1 - x_2 + 2x_3 - 3x_4 \\
x \in \mathbb{R}^4
\end{cases}
$$

starting from the point $(0, 0, 0, 0)$. [Use $\|\nabla f(x)\| < 10^{-6}$ as stopping criterion.]

$$\frac{\partial f}{\partial x_1} = 6x_1 - 4x_3 + 1 \qquad \frac{\partial f}{\partial x_3} = 6x_3 - 4x_1 + 2$$

$$\frac{\partial f}{\partial x_2} = 6x_2 - 4x_4 - 1 \qquad \frac{\partial f}{\partial x_4} = 6x_4 - 4x_2 - 3$$

$$Q = \begin{bmatrix} 6 & 0 & -4 & 0 \\ 0 & 6 & 0 & -4 \\ -4 & 0 & 6 & 0 \\ 0 & -4 & 0 & 6 \end{bmatrix}$$

When f is not a quadratic function, the exact line search may be computationally expensive.

Gradient method with the Armijo inexact line search ● ● ●

1. Set $\alpha, \gamma \in (0, 1)$ and $\bar{t} > 0$. Choose $x^0 \in \mathbb{R}^n$, set $k = 0$. Go to Step 2.
2. If $\nabla f(x^k) = 0$, STOP. Otherwise go to Step 3.
3. Let $d^k = -\nabla f(x^k)$, $t_k = \bar{t}$;
   while $f(x^k + t_k d^k) > f(x^k) + \alpha t_k (d^k)^\mathsf{T} \nabla f(x^k)$ **do**
   $$t_k = \gamma t_k$$
   end
   Set $x^{k+1} = x^k + t_k d^k$, $k = k + 1$
   Go to Step 2.

Theorem

If f is coercive, then for any starting point x^0 the generated sequence $\{x^k\}$ is bounded and any of its cluster points is a stationary point of f.

Example 3.3 Let $f(x_1, x_2) = x_1^4 + x_1^2 + x_2^2$. Set $\alpha = 10^{-4}$, $\gamma = 0.5$, $\bar{t} = 1$, choose $x^0 = (1, 1)$.
$d^0 = -\nabla f(x^0) = (-6, -2)$.

Line search. If $t_0 = 1$ then $x^0 + t_0 d^0 = (-5, -1)$ and

$$f(x^0 + t_0 d^0) = 651 > f(x^0) + \alpha\, t_0 (d^0)^{\mathsf{T}} \nabla f(x^0) = 2.996,$$

if $t_0 = 0.5$ then

$$f(x^0 + t_0 d^0) = 20 > f(x^0) + \alpha\, t_0 (d^0)^{\mathsf{T}} \nabla f(x^0) = 2.998,$$

if $t_0 = 0.25$ then

$$f(x^0 + t_0 d^0) = 0.5625 < f(x^0) + \alpha\, t_0 (d^0)^{\mathsf{T}} \nabla f(x^0) = 2.999$$

hence the step size is $t_0 = 0.25$ and the new iterate is

$$x^1 = x^0 + t_0\, d^0 = (1, 1) + \frac{1}{4}(-6, -2) = \left(-\frac{1}{2}, \frac{1}{2}\right).$$

Gradient method - Armijo inexact line search

Exercise 3.2. Solve the problem

$$\begin{cases} \min \; 2\,x_1^4 + 3\,x_2^4 + 2\,x_1^2 + 4\,x_2^2 + x_1\,x_2 - 3\,x_1 - 2\,x_2 \\ x \in \mathbb{R}^2 \end{cases}$$

by means of the gradient method with the Armijo inexact line search setting $\alpha = 0.1$, $\gamma = 0.9$, $\bar{t} = 1$ and starting from the point $(0, 0)$.
[Use $\|\nabla f(x)\| < 10^{-3}$ as stopping criterion.]

Exercise 3.3. Solve the problem

$$\begin{cases} \min \; x_1^4 + x_2^4 - 2\,x_1^2 + 4x_1\,x_2 - 2\,x_2^2 \\ x \in \mathbb{R}^2 \end{cases}$$

by means of the gradient method with the Armijo inexact line search setting $\alpha = 0.1$, $\gamma = 0.9$, $\bar{t} = 1$ and starting from the point $(10, -10)$.
[Use $\|\nabla f(x)\| < 10^{-3}$ as stopping criterion.]

Conjugate gradient method

The conjugate gradient method is a descent method where the search direction involves the gradient computed at the current iteration and the direction computed at the previous iteration.

We first consider the quadratic case:

$$f(x) = \frac{1}{2} x^\mathsf{T} Q x + c^\mathsf{T} x,$$

where Q is positive definite. Set $g^k = \nabla f(x^k) = Qx^k + c$.

At iteration k, the search direction is defined by

$$d^k = \begin{cases} -g^0 & \text{if } k = 0, \\ -g^k + \beta_k \, d^{k-1} & \text{if } k \geq 1, \end{cases}$$

where β_k is such that d^k and d^{k-1} are conjugate with respect to Q, i.e.,

$$(d^k)^\mathsf{T} Q \, d^{k-1} = 0.$$

- By the previous relation we can compute β_k:

$$\beta_k = \frac{(g^k)^\mathsf{T} Q \, d^{k-1}}{(d^{k-1})^\mathsf{T} Q \, d^{k-1}}$$

- If we perform an exact line search, then d^k is a descent direction
- The step size given by exact line search is $t_k = -\dfrac{(g^k)^\mathsf{T} d^k}{(d^k)^\mathsf{T} Q \, d^k}$

Conjugate gradient method for quadratic functions ● ● ●

① Choose $x^0 \in \mathbb{R}^n$, set $g^0 = Q \, x^0 + c$, $k := 0$; go to Step 2.

② Let $g^k = \nabla f(x^k)$. **If** $g^k = 0$ **then** STOP, **else** go to Step 3.

③ **If** $k = 0$ **then** $d^k = -g^k$

else $\beta_k = \dfrac{(g^k)^\mathsf{T} Q \, d^{k-1}}{(d^{k-1})^\mathsf{T} Q \, d^{k-1}}, \qquad d^k = -g^k + \beta_k \, d^{k-1}$

$\qquad t_k = -\dfrac{(g^k)^\mathsf{T} d^k}{(d^k)^\mathsf{T} Q \, d^k}$

$\qquad x^{k+1} = x^k + t_k \, d^k, \; g^{k+1} = Q \, x^{k+1} + c, \; k = k + 1$

Go to Step 2.

Conjugate gradient method

Example 3.4 Consider $f(x) = x_1^2 + 10\,x_2^2$, with starting point $x^0 = (10, 1)$.

$$Q = \begin{pmatrix} 2 & 0 \\ 0 & 20 \end{pmatrix} \quad \nabla f(x) = (2x_1, 20x_2)$$

- $k = 0$: $g^0 = (20, 20)$, $d^0 = -g^0 = (-20, -20)$,
  $t_0 = -((g^0)^\mathsf{T} d^0)/((d^0)^\mathsf{T} Q\, d^0) = 1/11$, and consequently

$$x^1 = x^0 + t_0\, d^0 = (10 - 20/11, 1 - 20/11) = (90/11, -9/11)$$

- $k = 1$: $g^1 = (180/11, -180/11)$, $\beta_1 = ((g^1)^\mathsf{T} Q\, d^0)/((d^0)^\mathsf{T} Q\, d^0) = 81/121$,
  $d^1 = -g^1 + \beta_1\, d^0 = (-3600/121, 360/121)$,
  $t_1 = -((g^1)^\mathsf{T} d^1)/((d^1)^\mathsf{T} Q\, d^1) = 11/40$,
  and $x^2 = x^1 + t_1\, d^1 = (0, 0)$ which is the global minimum of f.

Conjugate gradient method - convergence

Proposition

- An alternative formula for the step size is $t_k = \dfrac{\|g^k\|^2}{(d^k)^\mathsf{T} Q \, d^k}$

- An alternative formula for β_k is $\beta_k = \dfrac{\|g^k\|^2}{\|g^{k-1}\|^2}$

- If we did not find the global minimum after k iterations, then the gradients $\{g^0, g^1, \ldots, g^k\}$ are orthogonal

- If we did not find the global minimum after k iterations, then the directions $\{d^0, d^1, \ldots, d^k\}$ are conjugate w.r.t. Q and x^k is the minimum of f on $x^0 + \mathrm{Span}(d^0, d^1, \ldots, d^k)$

Theorem (Convergence)

- The CG method finds the global minimum in at most *n* iterations.

- If Q has *r* distinct eigenvalues, then CG method finds the global minimum in at most *r* iterations.

Conjugate gradient method - convergence rate

Theorem (Error bound)

If $0 < \lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$ are the eigenvalues of Q, then the following bounds hold:

- $$\|x^k - x^*\|_Q \le 2 \left(\frac{\sqrt{\frac{\lambda_n}{\lambda_1}} - 1}{\sqrt{\frac{\lambda_n}{\lambda_1}} + 1} \right)^k \|x^0 - x^*\|_Q, \qquad \forall\ k \ge 0,$$

- $$\|x^k - x^*\|_Q \le \left(\frac{\lambda_{n-k+1} - \lambda_1}{\lambda_{n-k+1} + \lambda_1} \right) \|x^0 - x^*\|_Q, \qquad \forall\ k \ge 0.$$

Conjugate gradient method

Exercise 3.4 Implement in MATLAB the conjugate gradient method for solving the problem

$$\begin{cases} \min \ \dfrac{1}{2}x^\mathsf{T} Qx + c^\mathsf{T} x \\ x \in \mathbb{R}^n \end{cases}$$

where Q is a positive definite matrix.
Solve the problem

$$\begin{cases} \min \ 3x_1^2 + 3x_2^2 + 3x_3^2 + 3x_4^2 - 4x_1x_3 - 4x_2x_4 + x_1 - x_2 + 2x_3 - 3x_4 \\ x \in \mathbb{R}^4 \end{cases}$$

starting from the point $(0, 0, 0, 0)$. [Use $\|\nabla f(x)\| < 10^{-6}$ as stopping criterion.]

Newton method − basic version

We want to find a stationary point $\nabla f(x) = 0$.

At iteration k, make a linear approximation of $\nabla f(x)$ at x^k, i.e.

$$\nabla f(x) \simeq \nabla f(x^k) + \nabla^2 f(x^k)(x - x^k),$$

the new iterate x^{k+1} is the solution of the linear system

$$\nabla f(x^k) + \nabla^2 f(x^k)(x - x^k) = 0.$$

Note that x^{k+1} is a stationary point of the quadratic approximation of f at x^k:

$$f(x) \simeq f(x^k) + (x - x^k)^\mathsf{T} \nabla f(x^k) + \frac{1}{2}(x - x^k)^\mathsf{T} \nabla^2 f(x^k)(x - x^k).$$

Newton method – basic version

Newton method (basic version) ● ● ●

1. Let $x^0 \in \mathbb{R}^n$, set $k = 0$. Go to Step 2.
2. **If** $\nabla f(x^k) = 0$ then STOP **else** go to Step 3.
3. Let d^k be the solution of the linear system $\nabla^2 f(x^k)d = -\nabla f(x^k)$. Set $x^{k+1} = x^k + d^k$, $k = k + 1$ and go to Step 2.

Theorem (Convergence)

If x^* is a local minimum of f and $\nabla^2 f(x^*)$ is positive definite, then there exists $\delta > 0$ such that for any $x^0 \in B(x^*, \delta)$ the sequence $\{x^k\}$ converges to x^* and

$$\|x^{k+1} - x^*\| \leq C \|x^k - x^*\|^2 \qquad \forall \, k > \bar{k}, \qquad \text{(quadratic convergence)}$$

for some $C > 0$ and $\bar{k} > 0$.

Newton method – basic version

Example 3.5 $f(x) = 2 x_1^4 + 3 x_2^4 + 2 x_1^2 + 4 x_2^2 + x_1 x_2 - 3 x_1 - 2 x_2$ is strongly convex because

$$\nabla^2 f(x) = \begin{pmatrix} 24 x_1^2 + 4 & 1 \\ 1 & 36 x_2^2 + 8 \end{pmatrix}.$$

k	x^k		$\|\nabla f(x^k)\|$
	x1	x2	
0	10.000000	5.000000	8189.6317378
1	6.655450	3.298838	2429.6437291
2	4.421132	2.149158	721.6330686
3	2.925965	1.361690	214.6381594
4	1.923841	0.811659	63.7752575
5	1.255001	0.428109	18.6170045
6	0.823359	0.209601	5.0058040
7	0.580141	0.171251	1.0538969
8	0.492175	0.179815	0.1022945
9	0.481639	0.180914	0.0013018
10	0.481502	0.180928	0.0000002

Newton method – basic version

Drawbacks of Newton method:

- at each iteration we need to compute both the gradient $\nabla f(x^k)$ and the hessian matrix $\nabla^2 f(x^k)$
- local convergence: if x^0 is too far from the optimum x^*, then the generated sequence may be not convergent to x^*

Example 3.6 Let $f(x) = -\dfrac{1}{16}x^4 + \dfrac{5}{8}x^2$.

Then $f'(x) = -\dfrac{1}{4}x^3 + \dfrac{5}{4}x$ and $f''(x) = -\dfrac{3}{4}x^2 + \dfrac{5}{4}$.

$x^* = 0$ is a local minimum of f with $f''(x^*) = 5/4 > 0$.
The sequence does not converge to x^* if it starts from $x^0 = 1$:
$x^1 = -1$, $x^2 = 1$, $x^3 = -1$, ...

Newton method with line search

If f is strongly convex, then we have global convergence because d^k is a descent direction, in fact:

$$\nabla f(x^k)^\mathsf{T} d^k = -\nabla f(x^k)^\mathsf{T} [\nabla^2 f(x^k)]^{-1} \nabla f(x^k) < 0.$$

Newton method with (inexact) line search ● ● ●

1. Let $\alpha, \gamma \in (0,1)$, $\bar{t} > 0$, $x^0 \in \mathbb{R}^n$, set $k = 0$. Go to Step 2.

2. **If** $\nabla f(x^k) = 0$ then STOP **else** go to Step 3.

3. Let d^k be the solution of the linear system $\nabla^2 f(x^k)d = -\nabla f(x^k)$.
   Set $t_k = \bar{t}$

   　　while $f(x^k + t_k d^k) > f(x^k) + \alpha\, t_k\, (d^k)^\mathsf{T} \nabla f(x^k)$ **do**

   　　　　$t_k = \gamma t_k$

   　end

   Set $x^{k+1} = x^k + t_k d^k$, $k = k + 1$
   Go to Step 2.

Newton method with line search

Theorem (Convergence)

If f is strongly convex, then for any starting point $x^0 \in \mathbb{R}^n$ the sequence $\{x^k\}$ converges to the global minimum of f. Moreover, if $\alpha \in (0, 1/2)$ and $\bar{t} = 1$ then the convergence is quadratic.

Exercise 3.5. Solve the problem

$$\begin{cases} \min \ 2 x_1^4 + 3 x_2^4 + 2 x_1^2 + 4 x_2^2 + x_1 x_2 - 3 x_1 - 2 x_2 \\ x \in \mathbb{R}^2 \end{cases}$$

by means of the Newton method with inexact line search setting $\alpha = 0.1$, $\gamma = 0.9$, $\bar{t} = 1$ and starting from the point $(0, 0)$. [Use $\|\nabla f(x)\| < 10^{-3}$ as stopping criterion.]

Karush-Kuhn-Tucker optimality conditions and Lagrangian duality

G. Mastroeni

Department of Computer Science, University of Pisa

- The Abadie constraints qualification (ACQ);
- Karush-Kuhn-Tucker optimality conditions;
- Lagrangian duality.

Consider the constrained optimization problem

$$
\begin{cases}
\min \ f(x) \\
x \in X := \{x \in \mathbb{R}^n : g_j(x) \leq 0, \ \ j = 1, \ldots, m, \ h_k(x) = 0, \ \ k = 1, \ldots, p\}
\end{cases} \quad \text{(P)}
$$

where f, g_j and h_k are continuously differentiable for any j, k.

Definition ● ● ●

- The *Tangent cone* at $x^* \in X$, is defined by

$$
T_X(x^*) = \left\{ d \in \mathbb{R}^n : \exists \ \{z_k\} \subset X, \ \exists \ \{t_k\} > 0, \ z_k \to x^*, \ t_k \to 0, \ \lim_{k \to \infty} \frac{z_k - x^*}{t_k} = d \right\}
$$

- $\mathcal{A}(x^*) = \{j : \ g_j(x^*) = 0\}$ is the set of inequality constraints which are active at $x^* \in X$.

- The set

$$
D(x^*) = \left\{ d \in \mathbb{R}^n : \ \begin{array}{ll} d^\mathsf{T} \nabla g_j(x^*) \leq 0 & \forall \ j \in \mathcal{A}(x^*), \\ d^\mathsf{T} \nabla h_k(x^*) = 0 & \forall \ k = 1, \ldots, p \end{array} \right\}
$$

is the *first-order feasible direction cone* at $x^* \in X$.

Definition – Abadie constraint qualification (ACQ) ●●●

We say that the Abadie constraint qualification (ACQ) holds at a point $x^* \in X$, if $T_X(x^*) = D(x^*)$.

Theorem 1 (Sufficient conditions for ACQ) ●●●

a) (*Affine constraints*)
If g_j and h_k are affine for all $j = 1, \ldots, m$ and $k = 1, \ldots, p$, then ACQ holds at any $x \in X$.

b) (*Slater condition for convex problems*)
If g_j are convex for all $j = 1, \ldots, m$, h_k are affine for all $k = 1, \ldots, p$ and there exists $\bar{x} \in X$ s.t. $g(\bar{x}) < 0$ and $h(\bar{x}) = 0$, then ACQ holds at any $x \in X$.

c) (*Linear independence of the gradients of active constraints*)
If $x^* \in X$ and the vectors

$$\begin{cases} \nabla g_j(x^*) & \text{for } j \in \mathcal{A}(x^*), \\ \nabla h_k(x^*) & \text{for } k = 1, \ldots, p \end{cases}$$

are linearly independent, then ACQ holds at x^*.

Theorem 2 (Karush-Kuhn-Tucker) ● ● ●

If x^* is a local minimum and ACQ holds at x^*, then there exist $\lambda^* \in \mathbb{R}^m$ and $\mu^* \in \mathbb{R}^p$ s.t. (x^*, λ^*, μ^*) satisfies the KKT system:

$$
\begin{cases}
\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i^* \, \nabla g_i(x^*) + \sum_{j=1}^{p} \mu_j^* \, \nabla h_j(x^*) = 0 \\
\lambda_i^* \, g_i(x^*) = 0 \qquad \forall \ i = 1, \dots, m \\
\lambda^* \geq 0 \\
g(x^*) \leq 0 \\
h(x^*) = 0
\end{cases}
$$

Define the Lagrangian function $L : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ by

$$L(x, \lambda, \mu) := f(x) + \sum_{i=1}^{m} \lambda_i \, g_i(x) + \sum_{j=1}^{p} \mu_j \, h_j(x)$$

Then the KKT system can be formulated as:

$$\begin{cases} \nabla_x L(x, \lambda, \mu) \ = \ 0 \\ \lambda_i g_i(x) \ = \ 0, \quad i = 1, .., m \\ \lambda \geq 0, \ h(x) = 0, \ g(x) \leq 0 \end{cases} \tag{1}$$

Note that condition $\lambda_i g_i(x) \ = \ 0$, per $i = 1, .., m$, is equivalent to $\lambda^T g(x) = 0$ or also, $\langle \lambda, g(x) \rangle = 0$.

Example

Find the the minimum points of the function $f(x_1, x_2) = 2x_1 + x_2$ on the set
$X = \{(x_1, x_2) \in \mathbb{R}^2 : x_1^2 + x_2^2 \leq 4\}$

Note that X is compact so that from Weierstrass Theorem it follows that f admits global maximum and global minimum on X.
The Lagrangian function is:

$$L(x_1, x_2, \lambda) = 2x_1 + x_2 + \lambda(x_1^2 + x_2^2 - 4)$$

The KKT system is given by:

$$\begin{cases} 2 + 2\lambda x_1 = 0 \\ 1 + 2\lambda x_2 = 0 \\ \lambda(x_1^2 + x_2^2 - 4) = 0 \\ x_1^2 + x_2^2 \leq 4 \\ \lambda \geq 0 \end{cases}$$

Note that for $\lambda = 0$ the system is impossible.

We are led to solve the system:

$$\begin{cases} x_1 = -\frac{1}{\lambda} \\ x_2 = -\frac{1}{2\lambda} \\ x_1^2 + x_2^2 = 4 \\ \lambda \geq 0 \end{cases}$$

Then:

$$\frac{1}{\lambda^2} + \frac{1}{4\lambda^2} = 4$$

from which

$$16\lambda^2 = 5, \quad \lambda = \pm\frac{\sqrt{5}}{4}.$$

- $\lambda = \dfrac{\sqrt{5}}{4} \quad \Rightarrow \quad x_1 = -\dfrac{4}{\sqrt{5}} = -\dfrac{4\sqrt{5}}{5}, \quad x_2 = -\dfrac{2}{\sqrt{5}} = -\dfrac{2\sqrt{5}}{5}$

It follows that $\bar{x} = \left(-\frac{4\sqrt{5}}{5}, -\frac{2\sqrt{5}}{5}\right)$ is a global minimum point.

Remark

Note that in the previous example, ACQ is fulfilled for every $x \in X$. Indeed, there is only the constraint $g(x) = x_1^2 + x_2^2 - 4 \leq 0$, with $\nabla g(x_1, x_2) \neq (0,0)$, for every $x \in X, s.t.\ x_1^2 + x_2^2 - 4 = 0$.

What about the maximum points of f on X ?

Notice that it is enough to set $\lambda \leq 0$ in the KKT system. In fact, in order to find the maxima of f we have to look for the minima of $-f$. The KKT system for the problem
$$\min(-f(x)) \quad x \in X$$
is:

$$\begin{cases} -2 + 2\lambda x_1 = 0 \\ -1 + 2\lambda x_2 = 0 \\ \lambda(x_1^2 + x_2^2 - 4) = 0 \\ x_1^2 + x_2^2 \leq 4 \\ \lambda \geq 0 \end{cases}$$

which is equivalent to set $\lambda \leq 0$ in the original one.
Choosing in the original system: $\lambda = -\frac{\sqrt{5}}{4}$ we obtain
$$x_1 = \frac{4}{\sqrt{5}} = \frac{4\sqrt{5}}{5}, \quad x_2 = \frac{2}{\sqrt{5}} = \frac{2\sqrt{5}}{5}$$
so that $\hat{x} = \left(\frac{4\sqrt{5}}{5}, \frac{2\sqrt{5}}{5}\right)$ is a global maximum point for f on the set X.

Karush-Kuhn-Tucker Theorem

Remark

ACQ assumption is crucial in the KKT Theorem.

Example

$$\begin{cases} \min x_1 + x_2 \\ (x_1 - 1)^2 + (x_2 - 1)^2 - 1 \leq 0 \\ x_2 \leq 0 \end{cases}$$

$x^* = (1, 0)$ is the global optimum.

$T_X(x^*) = \{0\}$, $D(x^*) = \{d \in \mathbb{R}^2 : d_2 = 0\}$, hence ACQ does not hold at x^*.

$\nabla g_1(x^*) = (0, -2)$, $\nabla g_2(x^*) = (0, 1)$, $\nabla f(x^*) = (1, 1)$, hence there is no λ^* s.t. (x^*, λ^*) solves KKT system.

Karush-Kuhn-Tucker Theorem

KKT Theorem gives necessary optimality conditions, but not sufficient ones.

Example

$$\begin{cases} \min x_1 + x_2 \\ -x_1^2 - x_2^2 + 2 \leq 0 \end{cases}$$

$x^* = (1, 1)$, $\lambda^* = \dfrac{1}{2}$ solves KKT system, but x^* is not a local optimum.

Theorem 3 ● ● ●

If the optimization problem is convex and (x^*, λ^*, μ^*) solves KKT system, then x^* is a global optimum.

Recall that (P) is convex if f and g are convex and h is affine.

Exercise 4.1. Prove the previous theorem.

Denote by $v(P)$ denotes the optimal value of (P).

Definition ●●●

Given $\lambda \geq 0$ and $\mu \in \mathbb{R}^p$, the problem

$$\begin{cases} \inf \ L(x, \lambda, \mu) \\ x \in \mathbb{R}^n \end{cases}$$

is called Lagrangian relaxation of (P) and
$\varphi(\lambda, \mu) = \inf\limits_{x \in \mathbb{R}^n} L(x, \lambda, \mu)$ is the Lagrangian dual function.

Lagrangian relaxation provides a lower bound to $v(P)$.

Theorem 4 ●●●

For any $\lambda \geq 0$ and $\mu \in \mathbb{R}^p$, we have $\varphi(\lambda, \mu) \leq v(P)$.

Proof. If $x \in X$, i.e. $g(x) \leq 0, h(x) = 0$, then

$$L(x, \lambda, \mu) = f(x) + \sum_{i=1}^{m} \lambda_i\, g_i(x) \leq f(x),$$

hence

$$\varphi(\lambda, \mu) = \inf_{x \in \mathbb{R}^n}\, L(x, \lambda, \mu) \leq \inf_{x \in X}\, L(x, \lambda, \mu) \leq \inf_{x \in X}\, f(x) = v(P),$$

assuming that (P) admits a finite optimal value. $\quad\square$

Properties of the dual function ● ● ●

The dual function φ

- is concave because inf of affine functions w.r.t (λ, μ)
- may be equal to $-\infty$ at some point
- may be not differentiable at some point

Lagrangian dual problem

Definition ● ● ●

The problem
$$\begin{cases} \max \ \varphi(\lambda, \mu) \\ \lambda \geq 0 \end{cases} \tag{D}$$
is called Lagrangian dual problem of (P) [and (P) is called primal problem].

- The dual problem (D) consists in finding the best lower bound of $v(P)$.

- (D) is always equivalent to a convex problem, even if (P) is a non-convex problem, indeed, it is a maximization of a concave function on a convex set.

Theorem 4, can be equivalently stated as:

Theorem 4 (weak duality) ● ● ●

For any optimization problem (P), we have $v(D) \leq v(P)$.
The previous inequality is called "weak duality property".

Example - Linear Programming.

Primal problem:
$$\begin{cases} \min \ c^\mathsf{T} x \\ Ax \geq b \end{cases} \tag{P}$$

Lagrangian function: $L(x, \lambda) = c^\mathsf{T} x + \lambda^\mathsf{T}(b - Ax) = \lambda^\mathsf{T} b + (c^\mathsf{T} - \lambda^\mathsf{T} A)x$

Dual function:

$$\varphi(\lambda) = \inf_{x \in \mathbb{R}^n} L(x, \lambda) = \begin{cases} -\infty & \text{if } c^\mathsf{T} - \lambda^\mathsf{T} A \neq 0 \\ \lambda^\mathsf{T} b & \text{if } c^\mathsf{T} - \lambda^\mathsf{T} A = 0 \end{cases}$$

Dual problem:

$$\begin{cases} \max \ \varphi(\lambda) \\ \lambda \geq 0 \end{cases} \longrightarrow \begin{cases} \max \ \lambda^\mathsf{T} b \\ \lambda^\mathsf{T} A = c^\mathsf{T} \\ \lambda \geq 0 \end{cases} \tag{D}$$

is a linear programming problem.

Exercise 4.2. Find the dual of (D).

Example - Least norm solution of linear equations

Primal problem:

$$\begin{cases} \min \ \dfrac{1}{2}x^\mathsf{T}x \\[2mm] Ax = b \end{cases} \tag{P}$$

Lagrangian function: $L(x,\mu) = \frac{1}{2}x^\mathsf{T}x + \mu^\mathsf{T}(b - Ax)$.
Dual function: $\varphi(\mu) = \inf\limits_{x\in\mathbb{R}^n} L(x,\mu)$.

$L(x,\mu)$ is quadratic and strongly convex with respect to x, therefore

$$\varphi(\mu) = \inf_{x\in\mathbb{R}^n} L(x,\mu) = \min_{x\in\mathbb{R}^n} L(x,\mu),$$

thus the global optimum is the stationary point:

$$\nabla_x L = x - A^\mathsf{T}\mu = 0 \iff x = A^\mathsf{T}\mu,$$

hence $\varphi(\mu) = -\frac{1}{2}\mu^\mathsf{T}AA^\mathsf{T}\mu + b^\mathsf{T}\mu$.
Dual problem:

$$\begin{cases} \max \ -\dfrac{1}{2}\mu^\mathsf{T}AA^\mathsf{T}\mu + b^\mathsf{T}\mu \\[2mm] \mu \in \mathbb{R}^p \end{cases} \tag{D}$$

is an unconstrained convex quadratic programming problem.

Exercise 4.3. Find the dual problem of a general convex quadratic programming problem

$$\begin{cases} \min\ \dfrac{1}{2}x^{\mathsf{T}}Qx + c^{\mathsf{T}}x \\ Ax \leq b \end{cases} \tag{P}$$

where Q is a symmetric positive definite matrix.

Definition (Strong duality) ● ● ●

We say that strong duality holds for (P) if $v(D) = v(P)$ and (D) admits an optimal solution.

Strong duality does not hold in general.

Example. Consider the following (non-convex) problem:

$$\begin{cases} \min \ -x^2 \\ x - 1 \leq 0 \\ -x \leq 0 \end{cases} \tag{P}$$

It is easy to check that $v(P) = -1$.
The Lagrangian function is $L(x, \lambda) = -x^2 + \lambda_1(x - 1) - \lambda_2 x$, hence

$$\varphi(\lambda) = \inf_{x \in \mathbb{R}} L(x, \lambda) = -\infty \qquad \forall \, (\lambda_1, \lambda_2) \in \mathbb{R}^2,$$

hence $v(D) = -\infty$.

Next theorem provides sufficient conditions which guarantee strong duality for (P).

Theorem 5 ● ● ●

Suppose f, g, h are continuously differentiable, the primal problem

$$\begin{cases} \min\ f(x) \\ g(x) \leq 0 \\ h(x) = 0 \end{cases} \tag{P}$$

is convex, there exists a global optimum x^* and ACQ holds at x^*. Then:

- Strong duality holds ($v(D) = v(P)$ and (D) admits an optimal solution);
- (λ^*, μ^*) is optimal for (D) if and only if (λ^*, μ^*) is a KKT multipliers vector associated with x^*.

Proof. $L(x, \lambda, \mu)$ is convex with respect to x since (P) is convex.
Let (λ^*, μ^*) be any KKT vector of multipliers associated with x^*. Then,

$$\nabla_x L(x^*, \lambda^*, \mu^*) = 0 \qquad \lambda^* \geq 0, \qquad (\lambda^*)^\mathsf{T} g(x^*) = 0.$$

Thus,

$$v(D) \geq \varphi(\lambda^*, \mu^*) = \inf_x L(x, \lambda^*, \mu^*) \underset{[L \text{ convex}]}{=} L(x^*, \lambda^*, \mu^*)$$

$$= f(x^*) + (\lambda^*)^\mathsf{T} g(x^*) + (\mu^*)^\mathsf{T} h(x^*) = f(x^*) = v(P) \underset{[\text{weak duality}]}{\geq} v(D).$$

Therefore, $v(P) = v(D)$ and (λ^*, μ^*) is optimal for (D).
Viceversa, if (λ^*, μ^*) is any optimal solution for (D), then

$$f(x^*) = v(P) = v(D) = \varphi(\lambda^*, \mu^*) = \inf_x L(x, \lambda^*, \mu^*) \leq L(x^*, \lambda^*, \mu^*)$$

$$= f(x^*) + (\lambda^*)^\mathsf{T} g(x^*) + (\mu^*)^\mathsf{T} h(x^*) = f(x^*) + (\lambda^*)^\mathsf{T} g(x^*) \leq f(x^*),$$

thus $(\lambda^*)^\mathsf{T} g(x^*) = 0$ and $\inf_x L(x, \lambda^*, \mu^*) = L(x^*, \lambda^*, \mu^*)$, hence $\nabla_x L(x^*, \lambda^*, \mu^*) = 0$,
i.e., (λ^*, μ^*) is a KKT multipliers vector associated with x^*. $\qquad \square$

Strong duality may hold also for some non-convex problems.

Example

Consider the (non-convex) problem

$$\begin{cases} \min \ -x_1^2 - x_2^2 \\ x_1^2 + x_2^2 - 1 \leq 0 \end{cases}$$

We have $v(P) = -1$. The Lagrangian function is

$$L(x, \lambda) = -x_1^2 - x_2^2 + \lambda(x_1^2 + x_2^2 - 1) = (\lambda - 1)x_1^2 + (\lambda - 1)x_2^2 - \lambda.$$

The dual function is

$$\varphi(\lambda) = \inf_{x \in \mathbb{R}} L(x, \lambda) = \begin{cases} -\infty & \text{if } \lambda < 1 \\ -\lambda & \text{if } \lambda \geq 1 \end{cases}$$

The dual problem is

$$\begin{cases} \max \ -\lambda \\ \lambda \geq 1 \end{cases}$$

hence its optimal solution is $\lambda^* = 1$ and $v(D) = -1$.

Theorem 6 (characterization of strong duality)

(x^*, λ^*, μ^*) is a saddle point of L, i.e.

$$L(x^*, \lambda, \mu) \leq L(x^*, \lambda^*, \mu^*) \leq L(x, \lambda^*, \mu^*) \qquad \forall \, x \in \mathbb{R}^n, \, \lambda \in \mathbb{R}^m_+, \, \mu \in \mathbb{R}^p,$$

if and only if x^* is optimum of (P), (λ^*, μ^*) is optimum of (D) and $v(P) = v(D)$.

Proof. If (x^*, λ^*, μ^*) is a saddle point of L, then we can prove that $x^* \in X$, $\langle \lambda^*, g(x^*) \rangle = 0$ which implies $\varphi(\lambda^*, \mu^*) = f(x^*)$.
Viceversa, we have that

$$f(x^*) = \varphi(\lambda^*, \mu^*) = \inf_{x \in \mathbb{R}^n} L(x, \lambda^*, \mu^*) \leq L(x^*, \lambda^*, \mu^*) = f(x^*) + \langle \lambda^*, g(x^*) \rangle,$$

hence $\langle \lambda^*, g(x^*) \rangle = 0$ and $L(x^*, \lambda^*, \mu^*) = f(x^*) = \varphi(\lambda^*, \mu^*) \leq L(x, \lambda^*, \mu^*)$ for all $x \in \mathbb{R}^n$. Moreover

$$L(x^*, \lambda, \mu) = f(x^*) + \langle \lambda, g(x^*) \rangle \leq f(x^*) = L(x^*, \lambda^*, \mu^*) \qquad \forall \, \lambda \in \mathbb{R}^m_+, \, \mu \in \mathbb{R}^p.$$

$\square$

5 - Support Vector Machines for supervised classification problems

G. Mastroeni and M. Passacantando

Department of Computer Science, University of Pisa

Supervised pattern classification

Support Vector Machines (SVM) provide a supervised classification method for a vector of data, concerning a given problem, according to previously obtained vectors of data that have already been classified.

We are given a set of vectors of data (objects) partitioned in several classes with known labels, we want to assign to a suitable class a new object with unknown label.

Examples:

- medical diagnosis
- spam filtering
- credit card fraud detection

Binary classification: Linear SVM

In a binary classification, we are given two finite sets $A, B \subset \mathbb{R}^n$ with known labels (1 for points in A, -1 for points in B).

- $\mathbb{R}^n$ is the input space,
- $A \cup B$ is the training set.

Assume that A and B are strictly linearly separable, i.e., there is an hyperplane $H = \{x \in \mathbb{R}^n : w^\mathsf{T} x + b = 0\}$ such that

$$
\begin{aligned}
w^\mathsf{T} x^i + b > 0 \qquad & \forall \ x^i \in A, \\
w^\mathsf{T} x^j + b < 0 \qquad & \forall \ x^j \in B.
\end{aligned}
\tag{1}
$$
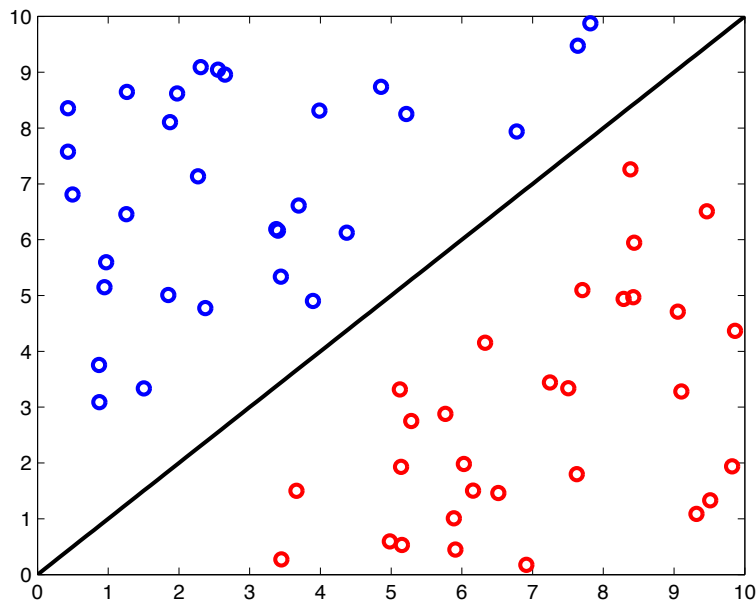
We have a new test data x:

use the decision function ● ● ●
$f(x) = \mathrm{sign}(w^\mathsf{T} x + b) =$
$$
\begin{cases}
1 & \text{if } w^\mathsf{T} x + b > 0, \\
-1 & \text{if } w^\mathsf{T} x + b < 0.
\end{cases}
$$

- A necessary and sufficient condition for (1) to hold is
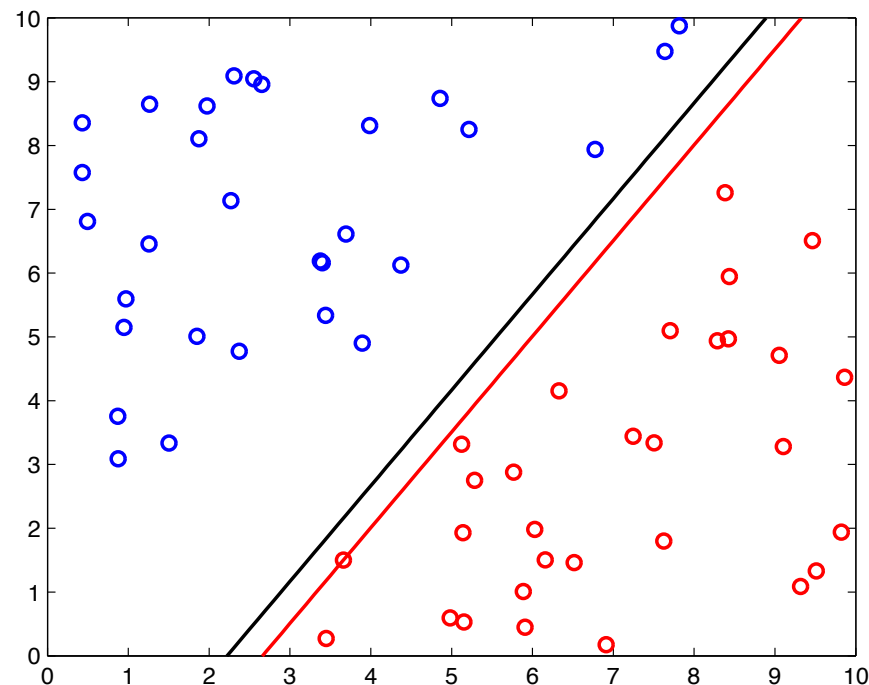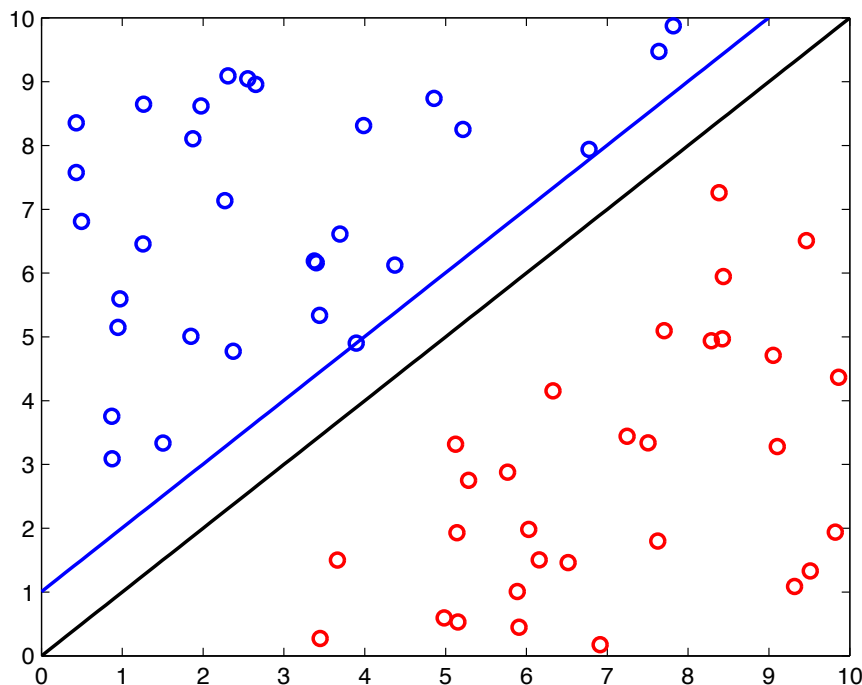
$$conv(A) \cap conv(B) = \emptyset$$

- Since there are many possible separating hyperplanes, we have to decide which hyperplane to choose.

Linear SVM
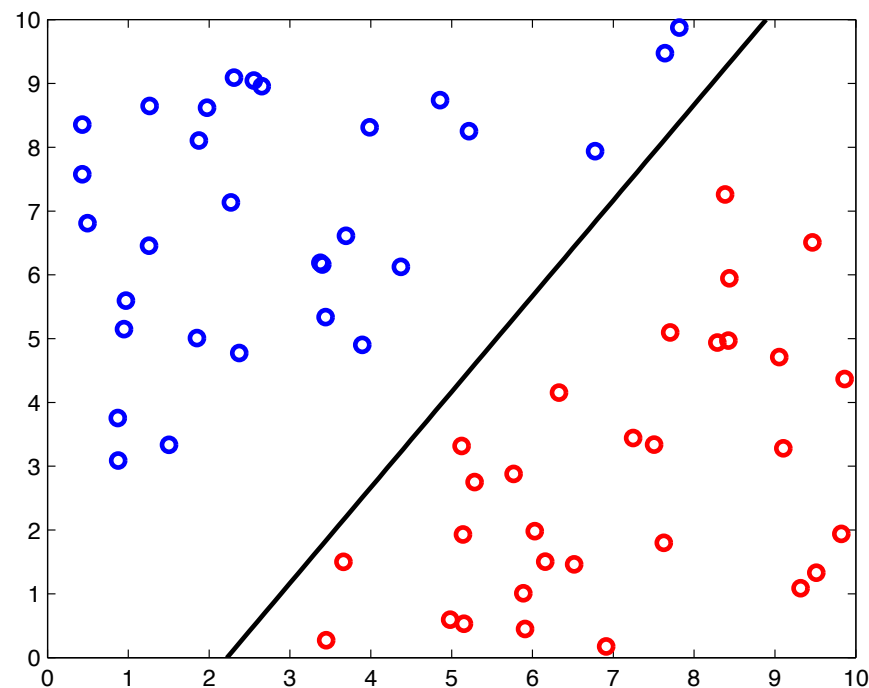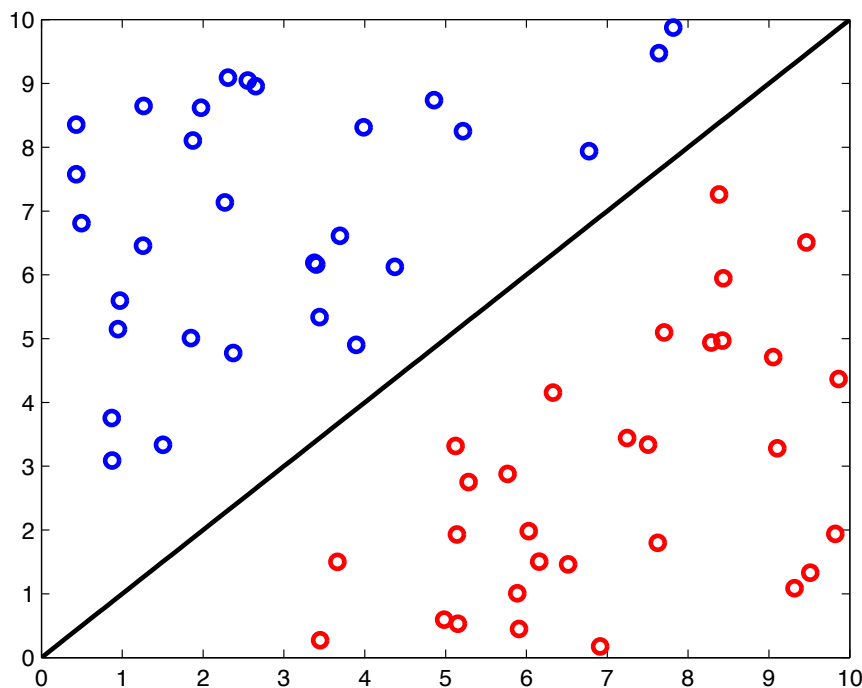
If H is a separating hyperplane, then the margin of separation of H is defined as the minimum distance between H and $A \cup B$, i.e.

$$\rho(H) = \min_{x \in A \cup B} \frac{|w^{\mathsf{T}} x + b|}{\|w\|}.$$

We look for the separating hyperplane with the maximum margin of separation.

Theorem ● ● ●

Finding the separating hyperplane with the maximum margin of separation is equivalent to solve the following convex quadratic programming problem:

$$
\begin{cases}
\displaystyle \min_{w,b} \ \frac{1}{2}\|w\|^2 \\
w^\mathsf{T} x^i + b \geq 1 \qquad \forall \ x^i \in A \\
w^\mathsf{T} x^j + b \leq -1 \qquad \forall \ x^j \in B
\end{cases}
\tag{2}
$$

Proof. It is possible to show that the distance between the hyperplanes:

$$
w^\mathsf{T} x + b = 1, \qquad\qquad w^\mathsf{T} x + b = -1
$$

is $\frac{2}{\|w\|}$. In fact, consider a point $\hat{x}$ such that $w^\mathsf{T}\hat{x} + b = 1$, then the distance between $\hat{x}$ and the other hyperplane $w^\mathsf{T} x + b + 1 = 0$ is

$$
\frac{|w^\mathsf{T}\hat{x} + b + 1|}{\|w\|} = \frac{2}{\|w\|}.
$$

Therefore, by minimizing $\|w\|$, we get two hyperplanes of maximum distance.

Moreover, we will see that problem (2) has a unique solution (w^*, b^*). $\qquad \square$

Example 5.1 Find the separating hyperplane with maximum margin for the data set:

$$
A = \begin{pmatrix}
0.4952 & 6.8088 \\
2.6505 & 8.9590 \\
3.4403 & 5.3366 \\
3.4010 & 6.1624 \\
5.2153 & 8.2529 \\
7.6393 & 9.4764 \\
1.5041 & 3.3370 \\
3.9855 & 8.3138 \\
1.8500 & 5.0079 \\
1.2631 & 8.6463 \\
3.8957 & 4.9014 \\
1.9751 & 8.6199 \\
1.2565 & 6.4558 \\
4.3732 & 6.1261 \\
0.4297 & 8.3551 \\
3.6931 & 6.6134 \\
7.8164 & 9.8767 \\
4.8561 & 8.7376 \\
6.7750 & 7.9386 \\
2.3734 & 4.7740 \\
0.8746 & 3.0892 \\
2.3088 & 9.0919 \\
2.5520 & 9.0469 \\
3.3773 & 6.1886 \\
0.8690 & 3.7550 \\
1.8738 & 8.1053 \\
0.9469 & 5.1476 \\
0.9718 & 5.5951 \\
0.4309 & 7.5763 \\
2.2699 & 7.1371
\end{pmatrix}
\qquad
B = \begin{pmatrix}
7.2450 & 3.4422 \\
7.7030 & 5.0965 \\
5.7670 & 2.8791 \\
3.6610 & 1.5002 \\
9.4633 & 6.5084 \\
9.8221 & 1.9383 \\
8.2874 & 4.9380 \\
5.9078 & 0.4489 \\
4.9810 & 0.5962 \\
5.1516 & 0.5319 \\
8.4363 & 5.9467 \\
8.4240 & 4.9696 \\
7.6240 & 1.7988 \\
3.4473 & 0.2725 \\
9.0528 & 4.7106 \\
9.1046 & 3.2798 \\
6.9110 & 0.1745 \\
5.1235 & 3.3181 \\
7.5051 & 3.3392 \\
6.3283 & 4.1555 \\
6.1585 & 1.5058 \\
8.3827 & 7.2617 \\
5.2841 & 2.7510 \\
5.1412 & 1.9314 \\
6.0290 & 1.9818 \\
5.8863 & 1.0087 \\
9.5110 & 1.3298 \\
9.3170 & 1.0890 \\
6.5170 & 1.4606 \\
9.8621 & 4.3674
\end{pmatrix}
$$

Assume $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{p \times n}$, $w = (w_1, ..., w_n)^T$;

Problem (2) is a quadratic problem defined by:

$$
\begin{cases}
\min_{w,b} \frac{1}{2}(w, b)^T C \begin{pmatrix} w \\ b \end{pmatrix} \\
D \begin{pmatrix} w \\ b \end{pmatrix} \leq d
\end{cases}
\tag{3}
$$

where, assuming $n = 2$, $w \in \mathbb{R}^2$, $b \in \mathbb{R}$,

$$
C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad D = \begin{pmatrix} -A & -e_m \\ B & e_p \end{pmatrix} \quad d = \begin{pmatrix} -e_m \\ -e_p \end{pmatrix}
$$

$$
-e_m = (-1, -1, ..., -1)^T \in \mathbb{R}^m, \quad -e_p = (-1, -1, ..., -1)^T \in \mathbb{R}^p
$$

The Matlab function "quadprog"

The previous problem can be solved by the Matlab function "quadprog" which solves a quadratic problem with linear constraints.

From the Matlab help

[x,fval,exitflag,output,lambda] = quadprog(H,f,A,b) attempts to solve the quadratic programming problem:
min 0.5*x'*H*x + f'*x subject to: A*x <= b x

[x,fval,exitflag,output,lambda] = quadprog(H,f,A,b,Aeq,beq) solves the problem above while additionally satisfying the equality constraints Aeq*x = beq. (Set A=[] and B=[] if no inequalities exist.)

[x,fval,exitflag,output,lambda] = quadprog(H,f,A,b,Aeq,beq,LB,UB) defines a set of lower and upper bounds on the design variables, X, so that the solution is in the range LB <= X <= UB. Use empty matrices for LB and UB if no bounds exist. Set LB(i) = -Inf if X(i) is unbounded below; set UB(i) = Inf if X(i) is unbounded above.

Matlab commands: primal problem

```
A=[........];
B=[........];
nA = size(A,1);
nB = size(B,1);
T = [A ; B];
Q = [ 1 0 0 ; 0 1 0 ; 0 0 0 ];
D = [-A -ones(nA,1); B ones(nB,1) ] ;
d = -ones(nA+nB,1) ;
sol = quadprog(Q,zeros(3,1),D,d);
w = sol(1:2)
b = sol(3)

% Optional: plot the solution

xx = 0:0.1:10 ;
uu = (-w(1)/w(2)).*xx - b/w(2);
vv = (-w(1)/w(2)).*xx + (1-b)/w(2);
vvv = (-w(1)/w(2)).*xx + (-1-b)/w(2);

plot(A(:,1),A(:,2),'bo',B(:,1),B(:,2),'ro',xx,uu,'k-',xx,vv,'b-',xx,vvv,'r-','Linewidth', 1.5)
axis([0 10 0 10])
```

w =

-0.9229

0.7627

b =

1.1976
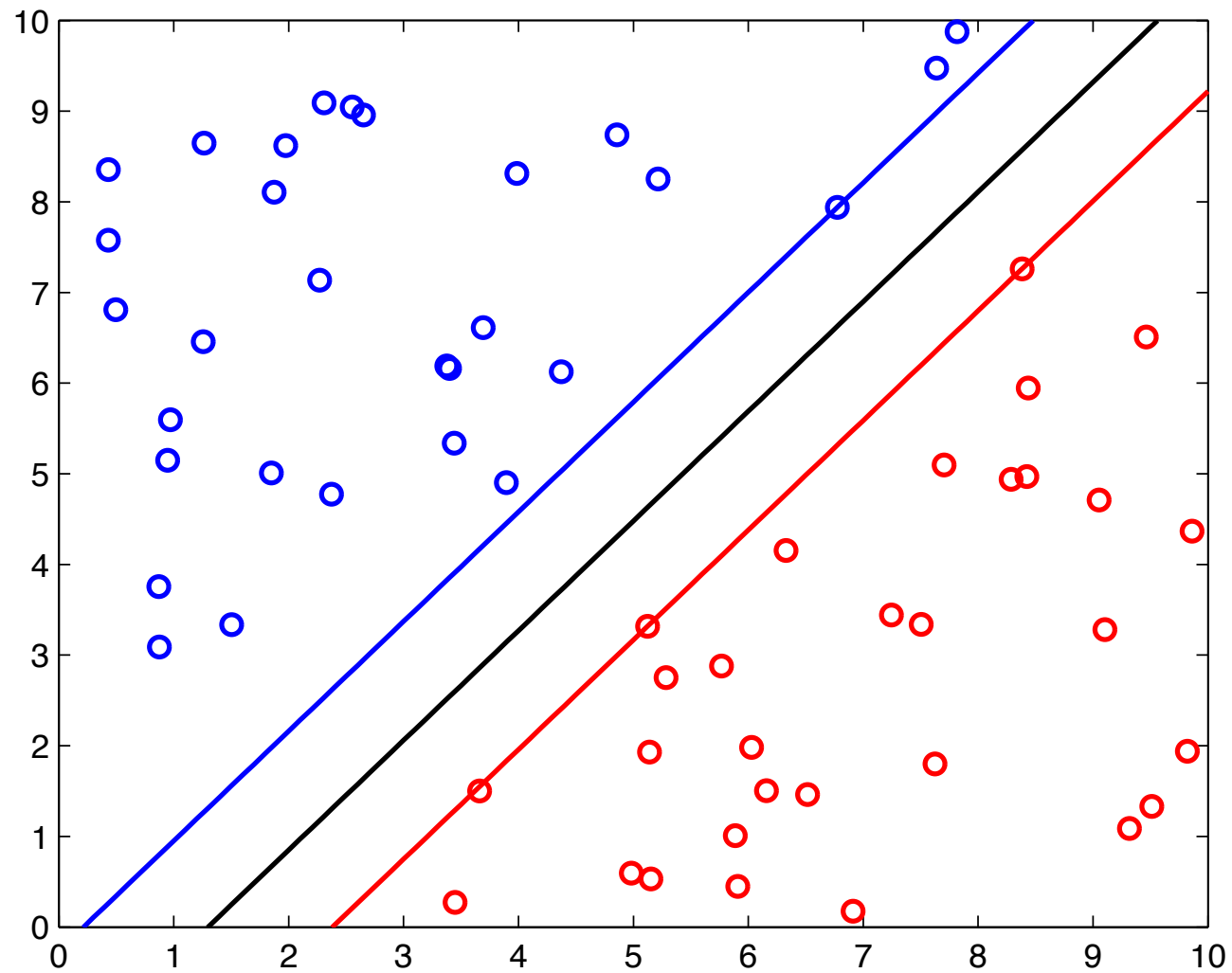
Let $\ell = |A \cup B|$. For any point $x^i \in A \cup B$, define a label

$$y^i = \begin{cases} 1 & \text{if } x^i \in A \\ -1 & \text{if } x^i \in B \end{cases} \qquad \forall\, i = 1, \ldots, \ell.$$

Then the problem

$$\begin{cases} \min\limits_{w,b} \ \dfrac{1}{2}\|w\|^2 \\ w^\mathsf{T} x^i + b \geq 1 & \forall\, x^i \in A \\ w^\mathsf{T} x^j + b \leq -1 & \forall\, x^j \in B \end{cases}$$

is equivalent to

linear SVM $\qquad \begin{cases} \min\limits_{w,b} \ \dfrac{1}{2}\|w\|^2 \\ \\ 1 - y^i(w^\mathsf{T} x^i + b) \leq 0 & \forall\, i = 1, \ldots, \ell \end{cases}$ $\qquad (4)$

Since problem (4) is convex, it is useful to consider the Lagrangian dual of (4).

$\bullet$ $\bullet$ $\bullet$

The Lagrangian function is

$$
\begin{aligned}
L(w, b, \lambda) \quad &= \frac{1}{2}\|w\|^2 + \sum_{i=1}^{\ell} \lambda_i \left[1 - y^i(w^\mathsf{T} x^i + b)\right] \\
&= \frac{1}{2}\|w\|^2 - \sum_{i=1}^{\ell} \lambda_i y^i w^\mathsf{T} x^i - b \sum_{i=1}^{\ell} \lambda_i y^i + \sum_{i=1}^{\ell} \lambda_i
\end{aligned}
$$

If $\sum_{i=1}^{\ell} \lambda_i y^i \neq 0$, then $\min_{w,b} L(w, b, \lambda) = -\infty$.

If $\sum_{i=1}^{\ell} \lambda_i y^i = 0$, then L does not depend on b, L is strongly convex wrt w and $\arg \min_{w} L(w, b, \lambda)$ is given by the (unique) stationary point

$$
\nabla_w L(w, b, \lambda) = w - \sum_{i=1}^{\ell} \lambda_i y^i x^i = 0. \tag{5}
$$

Note that, if (9) holds and $\sum_{i=1}^{\ell} \lambda_i y^i = 0$, then

$$L(w, b, \lambda) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{\ell} \lambda_i y^i w^\mathsf{T} x^i - b \sum_{i=1}^{\ell} \lambda_i y^i + \sum_{i=1}^{\ell} \lambda_i = \frac{1}{2} w^\mathsf{T} w - w^\mathsf{T} w + \sum_{i=1}^{\ell} \lambda_i$$

$$= -\frac{1}{2} w^\mathsf{T} w + \sum_{i=1}^{\ell} \lambda_i$$

Therefore, the dual function is

$$\varphi(\lambda) = \begin{cases} -\infty & \text{if } \sum_{i=1}^{\ell} \lambda_i y^i \neq 0 \\ -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} y^i y^j (x^i)^\mathsf{T} x^j \lambda_i \lambda_j + \sum_{i=1}^{\ell} \lambda_i & \text{if } \sum_{i=1}^{\ell} \lambda_i y^i = 0 \end{cases}$$

The dual of problem (4) is ● ● ●

$$\begin{cases} \max_{\lambda} \ -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} y^i y^j (x^i)^\mathsf{T} x^j \lambda_i \lambda_j + \sum_{i=1}^{\ell} \lambda_i \\ \sum_{i=1}^{\ell} \lambda_i y^i = 0 \\ \lambda \geq 0 \end{cases} \tag{6}$$

or

$$\begin{cases} \max_{\lambda} \ -\frac{1}{2} \lambda^\mathsf{T} X^\mathsf{T} X \lambda + e^\mathsf{T} \lambda \\ \sum_{i=1}^{\ell} \lambda_i y^i = 0 \\ \lambda \geq 0 \end{cases} \tag{7}$$

where $X = (y^1 x^1, y^2 x^2, \ldots, y^\ell x^\ell)$ is a $n \times \ell$ matrix and $e^\mathsf{T} = (1, \ldots, 1) \in \mathbb{R}^\ell$.

Remarks ● ● ●

- Since $X^T X$ is always positive semidefinite then the dual problem is a convex quadratic programming problem;

- A KKT multiplier λ^* associated to the primal optimum (w^*, b^*) is a dual optimum;

- If $\lambda_i^* > 0$, then x^i is said support vector;

- If λ^* is a dual optimum, then, by (9), we have:

$$w^* = \sum_{i=1}^{\ell} \lambda_i^* y^i x^i;$$

- b^* is obtained using the complementarity conditions:

$$\lambda_i^* \left[1 - y^i((w^*)^\mathsf{T} x^i + b^*) \right] = 0;$$

in fact, if i is such that $\lambda_i^* > 0$, then $b^* = \dfrac{1}{y^i} - (w^*)^\mathsf{T} x^i$.

This allows us to find the separating hyperplane $(w^*)^\mathsf{T} x + b^* = 0$ and the decision function

$$f(x) = \text{sign}((w^*)^\mathsf{T} x + b^*).$$

Determine the KKT conditions of the primal problem (4):

$$\begin{cases} \min_{w,b} \ \dfrac{1}{2}\|w\|^2 \\[2mm] 1 - y^i(w^\mathsf{T}x^i + b) \le 0 \qquad \forall\, i = 1,\dots,\ell \end{cases}$$

As previously seen, the Lagrangian function is:

$$L(w, b, \lambda) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{\ell}\lambda_i y^i w^\mathsf{T}x^i - b\sum_{i=1}^{\ell}\lambda_i y^i + \sum_{i=1}^{\ell}\lambda_i$$

Then, the KKT conditions are:

$$\begin{cases} \nabla_w L(w, b, \lambda) = w - \displaystyle\sum_{i=1}^{\ell}\lambda_i y^i x^i = 0 \\[4mm] \nabla_b L(w, b, \lambda) = -\displaystyle\sum_{i=1}^{\ell}\lambda_i y^i = 0 \\[4mm] \lambda_i(1 - y^i(w^\mathsf{T}x^i + b)) = 0 \qquad \forall\, i = 1,\dots,\ell \\[2mm] \lambda_i \ge 0, \quad 1 - y^i(w^\mathsf{T}x^i + b) \le 0 \qquad \forall\, i = 1,\dots,\ell \end{cases}$$

Example 5.2. Find the separating hyperplane with maximum margin for the data set given in Example 5.1 by solving the dual problem (6).

We have to solve the problem:

$$
\begin{cases}
-\min_{\lambda} \; \dfrac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} y^i y^j (x^i)^{\mathsf{T}} x^j \lambda_i \lambda_j - \sum_{i=1}^{\ell} \lambda_i \\[2mm]
\sum_{i=1}^{\ell} \lambda_i y^i = 0 \\[1mm]
\lambda \geq 0
\end{cases}
$$

Note that the generic component q_{ij} of the hessian matrix Q is given by

$$
q_{ij} = y^i y^j (x^i)^{\mathsf{T}} x^j
$$

Matlab commands: dual problem

```
A=[........]; B=[........]; nA = size(A,1); nB = size(B,1);
T = [A ; B]; y = [ones(nA,1) ; -ones(nB,1)]; l = length(y); Q = zeros(l,l);
for i = 1 : l
for j = 1 : l
Q(i,j) = y(i)*y(j)*(T(i,:))*T(j,:)' ;
end
end
la = quadprog(Q,-ones(l,1),[ ],[ ],y',0,zeros(l,1),[ ]);
wD = zeros(2,1);
for i = 1 : l
wD = wD + la(i)*y(i)*T(i,:)';
end
wD
ind = find(la > 0.001) ;
i = ind(1) ;
bD = 1/y(i) - wD'*T(i,:)'
```

Exercise

Plot the solution obtained in Example 5.2.

```
xx = 0:0.1:10 ;
uuD = (-wD(1)/wD(2)).*xx - bD/wD(2);
vvD = (-wD(1)/wD(2)).*xx + (1-bD)/wD(2);
vvvD = (-wD(1)/wD(2)).*xx + (-1-bD)/wD(2);
figure
plot(A(:,1),A(:,2),'bo',B(:,1),B(:,2),'ro',
xx,uuD,'k-',xx,vvD,'b-',xx,vvvD,'r-','Linewidth',1.5)
axis([0 10 0 10])
```

What if sets A and B are not linearly separable?

The linear system

$$1 - y^i(w^\mathsf{T}x^i + b) \leq 0 \qquad\qquad i = 1, \ldots, \ell$$

has no solutions.

We introduce slack variables $\xi_i \geq 0$ and consider the (relaxed) system:

$$
\begin{aligned}
1 - y^i(w^\mathsf{T}x^i + b) &\leq \xi_i && i = 1, \ldots, \ell \\
\xi_i &\geq 0 && i = 1, \ldots, \ell
\end{aligned}
$$

If x^i is misclassified, then $\xi_i > 1$, thus $\sum_{i=1}^{\ell} \xi_i$ is an upper bound of the number of misclassified points. In fact,

- $x^i \in A$, with $w^\mathsf{T}x^i + b < 0$ implies

$$1 < 1 - (w^\mathsf{T}x^i + b) = 1 - y^i(w^\mathsf{T}x^i + b) \leq \xi_i$$

- $x^i \in B$, with $w^\mathsf{T}x^i + b > 0$ implies

$$1 < 1 + (w^\mathsf{T}x^i + b) = 1 - y^i(w^\mathsf{T}x^i + b) \leq \xi_i$$

We add to the objective function the term $C \sum_{i=1}^{\ell} \xi_i$, where $C > 0$ is a parameter:

linear SVM
with soft margin
$$\begin{cases} \min_{w,b,\xi} \ \dfrac{1}{2}\|w\|^2 + C \sum_{i=1}^{\ell} \xi_i \\ 1 - y^i(w^{\mathsf{T}}x^i + b) \leq \xi_i & \forall \ i = 1, \ldots, \ell \\ \xi_i \geq 0 & \forall \ i = 1, \ldots, \ell \end{cases} \tag{8}$$

Exercise 5.2. Prove that the dual problem of (8) is

$$\begin{cases} \max_{\lambda} \ -\dfrac{1}{2}\sum_{i=1}^{\ell}\sum_{j=1}^{\ell} y^i y^j (x^i)^{\mathsf{T}} x^j \lambda_i \lambda_j + \sum_{i=1}^{\ell} \lambda_i \\ \sum_{i=1}^{\ell} \lambda_i y^i = 0 \\ 0 \leq \lambda_i \leq C & i = 1, \ldots, \ell \end{cases}$$

The Lagrangian function is

$$L(w, b, \xi, \lambda, \mu) = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{\ell} \xi_i + \sum_{i=1}^{\ell} \lambda_i \left[1 - y^i(w^\mathsf{T} x^i + b) - \xi_i\right] - \sum_{i=1}^{\ell} \mu_i \xi_i$$

$$= \frac{1}{2}\|w\|^2 - \sum_{i=1}^{\ell} \lambda_i y^i w^\mathsf{T} x^i - b\sum_{i=1}^{\ell} \lambda_i y^i + \sum_{i=1}^{\ell} \lambda_i + \sum_{i=1}^{\ell} \xi_i (C - \lambda_i - \mu_i)$$

For a fixed (λ, μ), we aim at finding $\min\limits_{w, b, \xi} L(w, b, \xi, \lambda, \mu)$.

Since L is convex w.r.t. (w, b, ξ) then a global minimum is a stationary point of $L(\cdot, \cdot, \cdot, \lambda, \mu)$, i.e. it is a solution of the system:

$$\begin{cases} \nabla_w L(w, b, \xi, \lambda, \mu) = w - \sum_{i=1}^{\ell} \lambda_i y^i x^i = 0 \\ \nabla_b L(w, b, \xi, \lambda, \mu) = -\sum_{i=1}^{\ell} \lambda_i y^i = 0 \\ \nabla_\xi L(w, b, \xi, \lambda, \mu) = C - \lambda_i - \mu_i = 0, \ \ i = 1, .., \ell \end{cases} \tag{9}$$

Eliminating the variable w, with the same arguments used for finding the dual of (4), we have that the dual of problem (8) is

$$
\begin{cases}
\max_{\lambda} \; -\dfrac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} y^i y^j (x^i)^\mathsf{T} x^j \lambda_i \lambda_j + \sum_{i=1}^{\ell} \lambda_i \\[2mm]
\sum_{i=1}^{\ell} \lambda_i y^i = 0 \\[2mm]
C - \lambda_i - \mu_i = 0 \qquad i = 1, \ldots, \ell \\[2mm]
\lambda \geq 0, \mu \geq 0
\end{cases}
\tag{10}
$$

and eliminating the variable μ, by noticing that $C - \lambda_i = \mu_i \geq 0$, we obtain the final dual formulation

$$
\begin{cases}
\max_{\lambda} \; -\dfrac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} y^i y^j (x^i)^\mathsf{T} x^j \lambda_i \lambda_j + \sum_{i=1}^{\ell} \lambda_i \\[2mm]
\sum_{i=1}^{\ell} \lambda_i y^i = 0 \\[2mm]
0 \leq \lambda_i \leq C \qquad i = 1, \ldots, \ell
\end{cases}
\tag{11}
$$

If λ^* is optimum for (11), then

$$w^* = \sum_{i=1}^{\ell} \lambda_i^* y^i x^i.$$

We can find b^* by choosing i s.t. $0 < \lambda_i^* < C$ and using the complementarity conditions:

$$\begin{cases} \lambda_i^* \left[1 - y^i((w^*)^\mathsf{T} x^i + b^*) - \xi_i^* \right] = 0 \\ \mu_i^* \xi_i^* = (C - \lambda_i^*) \xi_i^* = 0 \end{cases} \quad \bullet\bullet\bullet \, (12)$$

Thus $b^* = \dfrac{1}{y^i} - (w^*)^\mathsf{T} x^i$.

Remark

Note that

- $0 \le \lambda_i^* < C$ implies $\xi_i^* = 0$
- $0 < \lambda_i^* \le C$ implies $1 - y^i((w^*)^\mathsf{T} x^i + b^*) - \xi_i^* = 0$
- $\xi_i^* > 0$ implies $\lambda_i^* = C$

The previous conditions also allow us to find the errors ξ_i^*, $i = 1, .., \ell$.

Exercise 5.3

Determine the KKT conditions of the problem :

$$\begin{cases} \min_{w,b,\xi} \ \frac{1}{2}\|w\|^2 + C \sum_{i=1}^{\ell} \xi_i \\ 1 - y^i(w^{\mathsf{T}}x^i + b) \leq \xi_i & \forall \ i = 1,\ldots,\ell \\ \xi_i \geq 0 & \forall \ i = 1,\ldots,\ell \end{cases}$$

The KKT conditions are given by joining together (9), (12) plus the feasibility conditions of the given problem and the nonnegativity of the involved multipliers.

Exercise 5.4. Find the separating hyperplane with soft margin for the following data set by solving the dual problem (11) with $C = 10$.
Compute the vector ξ of the errors.

$$
A = \begin{pmatrix}
2.6505 & 8.9590 \\
3.4403 & 5.3366 \\
3.4010 & 6.1624 \\
5.2153 & 8.2529 \\
7.6393 & 9.4764 \\
1.5041 & 3.3370 \\
3.9855 & 8.3138 \\
1.8500 & 5.0079 \\
1.2631 & 8.6463 \\
3.8957 & 4.9014 \\
1.9751 & 8.6199 \\
1.2565 & 6.4558 \\
4.3732 & 6.1261 \\
0.4297 & 8.3551 \\
3.6931 & 6.6134 \\
7.8164 & 9.8767 \\
4.8561 & 8.7376 \\
6.7750 & 7.9386 \\
2.3734 & 4.7740 \\
0.8746 & 3.0892 \\
2.3088 & 9.0919 \\
2.5520 & 9.0469 \\
3.3773 & 6.1886 \\
0.8690 & 3.7550 \\
1.8738 & 8.1053 \\
0.9469 & 5.1476 \\
0.4309 & 7.5763 \\
2.2699 & 7.1371
\end{pmatrix}
\qquad
B = \begin{pmatrix}
7.7030 & 5.0965 \\
5.7670 & 2.8791 \\
3.6610 & 1.5002 \\
9.4633 & 6.5084 \\
9.8221 & 1.9383 \\
8.2874 & 4.9380 \\
5.9078 & 0.4489 \\
4.9810 & 0.5962 \\
5.1516 & 0.5319 \\
8.4363 & 5.9467 \\
8.4240 & 4.9696 \\
7.6240 & 1.7988 \\
3.4473 & 0.2725 \\
9.0528 & 4.7106 \\
9.1046 & 3.2798 \\
6.9110 & 0.1745 \\
5.1235 & 3.3181 \\
7.5051 & 3.3392 \\
6.3283 & 4.1555 \\
6.1585 & 1.5058 \\
8.3827 & 7.2617 \\
5.2841 & 2.7510 \\
5.1412 & 1.9314 \\
5.8863 & 1.0087 \\
9.5110 & 1.3298 \\
6.5170 & 1.4606 \\
9.8621 & 4.3674 \\
6.0000 & 8.0000
\end{pmatrix}
$$

Consider now two sets A and B which are not linearly separable.
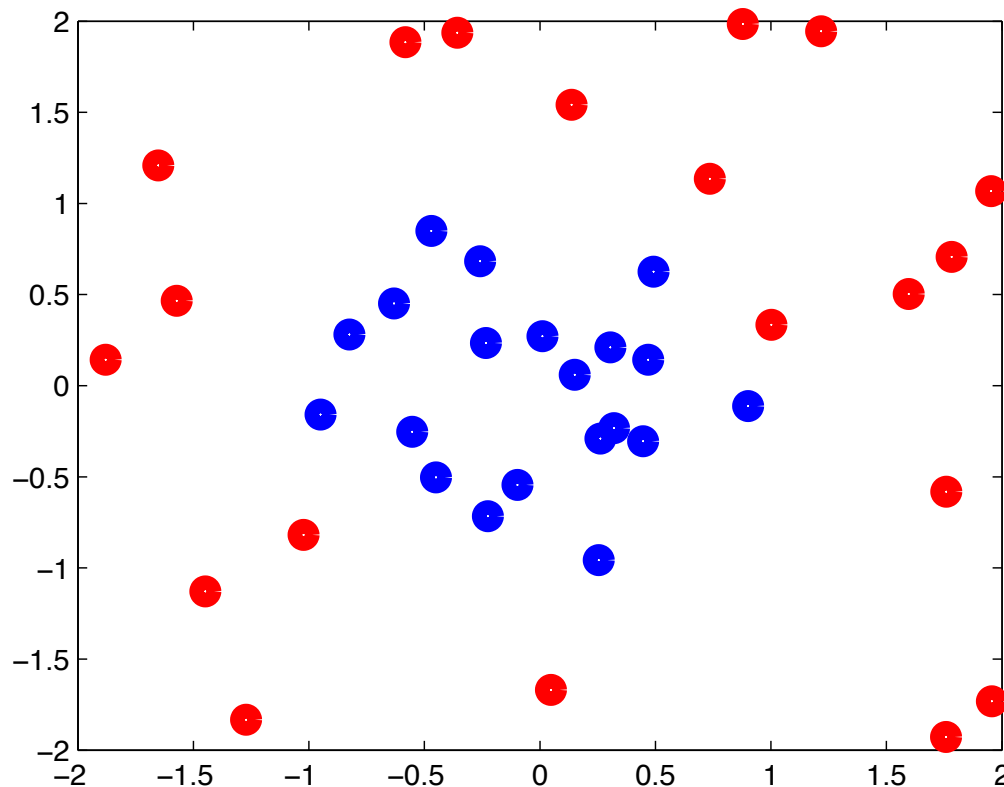
Are they linearly separable in other spaces?
Use a map $\phi : \mathbb{R}^n \to \mathcal{H}$, where $\mathcal{H}$ is an higher dimensional (maybe infinite) space.
$\mathcal{H}$ is called the features space
We try to linearly separate the images $\phi(x^i)$, $i = 1, \ldots, \ell$ in the feature space.

Nonlinear SVM

Primal problem:

$$
\begin{cases}
\min_{w,b,\xi} \ \dfrac{1}{2}\|w\|^2 + C\sum_{i=1}^{\ell}\xi_i \\[2mm]
1 - y^i(w^\mathsf{T}\phi(x^i) + b) \leq \xi_i & \forall\ i = 1,\dots,\ell \\[2mm]
\xi_i \geq 0 & \forall\ i = 1,\dots,\ell
\end{cases}
$$

w is a vector in a high dimensional space (maybe infinite variables)

Dual problem:

$$
\begin{cases}
\max_{\lambda} \ -\dfrac{1}{2}\sum_{i=1}^{\ell}\sum_{j=1}^{\ell} y^i y^j \phi(x^i)^\mathsf{T}\phi(x^j)\lambda_i\lambda_j + \sum_{i=1}^{\ell}\lambda_i \\[2mm]
\sum_{i=1}^{\ell}\lambda_i y^i = 0 \\[2mm]
0 \leq \lambda_i \leq C & \forall\ i = 1,\dots,\ell
\end{cases}
$$

number of variables = number of training data

- Let λ^* be a solution of the dual problem.

- Then $w^* = \sum_{i=1}^{\ell} \lambda_i^* y^i \phi(x^i)$.

- By any λ_i^* s.t. $0 < \lambda_i^* < C$ we can find b^*, by the complementarity relations that now become:

$$\begin{cases} \lambda_i^* \left[1 - y^i((w^*)^\mathsf{T}\phi(x^i) + b^*) - \xi_i^*\right] = 0 \\ \mu_i^* \xi_i^* = (C - \lambda_i^*)\xi_i^* = 0 \end{cases} \tag{13}$$

Then,

$$1 - y^i \left[(w^*)^\mathsf{T}\phi(x^i) + b^*\right] = 0 \quad \longrightarrow \quad b^* = \frac{1}{y^i} - \sum_{j=1}^{\ell} \lambda_j^* y^j \phi(x^j)^\mathsf{T}\phi(x^i)$$

The decision function is given by:

$$f(x) = \operatorname{sign}((w^*)^\mathsf{T}\phi(x) + b^*) = \operatorname{sign}\left(\sum_{i=1}^{\ell} \lambda_i^* y^i \phi(x^i)^\mathsf{T}\phi(x) + b^*\right)$$

Note that $f(x)$ depends on
- λ^* (that can be found knowing $\phi(x^i)^\mathsf{T}\phi(x^j)$)
- $\phi(x^i)^\mathsf{T}\phi(x)$
- b^* (that can be found knowing $\phi(x^i)^\mathsf{T}\phi(x^j)$)

Kernel functions

Definition (Kernel functions)

A function $k : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is called kernel if there exists a map $\phi : \mathbb{R}^n \to \mathcal{H}$ such that

$$k(x, y) = \langle \phi(x), \phi(y) \rangle,$$

where $\langle \cdot, \cdot \rangle$ is a scalar product in the features space $\mathcal{H}$.

Examples:

- $k(x, y) = x^\mathsf{T} y$
- $k(x, y) = (x^\mathsf{T} y + 1)^p$, with $p \geq 1$ (polynomial)
- $k(x, y) = e^{-\gamma \|x - y\|^2}$ (Gaussian)
- $k(x, y) = \tanh(\beta x^\mathsf{T} y + \gamma)$, with suitable β and γ

Theorem

If $k : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a kernel and $x^1, \ldots, x^\ell \in \mathbb{R}^n$, then the matrix K defined as follows

$$K_{ij} = k(x^i, x^j)$$

is positive semidefinite.

The dual problem depends on the kernel k:

$$
\begin{cases}
\max\limits_{\lambda} \quad -\dfrac{1}{2} \sum\limits_{i=1}^{\ell} \sum\limits_{j=1}^{\ell} y^i y^j \, {\color{red} k(x^i, x^j)} \lambda_i \lambda_j + \sum\limits_{i=1}^{\ell} \lambda_i \\
\sum\limits_{i=1}^{\ell} \lambda_i y^i = 0 \\
0 \leq \lambda_i \leq C \qquad i = 1, \ldots, \ell
\end{cases}
$$

The method:

- choose a kernel k

- find an optimal solution λ^* of the dual

- choose i s.t. $0 < \lambda_i^* < C$ and find b^*:

$$b^* = \frac{1}{y^i} - \sum_{j=1}^{\ell} \lambda_j^* y^j k(x^i, x^j)$$

- Decision function

$$f(x) = \text{sign}\left(\sum_{i=1}^{\ell} \lambda_i^* y^i k(x^i, x) + b^*\right)$$

The separating surface $f(x) = 0$ is

- linear in the features space

- nonlinear in the input space

Exercise 5.5. Find the optimal separating surface for the following data set using a Gaussian kernel with parameters $C = 1$ and $\gamma = 1$.

$$A = \begin{pmatrix} 0.0113 & 0.2713 \\ 0.9018 & -0.1121 \\ 0.2624 & -0.2899 \\ 0.3049 & 0.2100 \\ -0.2255 & -0.7156 \\ -0.9497 & -0.1578 \\ -0.6318 & 0.4516 \\ -0.2593 & 0.6831 \\ 0.4685 & 0.1421 \\ -0.4694 & 0.8492 \\ -0.5525 & -0.2529 \\ -0.8250 & 0.2802 \\ 0.4463 & -0.3051 \\ 0.3212 & -0.2323 \\ 0.2547 & -0.9567 \\ 0.4917 & 0.6262 \\ -0.2334 & 0.2346 \\ 0.1510 & 0.0601 \\ -0.4499 & -0.5027 \\ -0.0967 & -0.5446 \end{pmatrix} \qquad B = \begin{pmatrix} 1.2178 & 1.9444 \\ -1.8800 & 0.1427 \\ -1.6517 & 1.2084 \\ 1.9566 & -1.7322 \\ 1.7576 & -1.9273 \\ 0.7354 & 1.1349 \\ 0.1366 & 1.5414 \\ 1.5960 & 0.5038 \\ -1.4485 & -1.1288 \\ -1.2714 & -1.8327 \\ -1.5722 & 0.4658 \\ 1.7586 & -0.5822 \\ -0.3575 & 1.9374 \\ 1.7823 & 0.7066 \\ 1.9532 & 1.0673 \\ -1.0233 & -0.8180 \\ 1.0021 & 0.3341 \\ 0.0473 & -1.6696 \\ 0.8783 & 1.9846 \\ -0.5819 & 1.8850 \end{pmatrix}$$

$$g(x, y, \gamma) = e^{-\gamma \| x_i - x_j \|^2}$$

Matlab commands

```
A=[........]; B=[........]; nA = size(A,1); nB = size(B,1);
T = [A ; B]; y = [ones(nA,1) ; -ones(nB,1)]; l = length(y); C=1;

gamma = 1 ;                                        % Gaussian kernel
K = zeros(l,l);
for i = 1 : l
for j = 1 : l
K(i,j) = exp(-gamma*norm(T(i,:)-T(j,:))^ 2);
end
end

Q = zeros(l,l);                                    % define the problem
for i = 1 : l
for j = 1 : l
Q(i,j) = y(i)*y(j)*K(i,j) ;
end
end

la = quadprog(Q,-ones(l,1),[ ],[ ],y',0,zeros(l,1),C*ones(l,1));    % solve the problem

ind = find((la > 0.001) & (la < C-0.001));                         % compute b
i = ind(1);
```

```
b = 1/y(i);
for j = 1 : I
b = b - la(j)*y(j)*K(i,j);
end
```
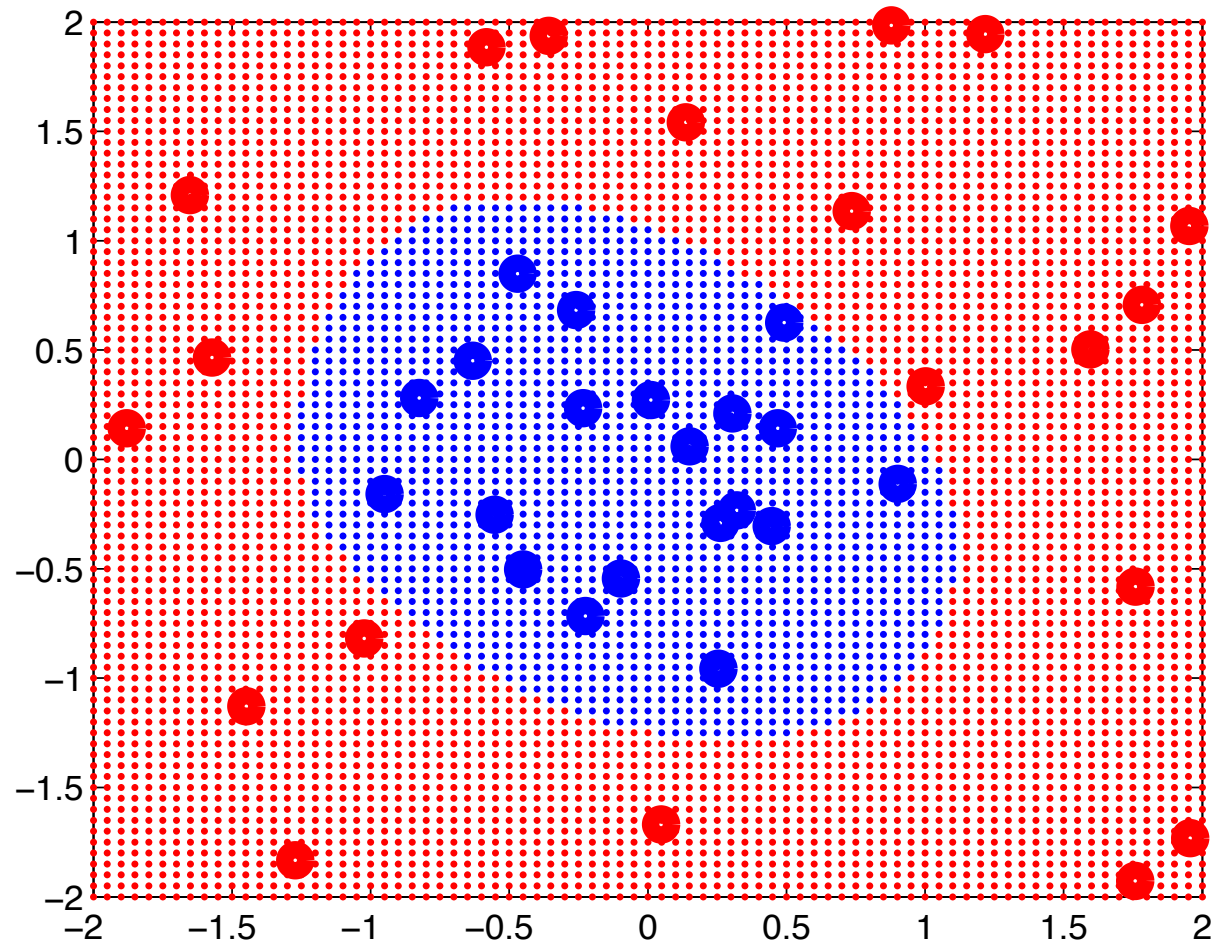
```
for xx = -2 : 0.01 : 2
for yy = -2 : 0.01 : 2
s = 0;
        for i = 1 : I
                s = s + la(i)*y(i)*exp(-gamma*norm(T(i,:)-[xx yy])^ 2);
        end
s = s + b;
        if (abs(s)< 0.01)
                plot(xx,yy,'g.');
                hold on
        end
end
end

plot(A(:,1),A(:,2),'bo',B(:,1),B(:,2),'ro','Linewidth',5)
```
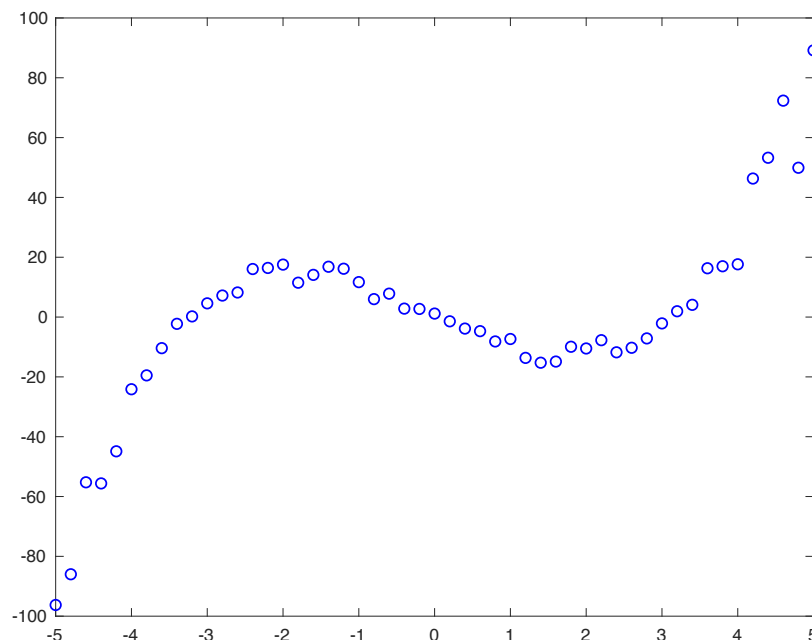
6 – Regression problems

G. Mastroeni and M. Passacantando

Department of Computer Science, University of Pisa

Polynomial regression

We have ℓ experimental data $y_1, y_2, \ldots, y_\ell \in \mathbb{R}$ corresponding to the observations related to the points $x_1, x_2, \ldots, x_\ell \in \mathbb{R}$.

We want to find the best approximation of experimental data with a polynomial p of degree $n - 1$, with $n \leq \ell$.
Polynomial p has coefficients $z_1, \ldots, z_n$:

$$p(x) = z_1 + z_2\, x + z_3\, x^2 + \cdots + z_n\, x^{n-1}$$

The residual is the vector $r \in \mathbb{R}^\ell$ such that $r_i = p(x_i) - y_i$, with $i = 1, \ldots, \ell$.

We want to find coefficients $z := (z_1, z_2, .., z_n)$ of polynomial p such that $\|r\|$ is minimum, which amounts to solve the following unconstrained problem

$$\begin{cases} \min \ \|A\,z - y\| \\ z \in \mathbb{R}^n \end{cases}$$

where

$$A = \begin{pmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \ldots & x_2^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_\ell & x_\ell^2 & \ldots & x_\ell^{n-1} \end{pmatrix} \in \mathbb{R}^{\ell \times n} \qquad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_\ell \end{pmatrix}$$

For any norm, the objective function $f(z) = \|Az - y\|$ is convex.

We will consider three special norms: $\|\cdot\|_2$, $\|\cdot\|_1$ and $\|\cdot\|_\infty$.

Euclidean norm $\|\cdot\|_2$ (least squares approximation)
$\rightarrow$ unconstrained quadratic programming problem:

$$\begin{cases} \min \ \dfrac{1}{2}\|A\,z - y\|_2^2 = \dfrac{1}{2}(Az - y)^{\mathsf{T}}(Az - y) = \dfrac{1}{2}z^{\mathsf{T}}A^{\mathsf{T}}Az - z^{\mathsf{T}}A^{\mathsf{T}}y + \dfrac{1}{2}y^{\mathsf{T}}y \\ z \in \mathbb{R}^n \end{cases}$$

It can be proved that $\mathrm{rank}(A) = n$, thus $A^{\mathsf{T}}A$ is positive definite.

Hence, the unique optimal solution is the stationary point of the objective function, i.e., the solution of the system of linear equations:

$$A^{\mathsf{T}}A\,z = A^{\mathsf{T}}y \tag{1}$$

Norm $\|\cdot\|_1 \rightarrow$ linear programming problem:

$$
\begin{cases}
\min \ \|Az - y\|_1 = \min \ \sum_{i=1}^{\ell} |A_i z - y_i| \\
z \in \mathbb{R}^n
\end{cases}
$$

is equivalent to

$$
\begin{cases}
\min\limits_{z,u} \ \sum_{i=1}^{\ell} u_i \\
u_i = |A_i z - y_i| \\
\quad = \max\{A_i z - y_i, y_i - A_i z\}
\end{cases}
\rightarrow
\begin{cases}
\min\limits_{z,u} \ \sum_{i=1}^{\ell} u_i \\
u_i \geq \max\{A_i z - y_i, y_i - A_i z\}
\end{cases}
$$

$$
\rightarrow
\begin{cases}
\min\limits_{z,u} \ \sum_{i=1}^{\ell} u_i \\
u_i \geq A_i z - y_i & \forall \ i = 1, \ldots, \ell \\
u_i \geq y_i - A_i z & \forall \ i = 1, \ldots, \ell
\end{cases}
\tag{2}
$$

In matrix form (2) can be written as

$$
\begin{cases}
\min_{z,u} \ e_\ell^T u \\
Az - u \le y \\
-Az - u \le -y
\end{cases}
$$

where $e^T = (1, \ldots, 1) \in \mathbb{R}^\ell$.
Set

$$
D = \begin{pmatrix} A & -I_\ell \\ -A & -I_\ell \end{pmatrix} \qquad d = \begin{pmatrix} y \\ -y \end{pmatrix}
$$

where I_ℓ is the identity matrix of order ℓ, then we obtain

$$
\begin{cases}
\min_{z,u} \ (0_n^T, e_\ell^T) \begin{pmatrix} z \\ u \end{pmatrix} \\
D \begin{pmatrix} z \\ u \end{pmatrix} \le d
\end{cases}
$$

Norm $\|\cdot\|_\infty \to$ linear programming problem:

$$\begin{cases} \min \ \|Az - y\|_\infty = \min \ \max_{i=1,\ldots,\ell} |A_i z - y_i| \\ z \in \mathbb{R}^n \end{cases}$$

is equivalent to

$$\begin{cases} \min_{z,u} \ u \\ u = \max_{i=1,\ldots,\ell} |A_i z - y_i| \end{cases} \to \begin{cases} \min_{z,u} \ u \\ u \geq A_i z - y_i & \forall \ i = 1, \ldots, \ell \\ u \geq y_i - A_i z & \forall \ i = 1, \ldots, \ell \end{cases} \quad (3)$$

Set

$$D = \begin{pmatrix} A & -e_\ell \\ -A & -e_\ell \end{pmatrix} \quad d = \begin{pmatrix} y \\ -y \end{pmatrix}$$

where $e_\ell = (1, \ldots, 1) \in \mathbb{R}^\ell$, in matrix form (3) becomes:

$$\begin{cases} \min_{z,u} \ (0, 0, \ldots, 0, 1) \begin{pmatrix} z \\ u \end{pmatrix} \\ D \begin{pmatrix} z \\ u \end{pmatrix} \leq d \end{cases}$$

Exercise 6.1.

Consider the experimental data (x_i, y_i), $i = 1, .., \ell$, given below:

$$
\begin{pmatrix}
-5.0000 & -96.2607 \\
-4.8000 & -85.9893 \\
-4.6000 & -55.2451 \\
-4.4000 & -55.6153 \\
-4.2000 & -44.8827 \\
-4.0000 & -24.1306 \\
-3.8000 & -19.4970 \\
-3.6000 & -10.3972 \\
-3.4000 & -2.2633 \\
-3.2000 & 0.2196 \\
-3.0000 & 4.5852 \\
-2.8000 & 7.1974 \\
-2.6000 & 8.2207 \\
-2.4000 & 16.0614 \\
-2.2000 & 16.4224 \\
-2.0000 & 17.5381 \\
-1.8000 & 11.4895 \\
-1.6000 & 14.1065 \\
-1.4000 & 16.8220 \\
-1.2000 & 16.1584 \\
-1.0000 & 11.6846 \\
-0.8000 & 5.9991 \\
-0.6000 & 7.8277 \\
-0.4000 & 2.8236 \\
-0.2000 & 2.7129 \\
0 & 1.1669
\end{pmatrix}
\qquad
\begin{pmatrix}
0.2000 & -1.4223 \\
0.4000 & -3.8489 \\
0.6000 & -4.7101 \\
0.8000 & -8.1538 \\
1.0000 & -7.3364 \\
1.2000 & -13.6464 \\
1.4000 & -15.2607 \\
1.6000 & -14.8747 \\
1.8000 & -9.9271 \\
2.0000 & -10.5022 \\
2.2000 & -7.7297 \\
2.4000 & -11.7859 \\
2.6000 & -10.2662 \\
2.8000 & -7.1364 \\
3.0000 & -2.1166 \\
3.2000 & 1.9428 \\
3.4000 & 4.0905 \\
3.6000 & 16.3151 \\
3.8000 & 16.9854 \\
4.0000 & 17.6418 \\
4.2000 & 46.3117 \\
4.4000 & 53.2609 \\
4.6000 & 72.3538 \\
4.8000 & 49.9166 \\
5.0000 & 89.1652
\end{pmatrix}
$$

Find the best approximating polynomials of degree 3 with respect to the norms $\| \cdot \|_2$, $\| \cdot \|_1$, $\| \cdot \|_\infty$.
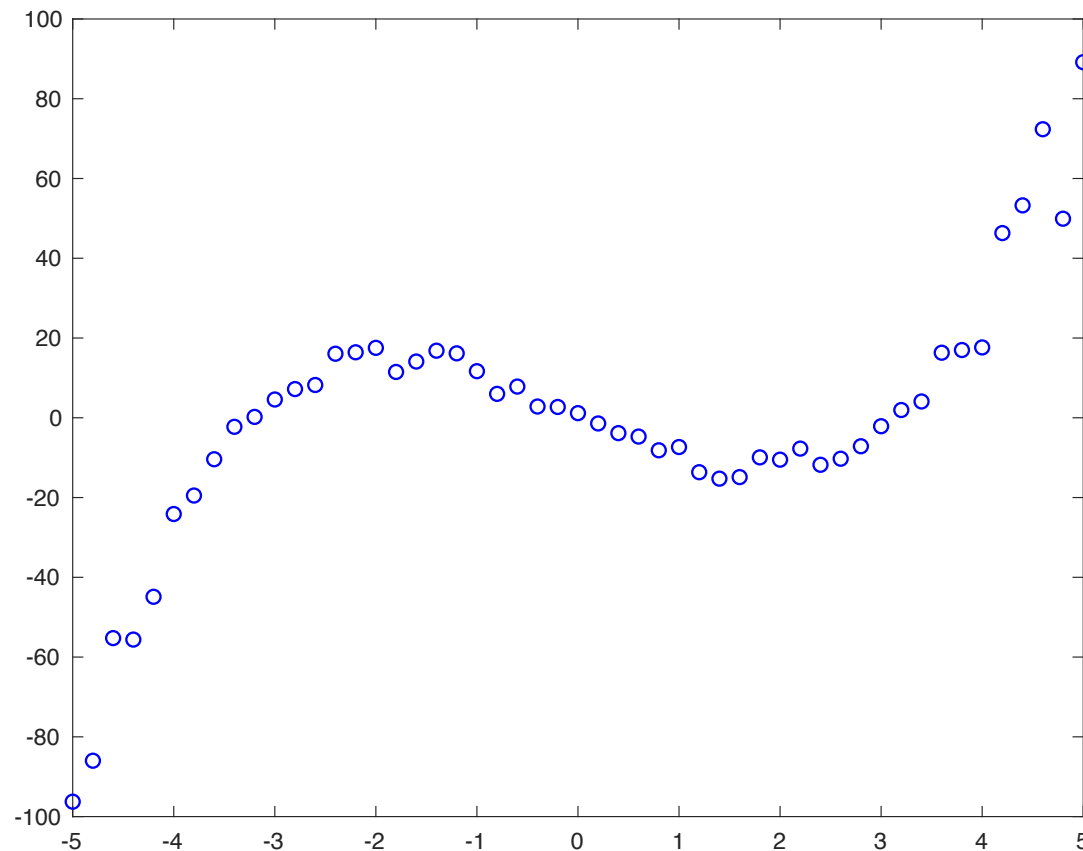
- For the case of norm $\| \cdot \|_2$, the solution is given by (1).
- For the cases of norms $\| \cdot \|_2$, $\| \cdot \|_1$, $\| \cdot \|_\infty$, we have to solve problems (2) and (3) written in matrix form.

We will use the Matlab function "linprog".

From the Matlab help

- X = linprog(f,A,b) attempts to solve the linear programming problem:

$$\min_{x} f' * x \text{ subject to: } A * x <= b$$

- X = linprog(f,A,b,Aeq,beq) solves the problem above while additionally satisfying the equality constraints $Aeq * x = beq$.
  (Set A=[] and B=[] if no inequalities exist.)
- X = linprog(f,A,b,Aeq,beq,LB,UB) defines a set of lower and upper bounds on the design variables, X, so that the solution is in the range LB <= X <= UB. Use empty matrices for LB and UB if no bounds exist. Set LB(i) = -Inf if X(i) is unbounded below; set UB(i) = Inf if X(i) is unbounded above.

```
data =[....];              %Matrix of given data

x = data(:,1) ;
y = data(:,2) ;
l = length(x) ;
n = 4 ;                              % number of coefficients of polynomial
A = [ ones(l,1) x x.^ 2 x.^ 3 ];     % Vandermonde matrix
```

% 2-norm problem

```
z2 = inv(A'*A)*(A'*y)
p2 = A*z2;               % regression values at the data
```

% 1-norm problem

```
c = [ zeros(n,1); ones(l,1) ];
D = [ A -eye(l); -A -eye(l) ];
d = [ y; -y ];
sol1 = linprog(c,D,d) ;
z1 = sol1(1:n)
p1 = A*z1;               % regression values at the data
```

% inf-norm problem

```
c = [ zeros(n,1); 1 ];
D = [ A -ones(l,1); -A -ones(l,1) ];
solinf = linprog(c,D,d) ;
zinf = solinf(1:n)
pinf = A*zinf;           % regression values at the data
```
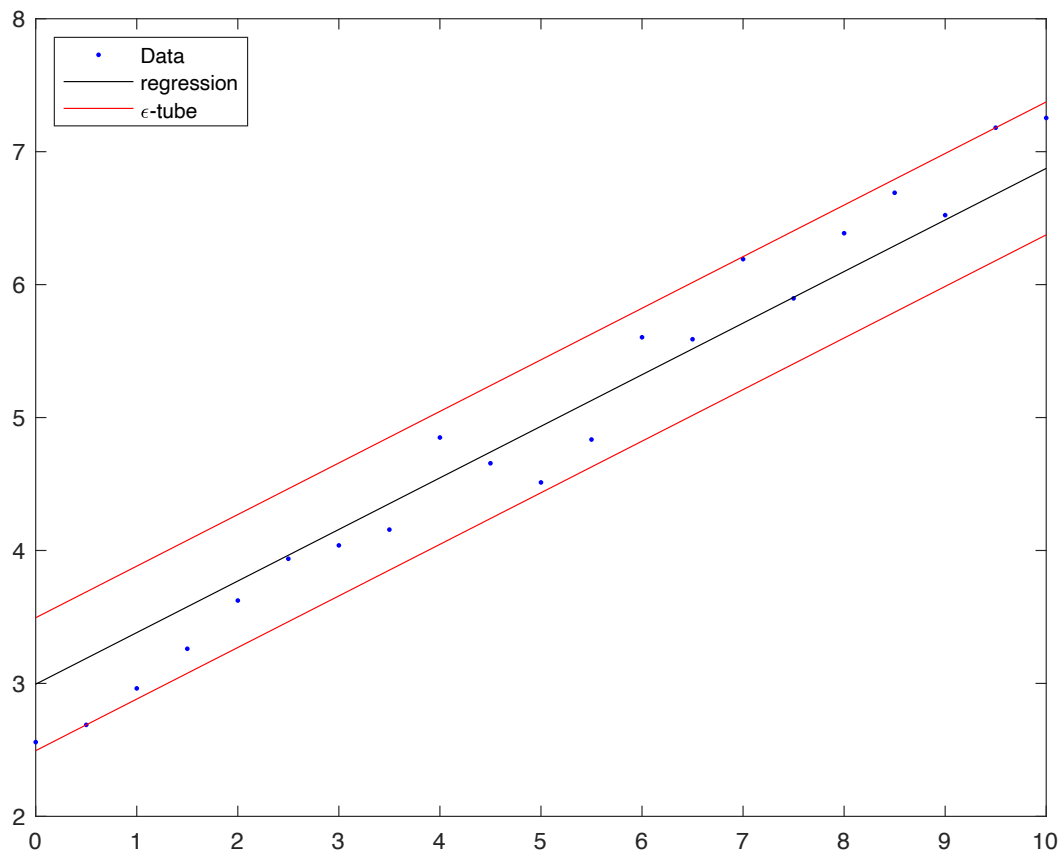
% plot the solutions

```
plot(x,y,'b.',x,p2,'r-',x,p1,'k-',x,pinf,'g-')
legend('Data','2-norm','1-norm','inf-norm','Location','NorthWest');
```

Given a set of training data $\{(x_1, y_1), \ldots, (x_\ell, y_\ell)\}$, where $x_i \in \mathbb{R}^n$, $y_i \in \mathbb{R}$, and a tolerance $\varepsilon > 0$, in ε-SV regression we aim at finding a function f that

$$|f(x_i) - y_i| \leq \varepsilon, \ i = 1, .., \ell$$

and it fulfills suitable properties (for example, it is as flat as possible)

In a linear regression, we consider an affine function $f(x) = w^{\mathsf{T}}x + b$ and set a tolerance parameter $\varepsilon > 0$.

If we want f to be flat, then we must seek for a small w, which leads us to solve the convex quadratic optimization problem

$$
\begin{cases}
\displaystyle\min_{w,b}\ \frac{1}{2}\|w\|^2 \\[2ex]
y_i \leq w^{\mathsf{T}}x_i + b + \varepsilon & \forall\, i = 1, \ldots, \ell \\
y_i \geq w^{\mathsf{T}}x_i + b - \varepsilon & \forall\, i = 1, \ldots, \ell
\end{cases}
\tag{4}
$$

In matrix form (4) becomes:

$$
\begin{cases}
\displaystyle\min_{w,b}\ \tfrac{1}{2}(w^T, b)Q\begin{pmatrix} w \\ b \end{pmatrix} \\[2ex]
D\begin{pmatrix} w \\ b \end{pmatrix} \leq d
\end{cases}
$$

where

$$
Q = \begin{pmatrix} I_n & 0_n \\ 0_n^T & 0 \end{pmatrix} \qquad D = \begin{pmatrix} -x & -e_\ell \\ x & e_\ell \end{pmatrix} \qquad d = \begin{pmatrix} \varepsilon e_\ell - y \\ \varepsilon e_\ell + y \end{pmatrix}
$$

Exercise 6.2. Apply the linear ε-SV regression model with $\varepsilon = 0.5$ to the following training data

$$
\begin{pmatrix}
0 & 2.5584 \\
0.5000 & 2.6882 \\
1.0000 & 2.9627 \\
1.5000 & 3.2608 \\
2.0000 & 3.6235 \\
2.5000 & 3.9376 \\
3.0000 & 4.0383 \\
3.5000 & 4.1570 \\
4.0000 & 4.8498 \\
4.5000 & 4.6561 \\
5.0000 & 4.5119 \\
5.5000 & 4.8346 \\
6.0000 & 5.6039 \\
6.5000 & 5.5890 \\
7.0000 & 6.1914 \\
7.5000 & 5.8966 \\
8.0000 & 6.3866 \\
8.5000 & 6.6909 \\
9.0000 & 6.5224 \\
9.5000 & 7.1803 \\
10.0000 & 7.2537
\end{pmatrix}
$$

Matlab commands

```
data=[ ]
x = data(:,1) ;
y = data(:,2) ;
l = length(x) ; % number of points
epsilon = 0.5 ;

Q = [ 1 0; 0 0 ];
c = [0;0];
D = [-x -ones(l,1); x ones(l,1)];
d = epsilon*ones(2*l,1) + [-y;y];

sol = quadprog(Q,c,D,d);
w = sol(1);
b = sol(2);
z = w.*x + b ;
zp = w.*x + b + epsilon ;
zm = w.*x + b - epsilon ;

% plot the solution

plot(x,y,'b.',x,z,'k-',x,zp,'r-',x,zm,'r-');
legend('Data','regression','ε-tube',... 'Location','NorthWest')
```
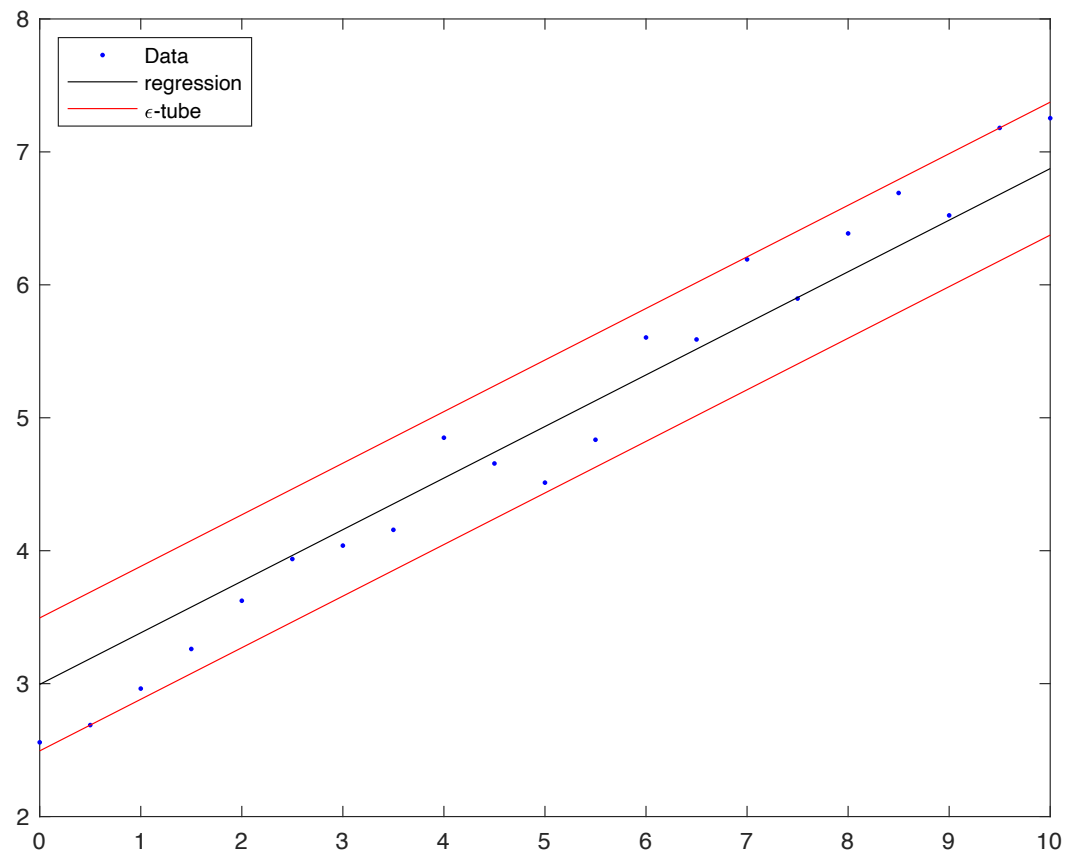
w =
0.3880

b =
2.9942

If ε is too small, the model (4) might not be feasible.

The linear ε-SV regression model can be extended by introducing slack variables ξ^+ and ξ^- to relax the constraints of problem (4):

$$\begin{cases} \min_{w,b,\xi^+,\xi^-} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{\ell}(\xi_i^+ + \xi_i^-) \\ y_i \leq w^\mathsf{T}x_i + b + \varepsilon + \xi_i^+ \qquad \forall\, i = 1,\ldots,\ell \\ y_i \geq w^\mathsf{T}x_i + b - \varepsilon - \xi_i^- \qquad \forall\, i = 1,\ldots,\ell \\ \xi^+ \geq 0 \\ \xi^- \geq 0 \end{cases} \tag{5}$$

where parameter C gives the trade-off between the flatness of f and tolerance to deviations larger than ε.

In matrix form (5) becomes:

$$
\begin{cases}
\min_{w,b} \; \frac{1}{2}(w^T, b, (\xi^+)^{\mathsf{T}}, (\xi^-)^{\mathsf{T}}) Q1 \begin{pmatrix} w \\ b \\ \xi^+ \\ \xi^- \end{pmatrix} + c^{\mathsf{T}} \begin{pmatrix} w \\ b \\ \xi^+ \\ \xi^- \end{pmatrix} \\[2em]
D1 \begin{pmatrix} w \\ b \\ \xi^+ \\ \xi^- \end{pmatrix} \leq d1 \\[2em]
\xi^+ \geq 0, \; \xi^- \geq 0
\end{cases}
$$

where

$$
Q1 = \begin{pmatrix} I_n & 0_n & O_{n \times 2\ell} \\ 0_n^T & 0 & 0_{2\ell}^T \\ O_{2\ell \times n} & 0_{2\ell} & O_{2\ell \times 2\ell} \end{pmatrix} \quad c^T = (O_n^T, 0, C * e_\ell^T, C * e_\ell^T)
$$

$$
D1 = \begin{pmatrix} -x & -e_\ell & -I_\ell & O_{\ell \times \ell} \\ x & e_\ell & O_{\ell \times \ell} & -I_\ell \end{pmatrix} \quad d = \begin{pmatrix} \varepsilon e_\ell - y \\ \varepsilon e_\ell + y \end{pmatrix}
$$

Exercise 6.3. Apply the linear ε-SV regression model with slack variables (set $\varepsilon = 0.2$ and $C = 10$) to the training data given in Exercise 6.2.
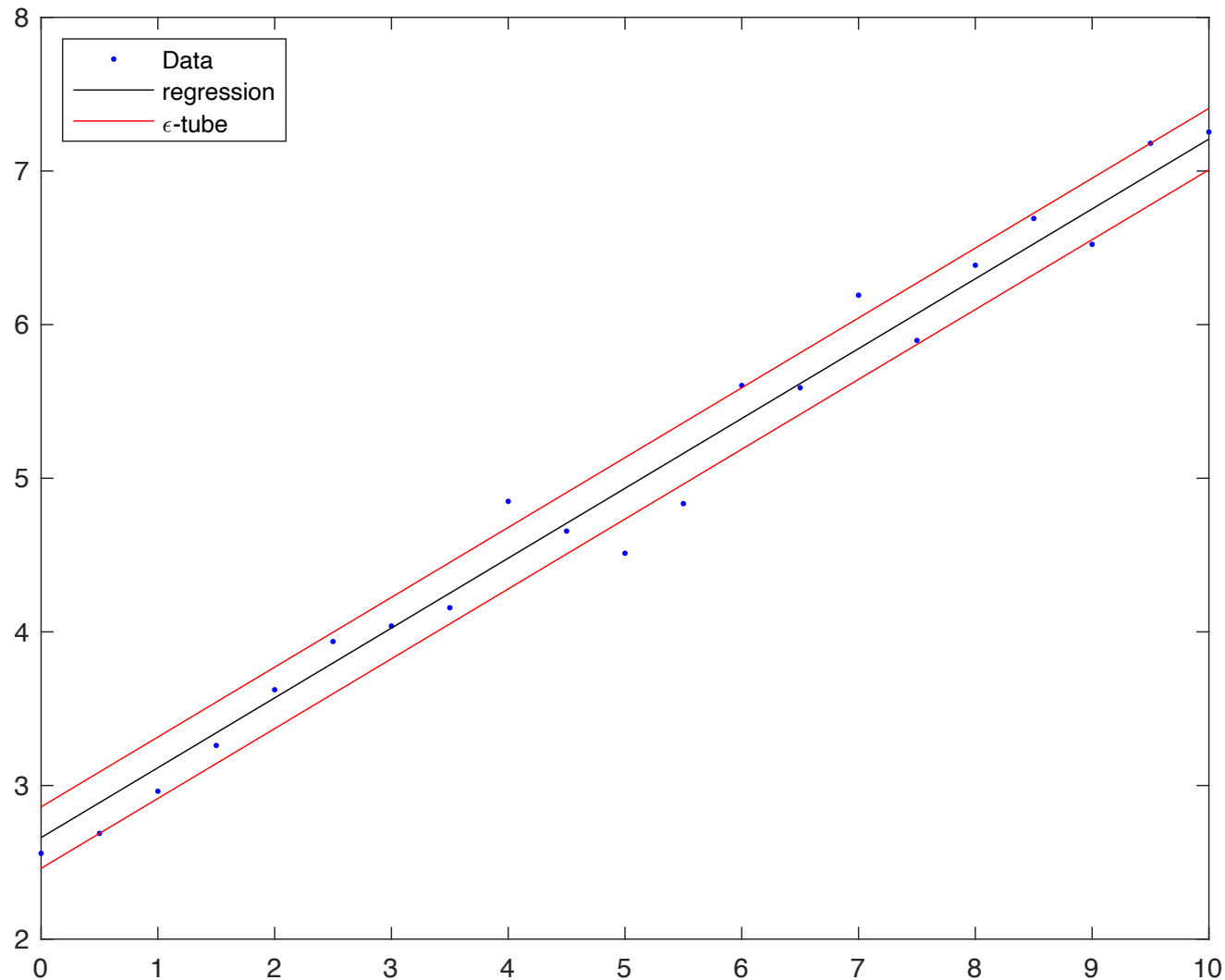
Linear ε-SV regression with slack variables - dual problem

Let us compute the dual of problem (5). The Lagrangian function is

$$L(\underbrace{w, b, \xi^+, \xi^-}_{\text{primal var.}}, \underbrace{\lambda^+, \lambda^-, \eta^+, \eta^-}_{\text{dual var.}}) = \frac{1}{2}\|w\|^2 - w^\mathsf{T}\left[\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)x_i\right] - b\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)$$

$$+ \sum_{i=1}^{\ell}\xi_i^+(C - \lambda_i^+ - \eta_i^+) + \sum_{i=1}^{\ell}\xi_i^-(C - \lambda_i^- - \eta_i^-) - \varepsilon\sum_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum_{i=1}^{\ell}y_i(\lambda_i^+ - \lambda_i^-)$$

If $\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) \neq 0$ or $C - \lambda_i^+ - \eta_i^+ \neq 0$ for some i or $C - \lambda_i^- - \eta_i^- \neq 0$ for some i, then $\min\limits_{w,b,\xi^+,\xi^-} L = -\infty$. Otherwise,

$$\nabla_w L = w - \sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)x_i = 0.$$

Operating as in previously made calculations, we substitute $w = \sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)x_i$ in the Lagrangian and we consider the above mentioned constraints.

The dual problem of (5) is

$$
\begin{cases}
\max_{\lambda^+,\lambda^-,\eta^+,\eta^-\geq 0} & -\frac{1}{2}\sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)(x_i)^\mathsf{T} x_j \\
& -\varepsilon\sum_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum_{i=1}^{\ell} y_i(\lambda_i^+ - \lambda_i^-) \\
\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) = 0 & \\
C - \lambda_i^+ - \eta_i^+ = 0, \ i = 1,..,\ell & \\
C - \lambda_i^- - \eta_i^- = 0, \ i = 1,..,\ell &
\end{cases}
$$

Finally, eliminating the variables η_i^+, η_i^- we obtain:

$$
\begin{cases}
\max_{\lambda^+,\lambda^-} & -\frac{1}{2}\sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)(x_i)^\mathsf{T} x_j \\
& -\varepsilon\sum_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum_{i=1}^{\ell} y_i(\lambda_i^+ - \lambda_i^-) \\
\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) = 0 & \\
\lambda_i^+ \in [0, C], \ i = 1,..,\ell & \\
\lambda_i^- \in [0, C], \ i = 1,..,\ell &
\end{cases}
$$

Let us write the dual problem in matrix form.

Consider first the quadratic part of the objective function.

It is possible to show that, setting

$$X = [(x_i)^\mathsf{T} x_j] \quad i,j = 1,..,\ell, \qquad Q = \begin{pmatrix} X & -X \\ -X & X \end{pmatrix}, \qquad (6)$$

then, we have:

$$-\frac{1}{2}\sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)(x_i)^\mathsf{T} x_j = -\frac{1}{2}((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T})Q\begin{pmatrix} \lambda^+ \\ \lambda^- \end{pmatrix}$$

Indeed, note that

$$\sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)(x_i)^\mathsf{T} x_j$$

$$= \sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+\lambda_j^+ - \lambda_i^+\lambda_j^- - \lambda_i^-\lambda_j^+ + \lambda_i^-\lambda_j^-)(x_i)^\mathsf{T} x_j \qquad (7)$$

Moreover,

$$((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T})Q\begin{pmatrix}\lambda^+\\\lambda^-\end{pmatrix} = ((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T})\begin{pmatrix}X & -X\\-X & X\end{pmatrix}\begin{pmatrix}\lambda^+\\\lambda^-\end{pmatrix} =$$

$$= [(\lambda^+)^\mathsf{T}X - (\lambda^-)^\mathsf{T}X]\lambda^+ + [(\lambda^+)^\mathsf{T}(-X) + (\lambda^-)^\mathsf{T}X]\lambda^-$$

$$= (\lambda^+)^\mathsf{T}X\lambda^+ - (\lambda^-)^\mathsf{T}X\lambda^+ - (\lambda^+)^\mathsf{T}X\lambda^- + (\lambda^-)^\mathsf{T}X\lambda^-$$

which equals (7).

Finally, we obtain:

Dual problem in matrix form

$$\begin{cases}\max_{\lambda^+,\lambda^-} -\dfrac{1}{2}((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T})Q\begin{pmatrix}\lambda^+\\\lambda^-\end{pmatrix} + [-\epsilon(e_\ell^\mathsf{T}, e_\ell^\mathsf{T}) + (y^\mathsf{T}, -y^\mathsf{T})]\begin{pmatrix}\lambda^+\\\lambda^-\end{pmatrix}\\[2mm] (e_\ell^\mathsf{T}, -e_\ell^\mathsf{T})\begin{pmatrix}\lambda^+\\\lambda^-\end{pmatrix} = 0\\[2mm] \lambda_i^+ \in [0, C], \ \ i = 1, .., \ell\\[2mm] \lambda_i^- \in [0, C], \ \ i = 1, .., \ell\end{cases}$$

where Q is defined by (6).

- Dual problem is a convex quadratic programming problem
- If $\lambda_i^+ > 0$ or $\lambda_i^- > 0$, then x_i is said support vector
- If (λ^+, λ^-) is a dual optimum, then

$$w = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-) x_i, \tag{8}$$

- b is obtained using the complementarity conditions:

$$\lambda_i^+ \left[\varepsilon + \xi_i^+ - y_i + w^\mathsf{T} x_i + b \right] = 0$$
$$\lambda_i^- \left[\varepsilon + \xi_i^- + y_i - w^\mathsf{T} x_i - b \right] = 0$$
$$\xi_i^+ (C - \lambda_i^+) = 0$$
$$\xi_i^- (C - \lambda_i^-) = 0$$

Hence, if there is some i s.t. $0 < \lambda_i^+ < C$, then

$$b = y_i - w^\mathsf{T} x_i - \varepsilon; \tag{9}$$

while, if there is some i s.t. $0 < \lambda_i^- < C$, then

$$b = y_i - w^\mathsf{T} x_i + \varepsilon. \tag{10}$$

Exercise 6.4. Solve the dual problem of the linear ε-SV regression model with slack variables (set $\varepsilon = 0.2$ and $C = 10$) applied to the training data given in Exercise 6.2.
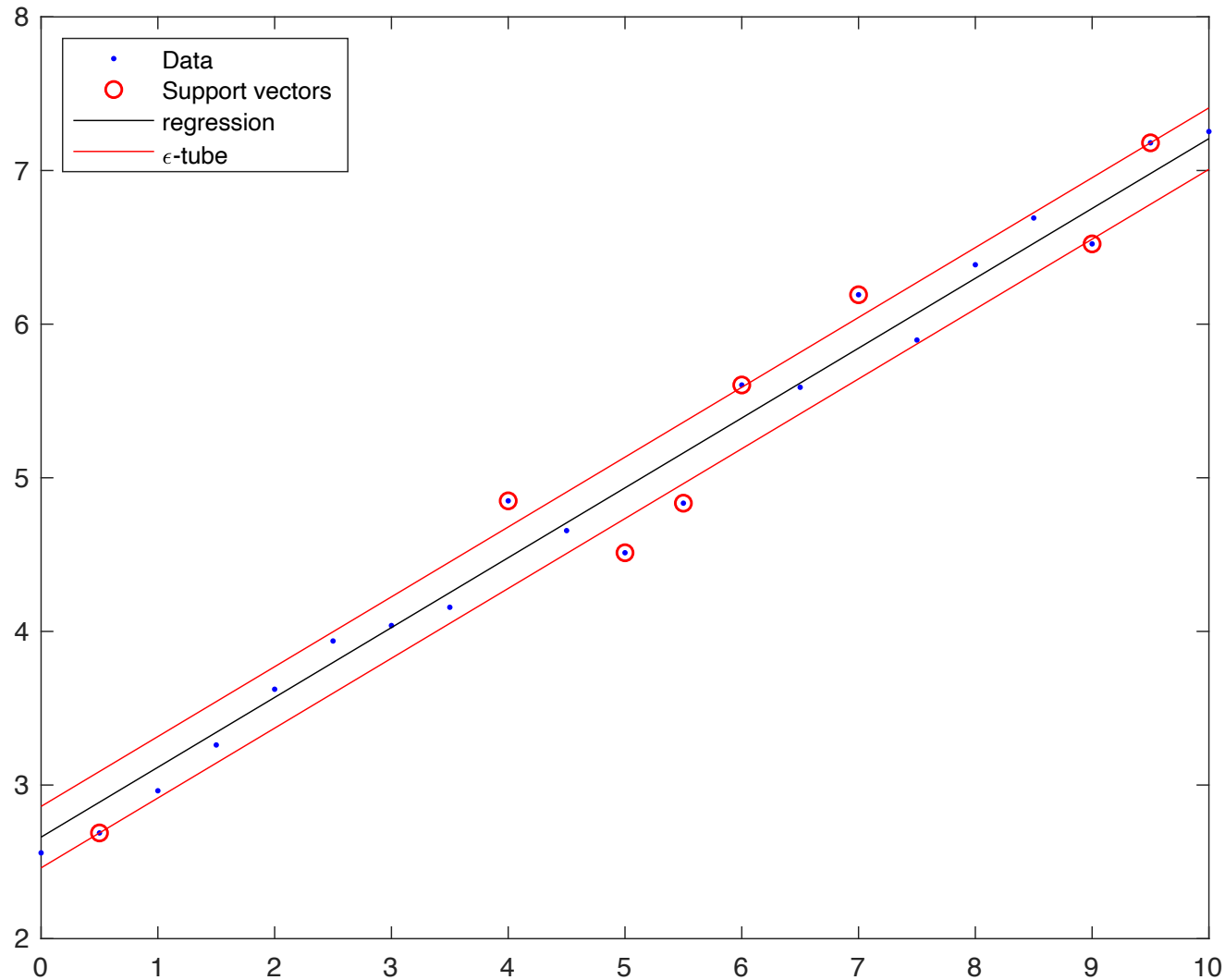
Matlab commands

```
data=[ .....]

x = data(:,1) ; y = data(:,2) ; l = length(x) ; epsilon = 0.2 ; C = 10;

X = zeros(l,l);
for i = 1 : l
    for j = 1 : l
        X(i,j) = x(i)*x(j);
    end
end
Q = [ X -X ; -X X ];
c = epsilon*ones(2*l,1) + [-y;y];

% solve the problem

sol = quadprog(Q,c,[],[],[ones(1,l) -ones(1,l)],0,zeros(2*l,1),C*ones(2*l,1));
lap = sol(1:l);
lam = sol(l+1:2*l);

% compute w

w = (lap-lam)'*x ;
```

```
% compute b

ind = find(lap > 0.001 & lap < C- 0.001);
if isempty(ind)==0
i = ind(1);
b = y(i) - w*x(i) - epsilon ;
else
ind = find(lam > 0.001 & lam < C- 0.001);
i = ind(1);
b = y(i) - w*x(i) + epsilon ;
end

% find regression and epsilon-tube

z = w.*x + b ;
zp = w.*x + b + epsilon ;
zm = w.*x + b - epsilon ;

% find support vectors and plot the solution

sv = [find(lap > 1e-3);find(lam > 1e-3)];
sv = sort(sv);

plot(x,y,'b.',x(sv),y(sv), 'ro',x,z,'k-',x,zp,'r-',x,zm,'r-');
```

In order to generate a nonlinear regression function f, we can use the kernel.

Define a map $\phi : \mathbb{R}^n \to \mathcal{H}$, where $\mathcal{H}$ (features space) is an higher dimensional (maybe infinite) space and find a linear regression for the points $\{(\phi(x_i), y_i)\}$ in the space $\mathcal{H} \times \mathbb{R}$.

The primal problem becomes:

$$
\begin{cases}
\min \ \dfrac{1}{2}\|w\|^2 + C \displaystyle\sum_{i=1}^{\ell}(\xi_i^+ + \xi_i^-) \\
y_i \leq w^{\mathsf{T}}\phi(x_i) + b + \varepsilon + \xi_i^+ \qquad \forall \ i = 1, \ldots, \ell \\
y_i \geq w^{\mathsf{T}}\phi(x_i) + b - \varepsilon - \xi_i^- \qquad \forall \ i = 1, \ldots, \ell
\end{cases}
$$

where w is a vector in a high (possibly infinite) dimensional space called the dual space of $\mathcal{H}$.

The dual problem is:

$$
\begin{cases}
\max\limits_{(\lambda^+,\lambda^-)} \quad -\dfrac{1}{2}\sum\limits_{i=1}^{\ell}\sum\limits_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)\textcolor{red}{\phi(x_i)^{\mathsf{T}}\phi(x_j)} \\
\qquad\qquad -\varepsilon\sum\limits_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum\limits_{i=1}^{\ell} y_i(\lambda_i^+ - \lambda_i^-) \\
\sum\limits_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) = 0 \\
\lambda_i^+, \lambda_i^- \in [0, C]
\end{cases}
$$

or,

$$
\begin{cases}
\max\limits_{(\lambda^+,\lambda^-)} \quad -\dfrac{1}{2}\sum\limits_{i=1}^{\ell}\sum\limits_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)\textcolor{red}{k(x_i, x_j)} \\
\qquad\qquad -\varepsilon\sum\limits_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum\limits_{i=1}^{\ell} y_i(\lambda_i^+ - \lambda_i^-) \\
\sum\limits_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) = 0 \\
\lambda_i^+, \lambda_i^- \in [0, C]
\end{cases}
$$

a finite dimensional problem with 2ℓ variables

- choose a kernel k
- solve the dual and find (λ^+, λ^-)
- Recall that, by (8) now we have:

$$w = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-)\phi(x_i), \qquad (11)$$

and, consequently,

$$w^T \phi(x) = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-)\phi(x_i)\phi(x) = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-)k(x_i, x).$$

By (9) and (10) we compute b:

Attenzione a λ, se esce fuori dall'intervallo

$$b = y_i - \varepsilon - \sum_{j=1}^{\ell} (\lambda_j^+ - \lambda_j^-)k(x_i, x_j), \qquad \text{for some } i \text{ s.t. } 0 < \lambda_i^+ < C$$

or

$$b = y_i + \varepsilon - \sum_{j=1}^{\ell} (\lambda_j^+ - \lambda_j^-)k(x_i, x_j), \qquad \text{for some } i \text{ s.t. } 0 < \lambda_i^- < C$$

(Recall that $k(x_i, x_j) = k(x_j, x_i)$.)

Finally, the regression function is:

$$f(x) = w^{\mathsf{T}}\phi(x) + b = \sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)k(x_i, x) + b \quad \bullet\bullet\bullet$$

Remark

The regression function is
- linear in the features space
- nonlinear in the input space

Exercise 6.5. Consider the training data given in Exercise 6.1. Apply the nonlinear ε-SV regression using a polynomial kernel with degree $p = 4$ and parameters $\varepsilon = 10$, $C = 10$. Moreover, find the support vectors.

```
data=[ .....]

x = data(:,1) ; y = data(:,2) ; l = length(x) ; epsilon = 10 ; C = 10;

X = zeros(l,l); for i = 1 : l
      for j = 1 : l
          X(i,j) =  kernel(x(i),x(j));
      end
end
Q = [ X -X ; -X X ];
c = epsilon*ones(2*l,1) + [-y;y];

% solve the problem

sol = quadprog(Q,c,[],[],[ones(1,l) -ones(1,l)],0,zeros(2*l,1),C*ones(2*l,1));
lap = sol(1:l);
lam = sol(l+1:2*l);

% compute b

ind = find(lap > 1e-3 & lap < C-1e-3);
if isempty(ind)==0
i = ind(1);
```

```
b = y(i) - epsilon;
for j = 1 : l
b = b - (lap(j)-lam(j))*kernel(x(i),x(j));
end
else
ind = find(lam > 1e-3 & lam < C-1e-3);
i = ind(1);
b = y(i) + epsilon ;
for j = 1 : l
b = b - (lap(j)-lam(j))*kernel(x(i),x(j));
end
end

% find regression and epsilon-tube evaluating f(x) at x(i), i=1,..,l

z = zeros(l,1);
for i = 1 : l
z(i) = b ;
for j = 1 : l
z(i) = z(i) + (lap(j)-lam(j))*kernel(x(i),x(j));
end
end
zp = z + epsilon ;
zm = z - epsilon ;
```

```
% find support vectors and plot the solution

sv = [find(lap > 1e-3);find(lam > 1e-3)];
sv = sort(sv);
plot(x,y,'b.',x(sv),y(sv), 'ro',x,z,'k-',x,zp,'r-',x,zm,'r-');

% kernel function

function v = kernel(x,y)

p = 4 ;

v = (x'*y + 1)^ p;

end
```
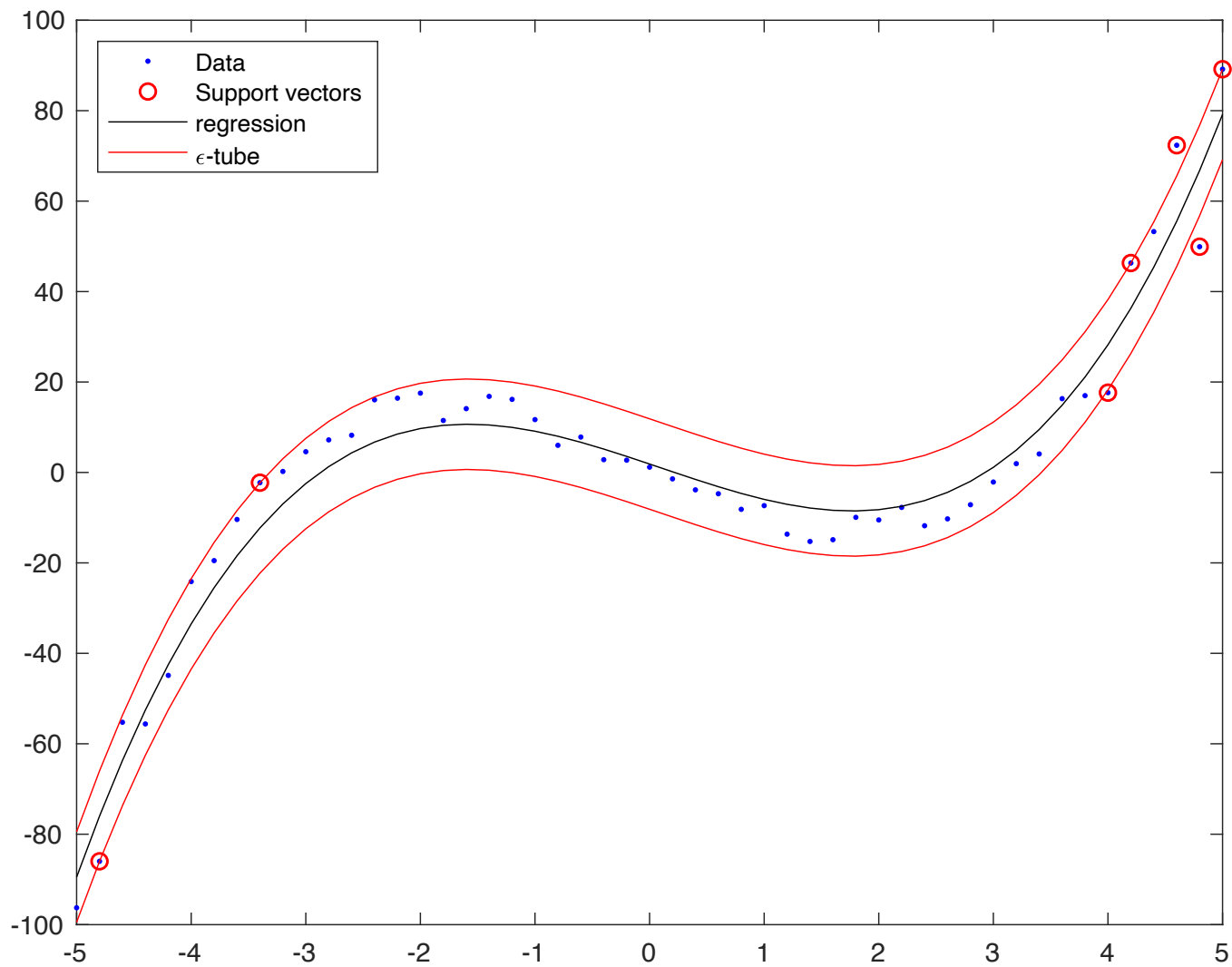
7 – Clustering problems

G. Mastroeni and M. Passacantando

Department of Computer Science, University of Pisa

Clustering problems

Definition

Given a set S of patterns and an integer number k, a clustering problem consists in finding a partition of S in k subsets $S_1, \ldots, S_k$ (clusters) that are homogeneous and well separated.
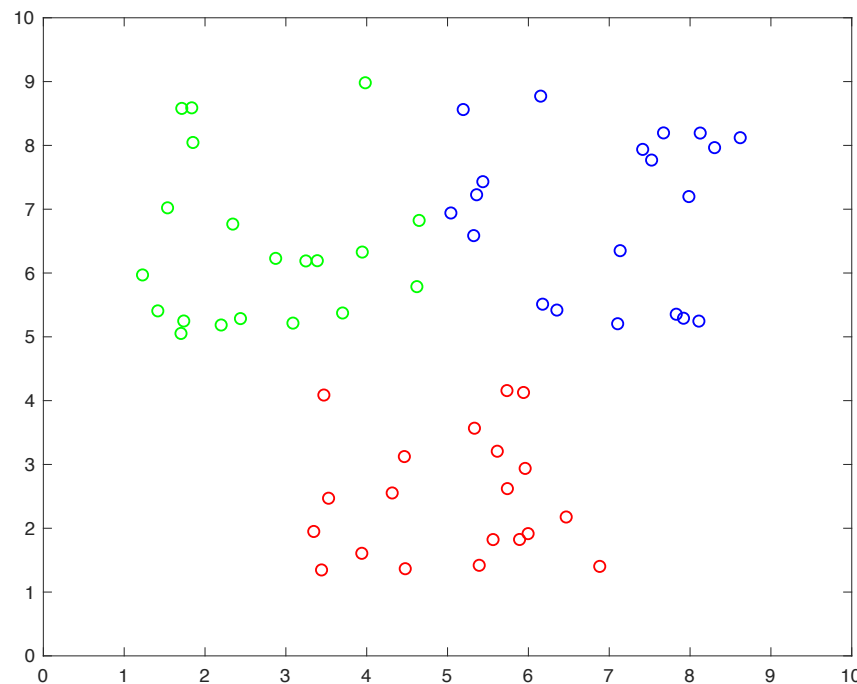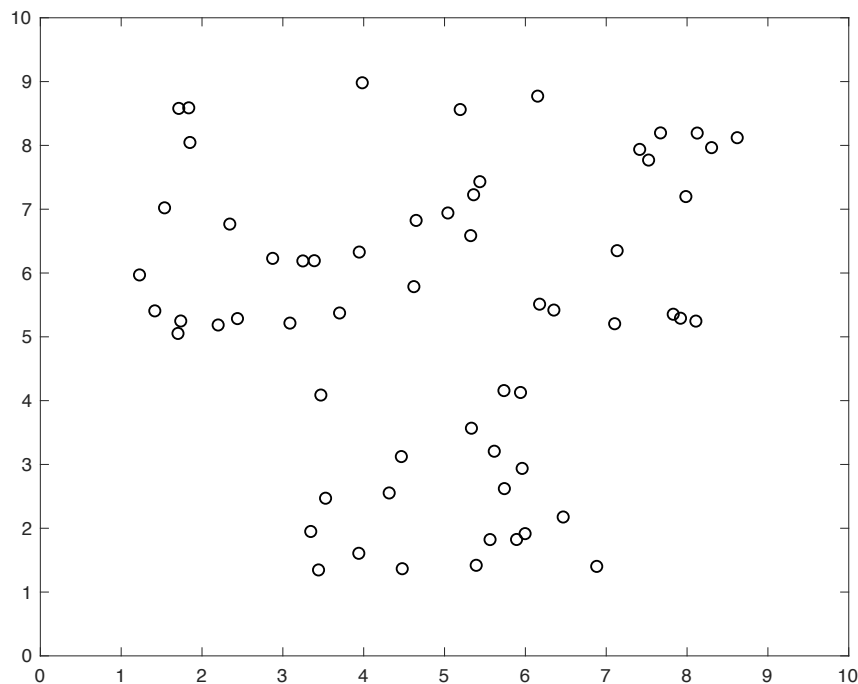
Clustering problem is of interest in unsupervisioned machine learning.

The optimization model

- Assume that patterns are vectors $p_1, \ldots, p_\ell \in \mathbb{R}^n$.

- Consider a distance $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ between vectors in $\mathbb{R}^n$.
  In what follows we will consider the square distance $d(x, y) = \|x - y\|_2^2$ or $d(x, y) = \|x - y\|_1$.

- For each cluster S_j introduce a centroid $x_j \in \mathbb{R}^n$ (unknown).

- Define clusters so that each pattern is associated to the closest centroid.

We aim to find k centroids in order to minimize the sum of the distances between each pattern and the closest centroid.

The model

$$
\begin{cases}
\min \; \displaystyle\sum_{i=1}^{\ell} \; \min_{j=1,\ldots,k} \; d(p_i, x_j) \\
x_j \in \mathbb{R}^n \qquad \forall \, j = 1, \ldots, k
\end{cases}
$$

Consider the square distance $d(x, y) = \|x - y\|_2^2$.
The optimization problem to solve is

$$
\begin{cases}
\min \ \displaystyle\sum_{i=1}^{\ell} \min_{j=1,\ldots,k} \|p_i - x_j\|_2^2 \\[2ex]
x_j \in \mathbb{R}^n \qquad \forall \, j = 1, \ldots, k
\end{cases}
$$

If $k = 1$ (one cluster), then it is a convex quadratic programming problem without constraints:

$$
\begin{cases}
\min \ \displaystyle\sum_{i=1}^{\ell} \|p_i - x\|_2^2 = \min \sum_{i=1}^{\ell} (x - p_i)^{\mathsf{T}} (x - p_i) \\[2ex]
x \in \mathbb{R}^n
\end{cases}
\tag{1}
$$

The global optimum is the stationary point:

$$
2\ell x - 2 \sum_{i=1}^{\ell} p_i = 0 \quad \iff \quad x = \frac{\displaystyle\sum_{i=1}^{\ell} p_i}{\ell} \quad \text{(mean or baricenter)}
$$

If $k > 1$ (at least two clusters), then the problem is nonconvex and nondifferentiable:

$$\begin{cases} \min_x \sum_{i=1}^{\ell} \min_{j=1,\ldots,k} \|p_i - x_j\|_2^2 \\ x_j \in \mathbb{R}^n \qquad \forall\, j = 1,\ldots,k \end{cases} \tag{2}$$

We observe that for fixed p_i and x_j, $j = 1,..,k$,

$$\min_{j=1,\ldots,k} \|p_i - x_j\|_2^2 = \begin{cases} \min \sum_{j=1}^{k} \alpha_{ij} \|p_i - x_j\|_2^2 \\ \sum_{j=1}^{k} \alpha_{ij} = 1 \\ \alpha_{ij} \geq 0 \qquad \forall\, j = 1,\ldots,k \end{cases} \tag{3}$$

Remark

It is enough to notice that $\displaystyle\min_{j=1,\ldots,k} \{a_j\} = \min\left\{ \sum_{j=1}^{k} \alpha_j a_j : \sum_{j=1}^{k} \alpha_j = 1,\ \alpha \geq 0 \right\}$.

An optimal solution of (3) is given by

$$\alpha_{ij}^* = \begin{cases} 1 & \text{if } \|p_i - x_j\|_2 = \min_{h=1,\dots,k} \|p_i - x_h\|_2 \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

Remark

Observe that $\alpha_{ij}^* = 1$ if pattern i is assigned to cluster j.

Theorem ● ● ●

Problem (2) is equivalent to the following nonconvex differentiable problem:

$$\begin{cases} \min_{x,\alpha} \ f(x,\alpha) := \sum_{i=1}^{\ell} \sum_{j=1}^{k} \alpha_{ij} \|p_i - x_j\|_2^2 \\[2mm] \sum_{j=1}^{k} \alpha_{ij} = 1 \quad \forall \ i = 1,\dots,\ell \\ \alpha_{ij} \geq 0 \qquad \forall \ i = 1,\dots,\ell, \ j = 1,\dots,k \\ x_j \in \mathbb{R}^n \qquad \forall \ j = 1,\dots,k. \end{cases} \tag{5}$$

The k-means algorithm is based on the following properties of problem (5):

- If x_j are fixed, then (5) is decomposable into ℓ simple LP problems of the form (3) : for any $i = 1, \ldots, \ell$, the optimal solution is

$$
\alpha_{ij}^* = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j\|_2 = \min_{h=1,\ldots,k} \|p_i - x_h\|_2 \\ & (x_j \text{ is the first closest centroid to } p_i), \\ 0 & \text{otherwise.} \end{cases}
$$

- If α_{ij} are fixed, then (5) is decomposable into k convex QP problems (in the unknown x_j) similar to (1), i.e.,

$$
\begin{cases} \min \ \sum_{i=1}^{\ell} \alpha_{ij} \|p_i - x_j\|_2^2 = \min \sum_{i=1}^{\ell} \alpha_{ij}(x_j - p_i)^{\mathsf{T}}(x_j - p_i) \\ x_j \in \mathbb{R}^n \end{cases} \tag{6}
$$

For any $j = 1, \ldots, k$, the optimal solution of (6) is

$$
x_j^* = \frac{\displaystyle\sum_{i=1}^{\ell} \alpha_{ij} p_i}{\displaystyle\sum_{i=1}^{\ell} \alpha_{ij}} \qquad \text{(mean of patterns).}
$$

Dimostrazione fatta alla lavagna. Potrebbe chiederla.

Clustering problem − k-means algorithm

The k-means algorithm consists in an alternating minimization of
$f(x, \alpha) = \sum_{i=1}^{\ell} \sum_{j=1}^{k} \alpha_{ij} \|p_i - x_j\|_2^2$ with respect to the two blocks of variables x and α.

0. (Inizialization) Set $t = 0$, choose centroids $x_1^0, \ldots, x_k^0 \in \mathbb{R}^n$ and assign patterns to clusters: for any $i = 1, \ldots, \ell$

$$\alpha_{ij}^0 = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j^0\|_2 = \min_{h=1,\ldots,k} \|p_i - x_h^0\|_2 \\ 0 & \text{otherwise.} \end{cases}$$

1. (Update centroids) For each $j = 1, \ldots, k$ compute the mean

$$x_j^{t+1} = \left(\sum_{i=1}^{\ell} \alpha_{ij}^t p_i \right) / \left(\sum_{i=1}^{\ell} \alpha_{ij}^t \right).$$

2. (Update clusters) For any $i = 1, \ldots, \ell$ compute

$$\alpha_{ij}^{t+1} = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j^{t+1}\|_2 = \min_{h=1,\ldots,k} \|p_i - x_h^{t+1}\|_2 \\ 0 & \text{otherwise.} \end{cases}$$

3. (Stopping criterion) If $f(x^{t+1}, \alpha^{t+1}) = f(x^t, \alpha^t)$ then STOP
else $t = t + 1$, go to Step 1.

Clustering problem – k-means algorithm

Theorem ●

The k-means algorithm stops after a finite number of iterations at a solution (x^*, α^*) of the KKT system of problem (5) such that

$$f(x^*, \alpha^*) \leq f(x^*, \alpha), \qquad \forall\, \alpha \geq 0 \ \text{ s.t. } \ \sum_{j=1}^{k} \alpha_{ij} = 1 \quad \forall\, i = 1, \ldots, \ell,$$

$$f(x^*, \alpha^*) \leq f(x, \alpha^*), \qquad \forall\, x \in \mathbb{R}^{kn}.$$

**Remark.** The k-means algorithm does not guarantee to find a global optimum.

Exercise 7.1. Consider the k-means algorithm, with $k = 3$, for the following set of patterns

$$
\begin{pmatrix}
1.2734 & 6.2721 \\
2.7453 & 7.4345 \\
1.6954 & 8.6408 \\
1.1044 & 8.6364 \\
4.8187 & 7.3664 \\
2.7224 & 6.3303 \\
4.8462 & 8.4123 \\
4.0497 & 6.7696 \\
1.0294 & 8.6174 \\
3.7202 & 5.1327 \\
3.8238 & 7.1297 \\
3.5805 & 7.8660 \\
3.2092 & 5.7172 \\
1.8724 & 6.3461 \\
4.0895 & 5.7509 \\
1.9121 & 6.2877 \\
2.4835 & 6.6154 \\
4.5637 & 7.1943 \\
4.4255 & 5.1950 \\
2.6097 & 7.2109
\end{pmatrix}
\quad
\begin{pmatrix}
6.0992 & 8.0496 \\
5.9660 & 7.3042 \\
5.9726 & 7.9907 \\
5.6166 & 7.5821 \\
8.8257 & 5.4929 \\
8.7426 & 7.0176 \\
8.2749 & 6.3890 \\
7.9130 & 5.3686 \\
5.7032 & 5.5914 \\
6.4415 & 5.7927 \\
5.7552 & 7.6891 \\
5.0048 & 6.7260 \\
6.2657 & 7.7776 \\
7.7985 & 6.0271 \\
7.5010 & 5.0390 \\
7.1722 & 7.1291 \\
6.7561 & 6.1176 \\
6.1497 & 8.7849 \\
7.0066 & 8.6258 \\
8.0462 & 6.5707
\end{pmatrix}
\quad
\begin{pmatrix}
3.0994 & 1.7722 \\
5.6857 & 2.3666 \\
6.3487 & 4.7316 \\
6.8860 & 2.5627 \\
3.2277 & 2.0929 \\
4.8013 & 1.6078 \\
5.3299 & 2.5884 \\
5.7466 & 2.4989 \\
5.8777 & 1.5245 \\
5.6002 & 2.7402 \\
5.9077 & 1.3661 \\
4.4954 & 3.4585 \\
5.3263 & 1.0439 \\
3.4645 & 3.2930 \\
3.2306 & 4.1589 \\
6.9191 & 1.9415 \\
4.1393 & 2.7921 \\
5.3799 & 3.2774 \\
6.8486 & 1.2456 \\
3.7431 & 2.9852
\end{pmatrix}
$$
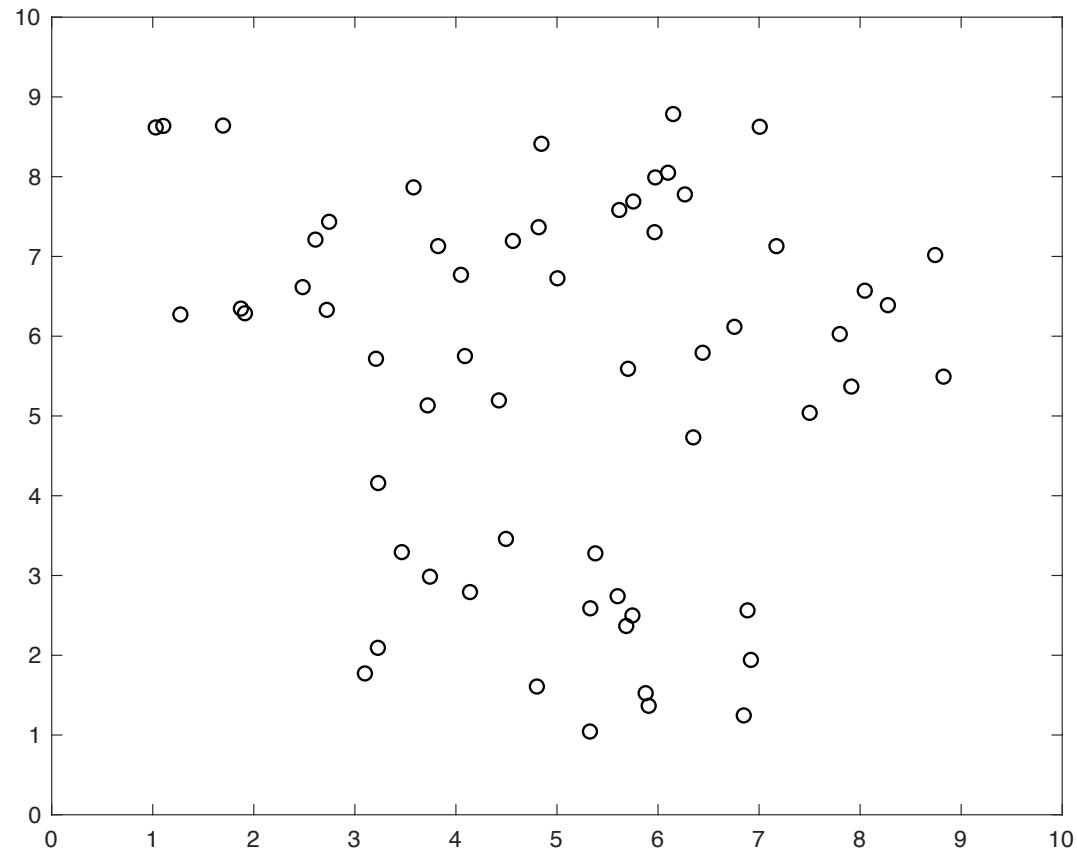
a) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 3)$.

b) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 4)$.

c) Is it possible to improve the solutions obtained in a) and b)?

Matlab commands

```
data=[...];

k=3;   % number of clusters

InitialCentroids=[5,7;6,3;4,3];

[x,cluster,v] = kmeans1(data,k,InitialCentroids)

% plot centroids
plot(x(1,1),x(1,2),'b*',x(2,1),x(2,2),'r*',x(3,1),x(3,2),'g*');

hold on

% plot clusters

c1 = data(cluster==1,:);
c2 = data(cluster==2,:);
c3 = data(cluster==3,:);

plot(c1(:,1),c1(:,2),'bo',c2(:,1),c2(:,2),'ro',c3(:,1),c3(:,2),'go');
```

```
function [x,cluster,v] = kmeans1(data,k,InitialCentroids)

l = size(data,1); % number of patterns
x = InitialCentroids; % initialize centroids

% initialize clusters
cluster = zeros(l,1);
for i = 1 : l
  d = inf;
   for j = 1 : k
    if norm(data(i,:)-x(j,:)) < d
    d = norm(data(i,:)-x(j,:));
    cluster(i) = j;
     end
   end
end

% compute the objective function value
vold = 0;
for i = 1 : l
   vold = vold + norm(data(i,:)-x(cluster(i),:))^ 2 ;
end

while true
```

```
% update centroids
for j = 1 : k
  ind = find(cluster == j);
   if isempty(ind)==0
    x(j,:) = mean(data(ind,:),1);
   end
end
```

```
% update clusters
for i = 1 : l
  d = inf;
   for j = 1 : k
   if norm(data(i,:)-x(j,:)) < d
   d = norm(data(i,:)-x(j,:));
   cluster(i) = j;
   end
   end
end
```

```
% update objective function
v = 0;
for i = 1 : l
  v = v + norm(data(i,:)-x(cluster(i),:))^ 2 ;
end
```

```
% stopping criterion

if vold - v < 1e-5
    break
else
    vold = v;
end

end

end
```

Consider now the distance $d(x, y) = \|x - y\|_1$.
The optimization problem to solve is

$$
\begin{cases}
\min \; \displaystyle\sum_{i=1}^{\ell} \; \min_{j=1,\ldots,k} \; \|p_i - x_j\|_1 \\[2ex]
x_j \in \mathbb{R}^n \qquad \forall \, j = 1, \ldots, k
\end{cases}
$$

If $k = 1$ (one cluster), then it is a convex problem decomposable into n convex problems of one variable:

$$
\begin{cases}
\min \; \displaystyle\sum_{i=1}^{\ell} \|p_i - x\|_1 = \min \sum_{i=1}^{\ell} \sum_{h=1}^{n} |x_h - (p_i)_h| = \min \sum_{h=1}^{n} \underbrace{\sum_{i=1}^{\ell} |x_h - (p_i)_h|}_{f_h(x_h)} \\[3ex]
x \in \mathbb{R}^n
\end{cases}
\tag{7}
$$

Given ℓ real numbers $a_1 < a_2 < \cdots < a_\ell$, what is the optimal solution of

$$\begin{cases} \min \; \sum_{i=1}^{\ell} |x - a_i| = f(x) \\ \\ x \in \mathbb{R} \end{cases} \quad ?$$

The objective function is convex and piecewise linear:

$$f(x) = \begin{cases} -\ell x + \sum_{i=1}^{\ell} a_i & \text{if } x < a_1 \\ (2 - \ell)x + \sum_{i=2}^{\ell} a_i - a_1 & \text{if } x \in [a_1, a_2] \\ \ldots & \ldots \\ (2r - \ell)x + \sum_{i=r+1}^{\ell} a_i - \sum_{i=1}^{r} a_1 & \text{if } x \in [a_r, a_{r+1}] \\ \ldots & \ldots \\ (\ell - 2)x + a_\ell - \sum_{i=1}^{\ell-1} a_i & \text{if } x \in [a_{\ell-1}, a_\ell] \\ \ell x - \sum_{i=1}^{\ell} a_i & \text{if } x > a_\ell \end{cases}$$

The global optimum is $\text{median}(a_1, \ldots, a_\ell) = \begin{cases} a_{(\ell+1)/2} & \text{if } \ell \text{ is odd,} \\ \dfrac{a_{\ell/2} + a_{1+\ell/2}}{2} & \text{if } \ell \text{ is even.} \end{cases}$

Example

(a) $f(x) = |x - 2| + |x - 4| + |x - 10|, \quad \ell = 3;$

(b) $f(x) = |x - 2| + |x - 4| + |x - 6| + |x - 10| \quad \ell = 4;$
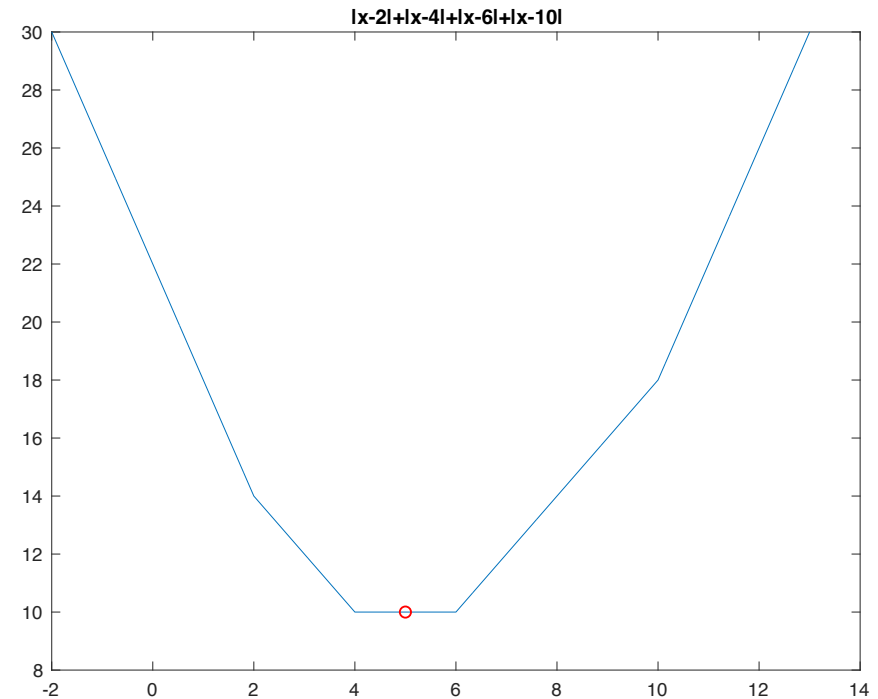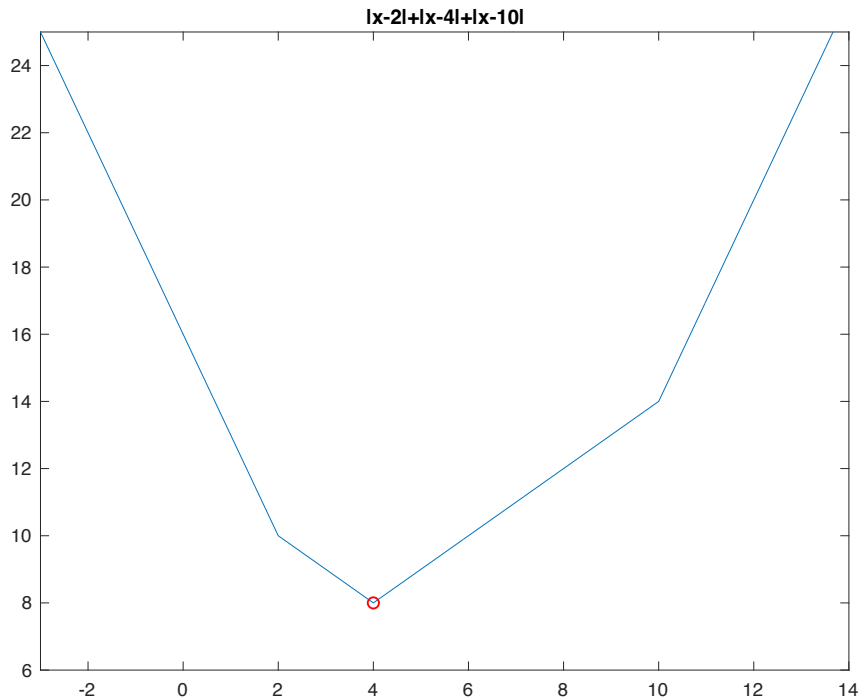
The global optimum is $\mathrm{median}(a_1, \ldots, a_\ell) = \begin{cases} a_{(\ell+1)/2} & \text{if } \ell = 3, \\[2mm] \dfrac{a_{\ell/2} + a_{1+\ell/2}}{2} & \text{if } \ell = 4 . \end{cases}$

If $k > 1$ (at least two clusters), then the problem is nonconvex and nonsmooth:

$$
\begin{cases}
\displaystyle\min_x \ \sum_{i=1}^{\ell} \min_{j=1,\ldots,k} \|p_i - x_j\|_1 \\[2ex]
x_j \in \mathbb{R}^n \qquad \forall\, j = 1, \ldots, k
\end{cases}
\tag{8}
$$

Theorem ● ● ●

Problem (8) is equivalent to the following problem:

$$
\begin{cases}
\displaystyle\min_{x,\alpha} \ \sum_{i=1}^{\ell}\sum_{j=1}^{k} \alpha_{ij}\|p_i - x_j\|_1 \\[2ex]
\displaystyle\sum_{j=1}^{k} \alpha_{ij} = 1 \quad \forall\, i = 1, \ldots, \ell \\[2ex]
\alpha_{ij} \geq 0 \qquad \forall\, i = 1, \ldots, \ell,\ j = 1, \ldots, k \\[1ex]
x_j \in \mathbb{R}^n \qquad \forall\, j = 1, \ldots, k.
\end{cases}
\tag{9}
$$

Note that

$$f(x, \alpha) := \sum_{i=1}^{\ell} \sum_{j=1}^{k} \alpha_{ij} \|p_i - x_j\|_1 = \sum_{i=1}^{\ell} \sum_{j=1}^{k} \sum_{h=1}^{n} \alpha_{ij} u_{ijh}$$

where we set

$$u_{ijh} = |(x_j)_h - (p_i)_h| = \max\{(x_j)_h - (p_i)_h, (p_i)_h - (x_j)_h\}$$

Consequently, we have the following result.

Theorem ●●●

Problem (9) is equivalent to the nonconvex differentiable (bilinear) problem:

$$
\begin{cases}
\min_{x, \alpha, u} \ \sum_{i=1}^{\ell} \sum_{j=1}^{k} \sum_{h=1}^{n} \alpha_{ij} u_{ijh} \\[2mm]
u_{ijh} \geq (p_i)_h - (x_j)_h \quad \forall \ i = 1, \dots, \ell, \ j = 1, \dots, k, \ h = 1, \dots, n \\
u_{ijh} \geq (x_j)_h - (p_i)_h \quad \forall \ i = 1, \dots, \ell, \ j = 1, \dots, k, \ h = 1, \dots, n \\
\sum_{j=1}^{k} \alpha_{ij} = 1 \quad \forall \ i = 1, \dots, \ell \\
\alpha_{ij} \geq 0 \quad \forall \ i = 1, \dots, \ell, \ j = 1, \dots, k \\
x_j \in \mathbb{R}^n \quad \forall \ j = 1, \dots, k.
\end{cases}
\tag{10}
$$

The k-median algorithm is based on the following properties of problem (9):

- If x_j are fixed, then (9) is decomposable into ℓ simple LP problems: for any $i = 1, \ldots, \ell$, the optimal solution is

$$
\alpha_{ij}^* = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j\|_1 = \min_{h=1,\ldots,k} \|p_i - x_h\|_1 \\ & (x_j \text{ is the first closest centroid to } p_i), \\ 0 & \text{otherwise.} \end{cases}
$$

- If $\alpha_{ij} \in \{0, 1\}$ are fixed, then (9) is decomposable into k simple convex problems similar to (7), i.e.,

$$
\begin{cases} \min \ \sum_{i=1}^{\ell} \alpha_{ij} \|p_i - x_j\|_1 = \min \sum_{i=1}^{\ell} \sum_{h=1}^{n} \alpha_{ij} |(x_j)_h - (p_i)_h| \\ x_j \in \mathbb{R}^n \end{cases} \tag{11}
$$

For any $j = 1, \ldots, k$, the optimal solution is

$$
x_j^* = \text{median}(p_i : \ \alpha_{ij} = 1).
$$

Clustering problem – k-median algorithm

The k-median algorithm consists in an alternating minimization of
$f(x, \alpha) = \sum_{i=1}^{\ell} \sum_{j=1}^{k} \alpha_{ij} \| p_i - x_j \|_1$ with respect to the two blocks of variables x and α.

0. (Inizialization) Set $t = 0$, choose centroids $x_1^0, \ldots, x_k^0 \in \mathbb{R}^n$ and assign patterns to clusters: for any $i = 1, \ldots, \ell$

$$\alpha_{ij}^0 = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \| p_i - x_j^0 \|_1 = \min_{h=1,\ldots,k} \| p_i - x_h^0 \|_1 \\ 0 & \text{otherwise.} \end{cases}$$

1. (Update centroids) For each $j = 1, \ldots, k$ compute

$$x_j^{t+1} = \text{median}(p_i : \ \alpha_{ij}^t = 1).$$

2. (Update clusters) For any $i = 1, \ldots, \ell$ compute

$$\alpha_{ij}^{t+1} = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \| p_i - x_j^{t+1} \|_1 = \min_{h=1,\ldots,k} \| p_i - x_h^{t+1} \|_1 \\ 0 & \text{otherwise.} \end{cases}$$

3. (Stopping criterion) If $f(x^{t+1}, \alpha^{t+1}) = f(x^t, \alpha^t)$ then STOP
else $t = t + 1$, go to Step 1.

The k-median algorithm stops after a finite number of iterations at a stationary point (x^*, α^*) of problem (8) such that

$$f(x^*, \alpha^*) \le f(x^*, \alpha), \qquad \forall\, \alpha \ge 0 \;\; \text{s.t.} \;\; \sum_{j=1}^{k} \alpha_{ij} = 1 \quad \forall\, i = 1, \ldots, \ell,$$

$$f(x^*, \alpha^*) \le f(x, \alpha^*), \qquad \forall\, x \in \mathbb{R}^{kn}.$$

Remark. ● ● ●

The k-median algorithm does not guarantee to find a global optimum.

Exercise 7.2. Consider the k-median algorithm, with $k = 3$, for the set of patterns given in Exercise 7.1.

a) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 3)$.

b) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 4)$.

c) Is it possible to improve the solutions obtained in a) and b)?

Matlab commands

Notice that the Matlab implementation of the k-median algorithm is analogous to the one of the k-means algorithm.

The changes with respect to the Matlab solution of Exercise 7.1 are given in blue.

```matlab
data=[...];

k=3;   % number of clusters

InitialCentroids=[5,7;6,3;4,3];

[x,cluster,v] = kmedian2(data,k,InitialCentroids)

% plot centroids
plot(x(1,1),x(1,2),'b*',x(2,1),x(2,2),'r*',x(3,1),x(3,2),'g*');

hold on

% plot clusters

c1 = data(cluster==1,:);
c2 = data(cluster==2,:);
c3 = data(cluster==3,:);

plot(c1(:,1),c1(:,2),'bo',c2(:,1),c2(:,2),'ro',c3(:,1),c3(:,2),'go');
```

```matlab
function [x,cluster,v] = kmedian2(data,k,InitialCentroids)

l = size(data,1); % number of patterns
x = InitialCentroids; % initialize centroids

% initialize clusters
cluster = zeros(l,1);
for i = 1 : l
  d = inf;
   for j = 1 : k
    if norm(data(i,:)-x(j,:),1) < d
    d = norm(data(i,:)-x(j,:),1);
    cluster(i) = j;
     end
   end
end

% compute the objective function value
vold = 0;
for i = 1 : l
   vold = vold + norm(data(i,:)-x(cluster(i),:),1) ;
end

while true
```

```matlab
% update centroids
for j = 1 : k
  ind = find(cluster == j);
   if isempty(ind)==0
    x(j,:) = median(data(ind,:),1);
   end
end

% update clusters
for i = 1 : l
  d = inf;
   for j = 1 : k
    if norm(data(i,:)-x(j,:),1) < d
    d = norm(data(i,:)-x(j,:),1);
    cluster(i) = j;
    end
   end
end

% update objective function
v = 0;
for i = 1 : l
  v = v + norm(data(i,:)-x(cluster(i),:),1) ;
end
```

```
% stopping criterion

if vold - v < 1e-5
    break
else
    vold = v;
end

end

end
```

••• 8 – Solution methods for constrained optimization problems

G. Mastroeni and M. Passacantando

Department of Computer Science, University of Pisa

Optimization Methods and Game Theory
Master of Science in Artificial Intelligence and Data Engineering
University of Pisa – A.Y. 2023/24

Solution methods

Consider the constrained optimization problem defined by

$$\begin{cases} \min \ f(x) \\ g_i(x) \leq 0 & \forall \ i = 1, \ldots, m \\ h_j(x) = 0 & \forall \ j = 1, \ldots, p \end{cases} \qquad (P)$$

Let $X = \{x \in \mathbb{R}^n : g(x) \leq 0, \ h(x) = 0\}$ be the feasible set of (P).

The methods for solving (P) are in general divided in the following classes:

- Primal methods that operate direct on the given problem (P) (e.g., methods of changing the variables, descent direction methods, as projected gradient method or Franke Wolfe method)
- Dual methods, that use the dual of (P), or related properties, (e.g., gradient methods for solving the dual problem, penalty methods)

As an example of a method of changing variables, we consider a problem with linear equality constraints only.

We observe that a constrained problem with linear equality constraints

$$
\begin{cases}
\min \ f(x) \\
Ax = b
\end{cases}
$$

where A is $p \times n$ matrix with $\text{rank}(A) = p$, is equivalent to an unconstrained problem:

indeed, write $A = (A_B, A_N)$ with $\det(A_B) \neq 0$, where A_B is a $(p \times p)$ matrix. Setting $x = \begin{pmatrix} x_B \\ x_N \end{pmatrix}$, then $Ax = b$ is equivalent to

$$
A_B x_B + A_N x_N = b \quad \Longrightarrow \quad x_B = A_B^{-1}(b - A_N x_N),
$$

thus, eliminating the variables x_B,

$$
\begin{cases}
\min \ f(x) \\
Ax = b
\end{cases}
\quad \text{is equivalent to} \quad
\begin{cases}
\min \ f(A_B^{-1}(b - A_N x_N), x_N) \\
x_N \in \mathbb{R}^{n-p}
\end{cases}
$$

Note that, if f is convex then the previous unconstrained problem is an unconstrained convex problem.

Example. Consider

$$\begin{cases} \min \ x_1^2 + x_2^2 + x_3^2 \\ x_1 + x_3 = 1 \\ x_1 + x_2 - x_3 = 2 \end{cases}$$

Since $x_1 = 1 - x_3$ and $x_2 = 2 - x_1 + x_3 = 1 + 2x_3$, the original constrained problem is equivalent to the following unconstrained problem:

$$\begin{cases} \min \ (1 - x_3)^2 + (1 + 2x_3)^2 + x_3^2 = 6x_3^2 + 2x_3 + 2 \\ x_3 \in \mathbb{R} \end{cases}$$

Therefore, the optimal solution is $x_3 = -1/6$, $x_1 = 7/6$, $x_2 = 2/3$.

Consider a constrained optimization problem

$$\begin{cases} \min \ f(x) \\ g_i(x) \leq 0 \qquad \forall \ i = 1, \ldots, m \end{cases}$$

(P)

Let $X = \{x \in \mathbb{R}^n : g(x) \leq 0\}$ the feasible set of (P).

Define the quadratic penalty function

$$p(x) = \sum_{i=1}^{m} \left(\max\{0, g_i(x)\}\right)^2$$

and consider the unconstrained penalized problem

$$\begin{cases} \min \ f(x) + \dfrac{1}{\varepsilon} p(x) := p_\varepsilon(x) \\ x \in \mathbb{R}^n \end{cases}$$

(P_ε)

Note that

$$p_\varepsilon(x) \begin{cases} = f(x) & \text{if } x \in X \\ > f(x) & \text{if } x \notin X \end{cases}$$

Proposition 8.1

1. If f, g_i are continuously differentiable, then p_ε is continuously differentiable and $\nabla p_\varepsilon(x) = \nabla f(x) + \dfrac{2}{\varepsilon} \sum_{i=1}^{m} \max\{0, g_i(x)\} \nabla g_i(x)$

2. If f and g_i are convex, then p_ε is convex

3. Any (P_ε) is a relaxation of (P), i.e., $v(P_\varepsilon) \leq v(P)$ for any $\varepsilon > 0$

4. If x_ε^* solves (P_ε) and $x_\varepsilon^* \in X$, then x_ε^* is optimal also for (P)

5. If $0 < \varepsilon_2 < \varepsilon_1$, then $v(P_{\varepsilon_1}) \leq v(P_{\varepsilon_2})$

Penalty method ● ● ●

0. Set $\varepsilon_0 > 0$, $\tau \in (0, 1)$, $k = 0$

1. Find an optimal solution x^k of the penalized problem (P_{ε_k})

2. **If** $x^k \in X$ **then** STOP
   else $\varepsilon_{k+1} = \tau \varepsilon_k$, $k = k + 1$ and go to step 1.

Theorem 8.2

- If f is coercive, then the sequence $\{x^k\}$ is bounded and any of its cluster points is an optimal solution of (P).
- If $\{x^k\}$ converges to x^*, then x^* is an optimal solution of (P).
- If $\{x^k\}$ converges to x^* and the gradients of active constraints at x^* are linear independent, then x^* is an optimal solution of (P) and the sequence of vectors $\{\lambda^k\}$ defined as

$$\lambda_i^k := \frac{2}{\varepsilon_k} \max\{0, g_i(x^k)\}, \qquad i = 1, \ldots, m$$

converges to a vector λ^* of KKT multipliers associated to x^*.

Remark

Notice that, by Proposition 8.1 (point 5), the sequence of the optimal values $v(P_{\varepsilon_k})$ generated by the penalty method, is increasing.

In fact, if x_ε^* solves (P_ε) and $x_\varepsilon^* \notin X$, then $v(P_\varepsilon) > v(P_{\varepsilon'})$ for any $\varepsilon < \varepsilon'$.

Exercise 8.1

a) Implement in MATLAB the penalty method for solving the problem

$$
\begin{cases}
\min \ \dfrac{1}{2}x^{\mathsf{T}}Qx + c^{\mathsf{T}}x \\
Ax \le b
\end{cases}
$$

where Q is a positive definite matrix.

b) Run the penalty method with $\tau = 0.1$ and $\varepsilon_0 = 5$ for solving the problem

$$
\begin{cases}
\min \ \dfrac{1}{2}(x_1 - 3)^2 + (x_2 - 2)^2 \\
-2x_1 + x_2 \le 0 \\
x_1 + x_2 \le 4 \\
-x_2 \le 0
\end{cases}
$$

[Use $\max(Ax - b) < 10^{-6}$ as stopping criterion.]

```
global Q c A b eps;

Q = [ 1 0 ; 0 2 ] ; c = [ -3 ; -4 ] ;   % data
A = [-2 1 ; 1 1 ; 0 -1 ]; b = [ 0 ; 4 ; 0 ];

tau = 0.1; eps0 = 5; tolerance = 1e-6 ;   % Penalty method
eps = eps0; x = [0;0]; iter = 0; SOL=[];

while true
[x,pval] = fminunc(@p_eps,x);
infeas = max(A*x-b);
SOL=[SOL;iter,eps,x',infeas,pval];
 if infeas < tolerance
  break
  else
  eps = tau*eps;
  iter = iter + 1 ;
 end
end

SOL
```

```
% The penalized function

function v= p_eps(x)

global Q c A b eps;

v = 0.5*x'*Q*x + c'*x ;

for i = 1 : size(A,1)
 v = v + (1/eps)*(max(0,A(i,:)*x-b(i)))^ 2 ;
end

end
```

The Matlab function 'fminunc' (from the Matlab help)

fminunc finds a local minimum of a function of several variables.
[X,FVAL] = fminunc(FUN,X0) starts at X0 and attempts to find a local minimizer X of the function FUN. FUN accepts input X and returns a scalar function value F evaluated at X. X0 can be a scalar, vector or matrix, FVAL is the optimal value of the function FUN.

FUN can be specified using @:
   [X,FVAL] = fminunc(@myfun,X0)
where myfun is a MATLAB function defined as:
   function F = myfun(x)
   F = ...;

Consider a convex constrained problem

$$\begin{cases} \min \ f(x) \\ g_i(x) \leq 0 \qquad \forall \ i = 1, \ldots, m \end{cases} \qquad (P)$$

and define the linear penalty function

$$\widetilde{p}(x) = \sum_{i=1}^{m} \max\{0, g_i(x)\}.$$

Consider the penalized problem

$$\begin{cases} \min \ \tilde{p}_\varepsilon(x) := f(x) + \dfrac{1}{\varepsilon} \, \widetilde{p}(x) \\ x \in \mathbb{R}^n \end{cases} \qquad (\widetilde{P}_\varepsilon)$$

which is unconstrained, convex and nonsmooth.

Note that
$$\tilde{p}_\varepsilon(x) \begin{cases} = f(x) & \text{if } x \in X \\ > f(x) & \text{if } x \notin X \end{cases}$$

For such penalized problem we do not need a sequence $\varepsilon_k \to 0$ to approximate an optimal solution of (P) (which avoid numerical issues), in fact there exists a suitable ε such that the minimum of $(\widetilde{P}_\varepsilon)$ coincides with the minimum of (P).

Proposition 8.3

Suppose that there exists an optimal solution x^* of (P) and λ^* is a KKT multipliers vector associated to x^*. Then, the sets of optimal solutions of (P) and $(\widetilde{P}_\varepsilon)$ coincide provided that $\varepsilon \in (0, 1/\|\lambda^*\|_\infty)$.

Exact penalty method

0. Set $\varepsilon_0 > 0$, $\tau \in (0, 1)$, $k = 0$

1. Find an optimal solution x^k of the penalized problem $(\widetilde{P}_{\varepsilon_k})$

2. If $x^k \in X$ **then** STOP
    else $\varepsilon_{k+1} = \tau \varepsilon_k$, $k = k + 1$ and go to step 1.

Theorem 8.4

The exact penalty method stops after a finite number of iterations at an optimal solution of (P).

Notice that penalty methods generate a sequence of unfeasible points that approximate an optimal solution of (P).

Exercise 8.2

Run the exact penalty method with $\tau = 0.5$ and $\varepsilon_0 = 4$ for solving the problem

$$
\begin{cases}
\min \ \dfrac{1}{2}(x_1 - 3)^2 + (x_2 - 2)^2 \\
-2x_1 + x_2 \leq 0 \\
x_1 + x_2 \leq 4 \\
-x_2 \leq 0
\end{cases}
$$

[Use $\max(Ax - b) < 10^{-6}$ as stopping criterion.]

Unlike penalty methods, barrier methods generate a sequence of feasible points that approximate an optimal solution of (P).

Consider

$$\begin{cases} \min \ f(x) \\ g_i(x) \leq 0 \quad i = 1, .., m \end{cases} \qquad (P)$$

under the following assumptions:

- f, g_i convex and twice continuously differentiable (on an open set containing X)
- there exists an optimal solution (e.g. f is coercive or X is bounded)
- Slater constraint qualification holds: there exists $\bar{x}$ such that

$$g_i(\bar{x}) < 0, \ \forall \ i = 1, \ldots, m$$

Hence strong duality holds.

Special cases: linear programming, convex quadratic programming

Logarithmic barrier

On the interior $\text{int}(X)$ of the feasible set X, we can approximate the given problem (P) with

$$\begin{cases} \min \ f(x) - \varepsilon \sum_{i=1}^{m} log(-g_i(x)) \\ x \in \text{int}(X) \end{cases}$$

Let $\psi_\varepsilon(x) := f(x) - \varepsilon \sum_{i=1}^{m} log(-g_i(x))$. Setting

$$B(x) := - \sum_{i=1}^{m} log(-g_i(x))$$

then

$$\psi_\varepsilon(x) := f(x) + \varepsilon B(x)$$

Note that, as x tends to the boundary of X, then $\psi_\varepsilon(x) \to +\infty$.

$B(x)$ is called logarithmic barrier function.

The function $B(x)$ has the following properties:

- $\text{dom}(B) = \text{int}(X)$
- B is convex
- B is smooth with

$$\nabla B(x) = -\sum_{i=1}^{m} \frac{1}{g_i(x)} \nabla g_i(x)$$

$$\nabla^2 B(x) = \sum_{i=1}^{m} \frac{1}{g_i(x)^2} \nabla g_i(x) \nabla g_i(x)^{\mathsf{T}} + \sum_{i=1}^{m} \frac{1}{-g_i(x)} \nabla^2 g_i(x)$$

Logarithmic barrier

If x_ε^* is the optimal solution of

$$\begin{cases} \min \ f(x) - \varepsilon \sum_{i=1}^m \log(-g_i(x)) \\ x \in \text{int}(X) \end{cases}$$

then

$$\nabla f(x_\varepsilon^*) + \sum_{i=1}^m \frac{\varepsilon}{-g_i(x_\varepsilon^*)} \nabla g_i(x_\varepsilon^*) = 0.$$

Define $\lambda_\varepsilon^* = \left(\dfrac{\varepsilon}{-g_1(x_\varepsilon^*)}, \dots, \dfrac{\varepsilon}{-g_m(x_\varepsilon^*)} \right) > 0.$

Consider the Lagrangian function L associated with the given problem (P),
$L(x, \lambda) := f(x) + \sum_{i=1}^m \lambda_i g_i(x)$. Then

$$L(x, \lambda_\varepsilon^*) = f(x) + \sum_{i=1}^m (\lambda_\varepsilon^*)_i g_i(x)$$

is convex and $\nabla_x L(x_\varepsilon^*, \lambda_\varepsilon^*) = 0$.

Recall that (P) is a convex problem and strong duality holds, hence

$$v(P) = \max_{\lambda \in \mathbb{R}_+^m} \inf_{x \in \mathbb{R}^n} L(x, \lambda)$$

Consequently,

$$v(P) \geq \min_x L(x, \lambda_\varepsilon^*) = L(x_\varepsilon^*, \lambda_\varepsilon^*).$$

Finally

$$f(x_\varepsilon^*) \geq v(P) \geq L(x_\varepsilon^*, \lambda_\varepsilon^*) = f(x_\varepsilon^*) + \sum_{i=1}^m (\lambda_\varepsilon^*)_i g_i(x_\varepsilon^*) = f(x_\varepsilon^*) - \underbrace{m\varepsilon}_{\text{optimality gap}}$$

Remark

Note that:

$$\text{As } \varepsilon \to 0, \qquad f(x_\varepsilon^*) \to v(P).$$

The KKT system of the original problem is

$$
\begin{cases}
\nabla f(x) + \sum\limits_{i=1}^{m} \lambda_i \nabla g_i(x) = 0 \\
-\lambda_i g_i(x) = 0 \quad i = 1, .., m \\
\lambda \geq 0 \\
g(x) \leq 0
\end{cases}
$$

Notice that $(x_\varepsilon^*, \lambda_\varepsilon^*)$ solves the system

$$
\begin{cases}
\nabla f(x) + \sum\limits_{i=1}^{m} \lambda_i \nabla g_i(x) = 0 \\
-\lambda_i g_i(x) = \varepsilon, \quad i = 1, .., m \\
\lambda \geq 0 \\
g(x) \leq 0
\end{cases}
$$

which is an approximation of the above KKT system.

Logarithmic barrier method ● ● ●

0. Set tolerance $\delta > 0$, $\tau \in (0,1)$ and $\varepsilon_1 > 0$. Choose $x^0 \in \text{int}(X)$, set $k = 1$

1. Find the optimal solution x^k of

$$
\begin{cases}
\min \ f(x) - \varepsilon_k \sum_{i=1}^{m} \log(-g_i(x)) \\
x \in \text{int}(X)
\end{cases}
$$

using x^{k-1} as starting point

2. If $m\varepsilon_k < \delta$ **then** STOP
else $\varepsilon_{k+1} = \tau\varepsilon_k$, $k = k+1$ and go to step 1

In order to find an initial point $x^0 \in \text{int}(X)$ we can consider the auxiliary problem

$$\begin{cases} \min_{x,s} \ s \\ g_i(x) \leq s, \quad i = 1, .., m \end{cases}$$

- Take any $\tilde{x} \in \mathbb{R}^n$, find $\tilde{s} > \max_{i=1,\ldots,m} g_i(\tilde{x})$

  $[(\tilde{x}, \tilde{s})$ is in the interior of the feasible region of the auxiliary problem]
- Find an optimal solution (x^*, s^*) of the auxiliary problem using a barrier method starting from $(\tilde{x}, \tilde{s})$
- If $s^* < 0$ then $x^* \in \text{int}(X)$
  else $\text{int}(X) = \emptyset$

Exercise 8.3.

a) Implement in MATLAB the logarithmic barrier method for solving the problem

$$\begin{cases} \min \ \dfrac{1}{2}x^\mathsf{T}Qx + c^\mathsf{T}x \\ Ax \le b \end{cases}$$

where Q is a positive definite matrix.

b) Run the logarithmic barrier method with $\delta = 10^{-3}$, $\tau = 0.5$, $\varepsilon_1 = 1$ and $x^0 = (1,1)$ for solving the problem

$$\begin{cases} \min \ \dfrac{1}{2}(x_1 - 3)^2 + (x_2 - 2)^2 \\ -2x_1 + x_2 \le 0 \\ x_1 + x_2 \le 4 \\ -x_2 \le 0 \end{cases}$$

```
global Q c A b eps;

Q = [ 1 0 ; 0 2 ] ; c = [ -3 ; -4 ] ;   % data
A = [-2 1 ; 1 1 ; 0 -1 ]; b = [ 0 ; 4 ; 0 ];

tau = 0.5; eps1 = 5; delta = 1e-3 ; x0=[1,1];   % barrier method

eps = eps1 ; m = size(A,1) ;
SOL=[];

while true
 [x,pval] = fminunc(@logbar,x);
  gap = m*eps;
  SOL=[SOL;eps,x',gap,pval];
   if gap < delta
    break
   else
    eps = eps*tau;
   end
end

SOL
```

```
function v= logbar(x)

global Q c A b eps;

v = 0.5*x'*Q*x + c'*x ;

for i = 1 : length(b)
 v = v - eps*log(b(i)-A(i,:)*x) ;
end

end
```

9 – Multiobjective optimization

G. Mastroeni, M. Passacantando

Department of Computer Science, University of Pisa
Department of Economic Sciences, University of Milano Bicocca

Optimization Methods and Game Theory
Master of Science in Artificial Intelligence and Data Engineering
University of Pisa – A.Y. 2023/24

Multiobjective optimization problems

Definition

A multiobjective optimization problem is defined by:

$$\begin{cases} \min\ f(x) = (f_1(x), f_2(x), \ldots, f_s(x)) \\ x \in X \end{cases} \tag{P}$$

where $f : \mathbb{R}^n \to \mathbb{R}^s$, $f(x) = (f_1(x), f_2(x), \ldots, f_s(x))$, $X \subseteq \mathbb{R}^n$.

- $f(x)$ is a vector in $\mathbb{R}^s$, i.e., there are several objectives to be simultaneously optimized.

- We need to define an order in $\mathbb{R}^s$.

Given $x, y \in \mathbb{R}^s$, we say that

$$x \geq y \quad \Longleftrightarrow \quad x_i \geq y_i \quad \text{for any } i = 1, \ldots, s.$$

This relation is a **partial order** in $\mathbb{R}^s$: it is

- reflexive: $x \geq x$
- asymmetric: if $x \geq y$ and $y \geq x$ then $x = y$
- transitive: if $x \geq y$ and $y \geq z$ then $x \geq z$

but it is not a total order: if $x = (1, 5)$ and $y = (4, 2)$ then $x \not\geq y$ and $y \not\geq x$

Definition ● ● ●

Given a subset $A \subseteq \mathbb{R}^s$, we say that

- $\bar{x} \in A$ is a Pareto ideal minimum (or ideal efficient point) of A if $y \geq \bar{x}$ for any $y \in A$.
- $\bar{x} \in A$ is a Pareto minimum (or efficient point) of A if there is no $y \in A$, $y \neq \bar{x}$, such that $\bar{x} \geq y$ (or, equivalently, there is no $y \in A$ such that $\bar{x} \geq y$ and $\bar{x}_j > y_j$, for some $j \in \{1, .., s\}$).
- $\bar{x} \in A$ is a Pareto weak minimum (or weakly efficient point) of A if there is no $y \in A$ such that $\bar{x} > y$, i.e., $\bar{x}_i > y_i$ for any $i = 1, \ldots, s$.

$IMin(A)$, $Min(A)$ and $WMin(A)$ denote the set of ideal minima, minima, weak minima of A, respectively.

Remark

$$IMin(A) \subseteq Min(A) \subseteq WMin(A).$$

Equivalent definitions of minimum points for a set of vectors

- $\bar{x} \in A$ is a Pareto ideal minimum if

$$A \subseteq (\bar{x} + \mathbb{R}^s_+)$$

- $\bar{x} \in A$ is a Pareto minimum of A if

$$A \cap (\bar{x} - \mathbb{R}^s_+) = \{\bar{x}\}$$

- $\bar{x} \in A$ is a Pareto weak minimum of A if

$$A \cap (\bar{x} - int(\mathbb{R}^s_+)) = \emptyset$$

Example 1

$$A = \{x \in \mathbb{R}^2 : \ x_1 \geq 0, \ x_2 \geq 0, \ x_1 + x_2 \leq 2\}.$$

Let $\bar{x} = (0,0)$.
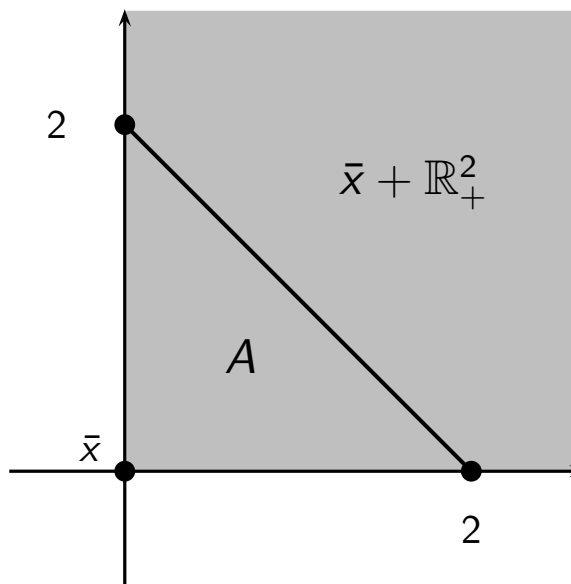
Let $\bar{x} = (0, a)$, $0 < a \leq 2$
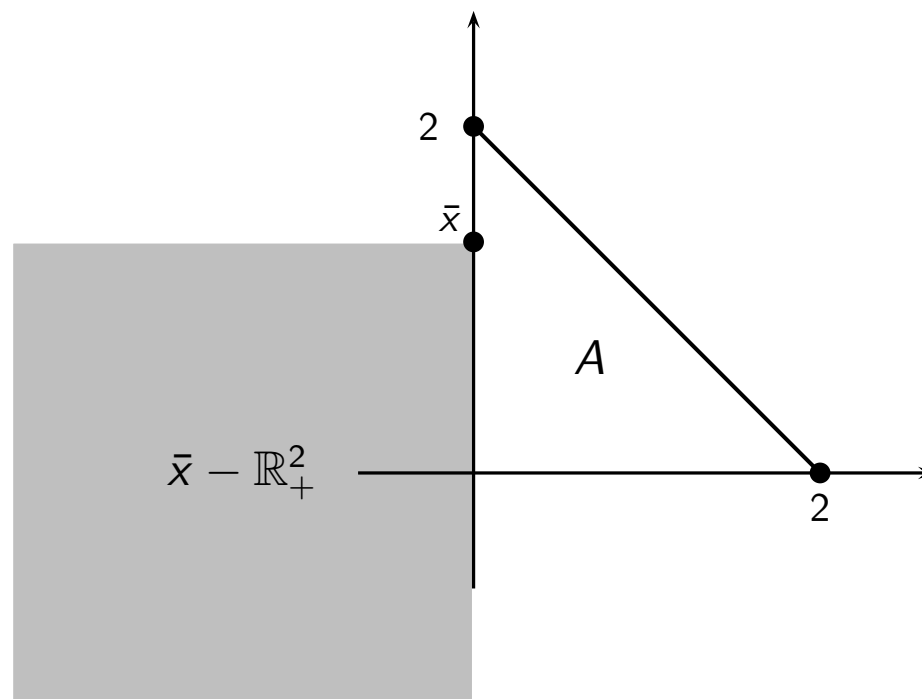
$IMin(A) = Min(A) = \{(0,0)\}, \quad WMin(A) = \{x \in A : \ x_1 = 0 \text{ or } x_2 = 0\}.$

Proposition ●

If $IMin(A) \neq \emptyset$, then $IMin(A) = Min(A) = \{\bar{x}\}$.

Proof. Let $x^1 \in IMin(A)$ and assume that there exists $x^2 \in Min(A)$, with $x^2 \neq x^1$.
We notice that:
- since $x^1 \in IMin(A)$ then $x_1 \leq x_2$ and
- since $x^2 \in Min(A)$, then $x_1 = x_2$.

Example 2

$B = \{x \in \mathbb{R}^2 : \ 0 \leq x_1 \leq 3, \ 0 \leq x_2 \leq 3, \ x_1 + x_2 \geq 2\}$.

- $IMin(B) = \emptyset$,
- $Min(B) = \{x \in B : x_1 + x_2 = 2\}$,
- $WMin(B) = \{x \in B : x_1 = 0 \text{ or } x_2 = 0 \text{ or } x_1 + x_2 = 2\}$.

We have the following fundamental existence result.

Theorem 1

If there exists $\hat{x} \in A$ such that the set $A \cap (\hat{x} - \mathbb{R}^s_+)$ is compact then $Min(A) \neq \emptyset$.

Definition ● ● ●

Given a multiobjective optimization problem

$$\begin{cases} \min\ f(x) = (f_1(x), f_2(x), \ldots, f_s(x)) \\ x \in X \end{cases} \qquad \text{(P)}$$

- $x^* \in X$ is a Pareto ideal minimum of (P) if $f(x^*)$ is a Pareto ideal minimum of $f(X)$, i.e., $f(x) \geq f(x^*)$ for any $x \in X$.

- $x^* \in X$ is a Pareto minimum of (P) if $f(x^*)$ is a Pareto minimum of $f(X)$, i.e., if there is no $x \in X$ such that

$$\begin{array}{ll} f_i(x^*) \geq f_i(x) & \text{for any } i = 1, \ldots, s, \\ f_j(x^*) > f_j(x) & \text{for some } j \in \{1, \ldots, s\}. \end{array}$$

- $x^* \in X$ is a Pareto weak minimum of (P) if $f(x^*)$ is a Pareto weak minimum of $f(X)$, i.e., if there is no $x \in X$ such that

$$f_i(x^*) > f_i(x) \qquad \text{for any } i = 1, \ldots, s.$$

Example 3

$$
\begin{cases}
\min \ (x_1 - x_2, \ -2x_1 + x_2) \\
x_1 \leq 1 \\
-x_1 \leq 0 \\
-x_1 + x_2 \leq 2 \\
2x_1 - x_2 \leq 0
\end{cases}
\tag{P}
$$

The image $f(X) = \{(y_1, y_2) : \ y_1 = x_1 - x_2, \ y_2 = -2x_1 + x_2, \ x \in X\}$.

We obtain $x_1 = -y_1 - y_2$ and $x_2 = -2y_1 - y_2$, hence

$$
f(X) = \{(y_1, y_2) : \ -y_1 - y_2 \leq 1, \ y_1 + y_2 \leq 0, -y_1 \leq 2, \ -y_2 \leq 0\}.
$$

$IMin(f(X)) = \emptyset$. $Min(f(X)) = \{y \in f(X) : \ -y_1 - y_2 = 1\}$, thus

$$
\{\text{minima of (P)}\} = \{x \in X : \ -x_1 + x_2 + 2x_1 - x_2 = 1\} = \{x \in X : \ x_1 = 1\}.
$$

$WMin(f(X)) = \{y \in f(X) : \ -y_1 - y_2 = 1 \text{ or } y_1 = -2 \text{ or } y_2 = 0\}$, thus

$$
\{\text{weak minima of (P)}\} = \{x \in X : \ x_1 = 1 \text{ or } x_1 - x_2 = -2 \text{ or } -2x_1 + x_2 = 0\}.
$$

We explicitly obtain

$$\text{minima of (P)} = (x_1, x_2) : \begin{cases} x_1 = 1 \\ -x_1 \leq 0 \\ -x_1 + x_2 \leq 2 \\ 2x_1 - x_2 \leq 0 \end{cases}$$

Weak minima of (P)=

$$= (x_1, x_2) : \begin{cases} x_1 = 1 \\ -x_1 \leq 0 \\ -x_1 + x_2 \leq 2 \\ 2x_1 - x_2 \leq 0 \end{cases} \cup \begin{cases} x_1 \leq 1 \\ -x_1 \leq 0 \\ -x_1 + x_2 = 2 \\ 2x_1 - x_2 \leq 0 \end{cases} \cup \begin{cases} x_1 \leq 1 \\ -x_1 \leq 0 \\ -x_1 + x_2 \leq 2 \\ 2x_1 - x_2 = 0 \end{cases}$$

Remark

If (P) is a multiobjective linear problem, then $Min(P)$ and $WMin(P)$ are union of faces of the polyhedron X.

Existence results

Theorem 2 ● ● ●

If f_i is continuous for any $i = 1 \ldots, s$ and X is compact, then there exists a minimum of (P).

Proof. It is an immediate consequence of Theorem 1. Indeed, since f is continuous and X is compact, then $f(X)$ is a compact set.

Theorem 3 ● ● ●

If f_i is continuous for any $i = 1 \ldots, s$, X is closed and there exist $v \in \mathbb{R}$ and $j \in \{1, \ldots, s\}$ such that the sublevel set

$$\{x \in X : \ f_j(x) \leq v\}$$

is nonempty and bounded, then there exists a minimum of (P).

Proof. It is a further consequence of Theorem 1. We need to prove that there exists $\hat{y} \in f(X)$ such that

$$S_{\hat{y}} := f(X) \cap (\hat{y} - \mathbb{R}^s_+)$$

is compact, so that $Min(f(X)) \neq \emptyset$.

Set $\hat{y}_j = f_j(x)$ for some x in the level set $\{x \in X : f_j(x) \le v\}$ and $\hat{y}_i = f_i(x)$, for $i \ne j$. Consider the subset B of X such that $f(B) = S_{\hat{y}}$, i.e.,

$$B := \{x \in X : f(x) \in S_{\hat{y}}\} = \{x \in X : f(x) \le \hat{y}\}$$

or, equivalently, the solution set of the system

$$\begin{cases} f_1(x) \le \hat{y}_1 \\ \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ f_s(x) \le \hat{y}_s \\ x \in X \end{cases}$$

By the continuity and compactness assumptions, the closed subset $\{x \in X : f_j(x) \le \hat{y}_j\} \subseteq \{x \in X : f_j(x) \le v\}$ is compact.
Moreover, since f is continuous then B is compact too, being a closed subset of the compact set $\{x \in X : f_j(x) \le \hat{y}_j\}$ and consequently $f(B) = S_{\hat{y}}$ is compact, which completes the proof.

Corollary 1 ●●●

If f_i is continuous for any $i = 1 \ldots, s$, X is closed and f_j is coercive for some $j \in \{1, \ldots, s\}$, then there exists a minimum of (P).

Example 4

Consider the multiobjective problem

$$\begin{cases} \min \ (x_1 + x_2^2, \ (x_1 - 1)^2 + (x_2 - 1)^2) \\ x \in X := \mathbb{R}_+^2 \end{cases}$$

Optimality conditions

Theorem 4

$x^* \in X$ is a minimum of (P) if and only if the auxiliary optimization problem

$$\begin{cases} \max \; \sum_{i=1}^{s} \varepsilon_i \\ f_i(x) + \varepsilon_i \leq f_i(x^*) \qquad \forall \; i = 1, \ldots, s \\ x \in X \\ \varepsilon \geq 0 \end{cases}$$

has optimal value equal to 0.

Proof. Let $(\bar{x}, \bar{\varepsilon})$ be an optimal solution of the auxiliary problem. Assume that x^* is a minimum of (P) and the optimal value $\sum_{i=1}^{s} \bar{\varepsilon}_i > 0$.

Then, there exists $j \in \{1, \ldots, s\}$ such that $\bar{\varepsilon}_j > 0$ and

$$f_i(x^*) \geq f_i(\bar{x}) \qquad \text{for any } i = 1, \ldots, s,$$
$$f_j(x^*) \geq f_j(\bar{x}) + \bar{\varepsilon}_j > f_j(\bar{x}).$$

which contradicts x^* is a minimum of (P).

Conversely, assume that the optimal value $\sum_{i=1}^{s} \bar{\varepsilon}_i = 0$ and x^* is not a minimum of (P).

Then for some $x \in X$

$$f_i(x^*) \geq f_i(x) \qquad \text{for any } i = 1, \ldots, s,$$
$$f_j(x^*) > f_j(x) \qquad \text{for some } j \in \{1, \ldots, s\}.$$

Setting $\varepsilon_j = f_j(x^*) - f_j(x) > 0$, the solution (x, ε), with $\varepsilon_i = 0, i \neq j$ is feasible for the auxiliary problem and $\sum_{i=1}^{s} \bar{\varepsilon}_i > 0$ which contradicts that the optimal value is zero.

Theorem 5

$x^* \in X$ is a weak minimum of (P) if and only if the auxiliary optimization problem

$$\begin{cases} \max\ v \\ v \leq \varepsilon_i & \forall\ i = 1, \ldots, s \\ f_i(x) + \varepsilon_i \leq f_i(x^*) & \forall\ i = 1, \ldots, s \\ x \in X \\ \varepsilon \geq 0 \end{cases}$$

has optimal value equal to 0.

Example 5

Consider the linear multiobjective problem

$$
\begin{cases}
\min \ (x_1 + 2x_2 - 3x_3 \ , \ -x_1 - x_2 - x_3 \ , \ -4x_1 - 2x_2 + x_3) \\
x_1 + x_2 + x_3 \leq 10 \\
x_3 \leq 5 \\
x_1, x_2, x_3 \geq 0
\end{cases}
$$

(a) Check if the point $x^* = (5, 0, 5)$, is a weak minimum by solving the corresponding auxiliary problem.

(b) Check if $x^* = (5, 0, 5)$, is a minimum by solving the corresponding auxiliary problem.

Let us check if $x^* = (5, 0, 5)$ is a weak minimum. Then, $f(x^*) = (-10, -10, -15,)^T$ and the corresponding auxiliary problem is given by

$$
\begin{cases}
\max \ v \\
v \leq \varepsilon_i, \quad i = 1, 2, 3 \\
x_1 + 2x_2 - 3x_3 + \varepsilon_1 \leq -10 \\
-x_1 - x_2 - x_3 + \varepsilon_2 \leq -10 \\
-4x_1 - 2x_2 + x_3 + \varepsilon_3 \leq -15 \\
x_1 + x_2 + x_3 \leq 10 \\
x_3 \leq 5 \\
x_1, x_2, x_3 \geq 0, \ \varepsilon_1, \varepsilon_2, \varepsilon_3 \geq 0
\end{cases}
$$

Let us solve the auxiliary problem by Matlab. In matrix form the problem can be written as:

$$
\begin{cases}
-\min \ -v \\
A \begin{pmatrix} x \\ \varepsilon \\ v \end{pmatrix} \leq b \\
x \geq 0, \ \varepsilon \geq 0
\end{cases}
\tag{1}
$$

where

$$
A = \begin{pmatrix}
0 & 0 & 0 & -1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & -1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & -1 & 1 \\
1 & 2 & -3 & 1 & 0 & 0 & 0 \\
-1 & -1 & -1 & 0 & 1 & 0 & 0 \\
-4 & -2 & 1 & 0 & 0 & 1 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0
\end{pmatrix}
\qquad
b = \begin{pmatrix}
0 \\
0 \\
0 \\
-10 \\
-10 \\
-15 \\
10 \\
5
\end{pmatrix}
$$

object. funct.	c=[0, 0, 0, 0, 0, 0, -1]'

constr.	A=[0 0 0 -1 0 0 1; 0 0 0 0 -1 0 1 ; 0 0 0 0 0 -1 1; 1 2 -3 1 0 0 0 ; -1 -1 -1 0 1 0 0; -4 -2 1 0 0 1 0; 1 1 1 0 0 0 0; 0 0 1 0 0 0 0]
	b= [0;0;0;-10; -10;-15;10;5]
	Aeq=[ ];
	beq=[ ];
	lb= [zeros(6,1); -Inf]
	ub= [ ];

Solut. Command	[x,fval]=linprog(c, A, b,[ ],[ ],lb,ub)

Solution

Optimal solution	(5,0,5,0,0,0,0)
Optimal value	0

Let us check if $x^* = (5, 0, 5)$ is a minimum. The corresponding auxiliary problem is:

$$\begin{cases} \max \ \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \\ x_1 + 2x_2 - 3x_3 + \varepsilon_1 \leq -10 \\ -x_1 - x_2 - x_3 + \varepsilon_2 \leq -10 \\ -4x_1 - 2x_2 + x_3 + \varepsilon_3 \leq -15 \\ x_1 + x_2 + x_3 \leq 10 \\ x_3 \leq 5 \\ x_1, x_2, x_3 \geq 0, \ \varepsilon_1, \varepsilon_2, \varepsilon_3 \geq 0 \end{cases}$$

In matrix form the problem can be written as:

$$\begin{cases} -\min \ -\varepsilon_1 - \varepsilon_2 - \varepsilon_3 \\ A \begin{pmatrix} x \\ \varepsilon \end{pmatrix} \leq b \\ x \geq 0, \ \varepsilon \geq 0 \end{cases} \tag{2}$$

where

$$A = \begin{pmatrix} 1 & 2 & -3 & 1 & 0 & 0 \\ -1 & -1 & -1 & 0 & 1 & 0 \\ -4 & -2 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \qquad b = \begin{pmatrix} -10 \\ -10 \\ -15 \\ 10 \\ 5 \end{pmatrix}$$

object. funct.	`c=[0, 0, 0, -1, -1, -1]'`

constr.	`A=[1 2 -3 1 0 0 ; -1 -1 -1 0 1 0 ; -4 -2 1 0 0 1 ; 1 1 1 0 0 0; 0 0 1 0 0 0]`
	`b= [-10; -10;-15;10;5]`
	`Aeq=[ ];`
	`beq=[ ];`
	`lb= zeros(6,1)`
	`ub= [ ];`

Solut. Command	`[x,fval]=linprog(c, A, b,[ ],[ ],lb,ub)`

Solution

Optimal solution	(5,0,5,0,0,0)
Optimal value	0

Exercise

Consider the linear multiobjective problem defined in Example 5,

$$
\begin{cases}
\min \left(x_1 + 2x_2 - 3x_3 \ , \ -x_1 - x_2 - x_3 \ , \ -4x_1 - 2x_2 + x_3\right) \\
x_1 + x_2 + x_3 \leq 10 \\
x_3 \leq 5 \\
x_1, x_2, x_3 \geq 0
\end{cases}
$$

- Prove that a Pareto minimum point exists;
- Check if the point $x^* = (3, 3, 4)$, is a weak minimum or a minimum by solving the corresponding auxiliary problems.

Consider an unconstrained multiobjective problem

$$\begin{cases} \min \ f(x) = (f_1(x), f_2(x), \ldots, f_s(x)) \\ x \in \mathbb{R}^n \end{cases} \qquad (P_u)$$

where f_i is continuously differentiable for any $i = 1, \ldots, s$.

Remark.

If x^* is a weak minimum of (P_u), then the system

$$\begin{cases} \nabla f_i(x^*)^\top d < 0, \quad i = 1, .., s, \\ d \in \mathbb{R}^n \end{cases} \qquad (S1)$$

is impossible.

Proposition 2 (Necessary optimality condition)

If x^* is a weak minimum of (P_u), then there exists $\theta^* \in \mathbb{R}^s$ such that (x^*, θ^*) is a solution of the system

$$\begin{cases} \sum\limits_{i=1}^{s} \theta_i \, \nabla f_i(x) = 0 \\[2mm] \theta \geq 0, \quad \sum\limits_{i=1}^{s} \theta_i = 1, \\[2mm] x \in \mathbb{R}^n \end{cases} \qquad \text{(S)}$$

Proof. By the previous remark the system (S1) is impossible. Let $\Gamma := \{ u \in \mathbb{R}^s : u_i = \nabla f_i(x^*)^\top d, \ d \in \mathbb{R}^n, \ i = 1, ..., s \}$. Then the impossibility of (S1) is equivalent to:

$$\Gamma \cap (-int(\mathbb{R}_+^s)) = \emptyset.$$

Since Γ and $-int(\mathbb{R}_+^s)$ are disjoint convex sets then there exists an hyperplane of equation $\langle \theta, u \rangle = 0$, $\theta \in \mathbb{R}_+^s$, $\theta \neq 0$, which separates them, i.e.,

$$\langle \theta, u \rangle \geq 0, \quad \forall u \in \Gamma, \quad \langle \theta, u \rangle \leq 0, \quad \forall u \in (-int(\mathbb{R}_+^s)).$$

The first inequality can be written as

$$\sum_{i=1}^{s} \theta_i \nabla f_i(x^*)^T d \geq 0, \quad \forall d \in \mathbb{R}^n.$$

Since v is arbitrary, we have:

$$\sum_{i=1}^{s} \theta_i \nabla f_i(x^*) = 0$$

and setting

$$\theta^* = \frac{\theta}{\sum_{i=1}^{s} \theta_i}$$

we obtain that system (S) is fulfilled.

Proposition 3 (Sufficient optimality condition)

Assume that the problem (P_u) is convex, i.e., f_i is convex for any $i = 1, \ldots, s$, and (x^*, θ^*) is a solution of the system (S). Then:

- x^* is a weak minimum of (P_u).

- If, additionally, $\theta^* > 0$, then x^* is a minimum of (P_u).

Proof. Consider the function $L(\theta, x) := \sum\limits_{i=1}^{s} \theta_i \, f_i(x)$, with $\theta \in \mathbb{R}_+^s$.

Since f is convex then $L(\theta, \cdot)$ is convex, and

$$\sum_{i=1}^{s} \theta_i^* \, \nabla f_i(x^*) = 0 \quad \Longrightarrow \quad L(\theta^*, x^*) \leq L(\theta^*, x), \quad \forall x \in \mathbb{R}^n,$$

i.e.,

$$\sum_{i=1}^{s} \theta_i^* (f_i(x^*) - f_i(x)) \leq 0, \quad \forall x \in \mathbb{R}^n. \tag{3}$$

As, $\theta^* \in \mathbb{R}_+^s$ and $\theta^* \neq 0$, the system

$$f(x^*) - f(x) > 0, \quad x \in \mathbb{R}^n,$$

is impossible,

in fact, if not, we would have:

$$\sum_{i=1}^{s} \theta_i^*(f_i(x^*) - f_i(x)) > 0, \quad \text{for some } x \in \mathbb{R}^n,$$

which contradicts (3). Therefore, x^* is a weak minimum of (P_u).

Similarly, we can prove that, if, additionally, $\theta^* > 0$, then x^* is a minimum of (P_u). Indeed, $x^* \in X$ is a minimum of (P_u) if the following system is impossible:

$$\begin{aligned} f_i(x^*) - f_i(x) \geq 0 \qquad & \text{for any } i = 1, \ldots, s, \quad i \neq j \\ f_j(x^*) - f_j(x) > 0 \qquad & \text{for some } j \in \{1, \ldots, s\}. \end{aligned}$$

By contradiction, assume that it is possible for some x. Since $\theta^* > 0$, then multiplying the inequality i by θ_i^* and summing all the inequalities we obtain:

$$\sum_{i=1}^{s} \theta_i^*(f_i(x^*) - f_i(x)) > 0$$

which contradicts (3). Hence, $x^* \in X$ is a minimum of (P_u).

Example 6

Let us determine the set of weak minima of the following nonlinear multiobjective problem (P_u) exploiting the first-order optimality conditions.

$$\begin{cases} \min \ (x_1^2 + x_2^2, \ (x_1 - 1)^2 + (x_2 - 1)^2) \\ x \in \mathbb{R}^2 \end{cases}$$

We preliminarly note the given problem is convex and differentiable: then system (S) provided a necessary and sufficient condition for a weak minimum.
In this case system (S) becomes:

$$\begin{cases} \theta_1 (2x_1) + \theta_2 2(x_1 - 1) = 0 \\ \theta_1 (2x_2) + \theta_2 2(x_2 - 1) = 0 \\ \theta_1, \theta_2 \geq 0, \ \theta_1 + \theta_2 = 1 \end{cases}$$

i.e.

$$\begin{cases} x_1(\theta_1 + \theta_2) - \theta_2 = 0 \\ x_2(\theta_1 + \theta_2) - \theta_2 = 0 \\ \theta_1, \theta_2 \geq 0, \ \theta_1 + \theta_2 = 1 \end{cases} \implies \begin{cases} x_1 = \theta_2 \\ x_2 = \theta_2 \\ 0 \leq \theta_2 \leq 1 \end{cases}$$

Therefore, the set of weak minima is given by

$$WMin(P_u) = \{(x_1, x_2) : x_1 = x_2, \ 0 \leq x_1 \leq 1\}$$

Exercise

Find the set of minima of the problem (P_u) defined in Example 6.

Notice that, by Proposition 3

$$\{(x_1, x_2) : x_1 = x_2, \ 0 < x_1 < 1\} \subseteq Min(P_u) \subseteq WMin(P_u)$$

We need only to check if the points $(0, 0)$ and $(1, 1)$ are minima for (P_u).

This can be done directly exploiting the definition of a minimum or by means of Theorem 4.

Consider a constrained multiobjective problem

$$\begin{cases} \min \ f(x) = (f_1(x), f_2(x), \ldots, f_s(x)) \\ x \in X := \{x \in \mathbb{R}^n : g_j(x) \leq 0, \ j = 1, \ldots, m, \ h_k(x) = 0, \ k = 1, \ldots, p\} \end{cases} \quad \text{(P)}$$

where f_i, g_j and h_k are continuously differentiable for any i, j, k.

We briefly recall the Abadie constraint qualification introduced in the analysis of scalar optimization problems.

Recall that:

- The *Tangent cone* at $x^* \in X$, is defined by

$$T_X(x^*) = \left\{ d \in \mathbb{R}^n : \exists \ \{z_k\} \subset X, \ \exists \ \{t_k\} > 0, \ z_k \to x^*, \ t_k \to 0, \ \lim_{k \to \infty} \frac{z_k - x^*}{t_k} = d \right\}$$

- $\mathcal{A}(x^*) = \{j : \ g_j(x^*) = 0\}$ denotes the set of inequality constraints which are active at $x^* \in X$.

- The set

$$D(x^*) = \left\{ d \in \mathbb{R}^n : \begin{array}{ll} d^{\mathsf{T}} \nabla g_j(x^*) \leq 0 & \forall \ j \in \mathcal{A}(x^*), \\ d^{\mathsf{T}} \nabla h_k(x^*) = 0 & \forall \ k = 1, \ldots, p \end{array} \right\}$$

is the *first-order feasible direction cone* at $x^* \in X$.

Definition – Abadie constraint qualification (ACQ)

We say that the Abadie constraint qualification (ACQ) holds at a point $x^* \in X$, if $T_X(x^*) = D(x^*)$.

Theorem (Sufficient conditions for ACQ)

a) (*Affine constraints*)
   If g_j and h_k are affine for all $j = 1, \ldots, m$ and $k = 1, \ldots, p$, then ACQ holds at any $x \in X$.

b) (*Slater condition for convex problems*)
   If g_j are convex for all $j = 1, \ldots, m$, h_k are affine for all $k = 1, \ldots, p$ and there exists $\bar{x} \in X$ s.t. $g(\bar{x}) < 0$ and $h(\bar{x}) = 0$, then ACQ holds at any $x \in X$.

c) (*Linear independence of the gradients of active constraints*)
   If $x^* \in X$ and the vectors

$$\begin{cases} \nabla g_j(x^*) & \text{for } j \in \mathcal{A}(x^*), \\ \nabla h_k(x^*) & \text{for } k = 1, \ldots, p \end{cases}$$

   are linearly independent, then ACQ holds at x^*.

Theorem (KKT necessary optimality conditions)

If x^* is a weak minimum of (P) and ACQ holds at x^*, then there exist $\theta^* \in \mathbb{R}^s$, $\lambda^* \in \mathbb{R}^m$ and $\mu^* \in \mathbb{R}^p$ such that $(x^*, \theta^*, \lambda^*, \mu^*)$ solves the KKT system

$$
\begin{cases}
\displaystyle\sum_{i=1}^{s} \theta_i \nabla f_i(x) + \sum_{j=1}^{m} \lambda_j \nabla g_j(x) + \sum_{k=1}^{p} \mu_k \nabla h_k(x) = 0 \\
\theta \geq 0, \quad \displaystyle\sum_{i=1}^{s} \theta_i = 1 \\
\lambda \geq 0 \\
\lambda_j \, g_j(x) = 0 \qquad \forall \, j = 1, \ldots, m \\
g(x) \leq 0, \ h(x) = 0
\end{cases}
\tag{4}
$$

Remark

Notice that for an unconstrained problem, i.e. $X = \mathbb{R}^n$, then the KKT system (4) reduces to system (S).

Necessary optimality conditions

Theorem

If x^* is a weak minimum of (P), then the system

$$\begin{cases} \nabla f_i(x^*)^\mathsf{T} d < 0, i = 1, ..., s \\ \quad d \in T_X(x^*). \end{cases}$$

has no solutions.

Proof. By contradiction, assume that there exists $d \in T_X(x^*)$ s.t. $\nabla f_i(x^*)^\mathsf{T} d < 0, i = 1, .., s$. Take the sequences $\{z_k\} \subseteq X$ and $\{t_k\} > 0$ s.t. $\lim_{k \to \infty} (z_k - x^*)/t_k = d$. Then $z_k = x^* + t_k d + o(t_k)$, where $o(t_k)/t_k \to 0$. Let $i \in 1, ..., s$. The first order approximation of f_i gives

$$f_i(z_k) = f_i(x^*) + t_k \nabla f_i(x^*)^\mathsf{T} d + o(t_k),$$

thus there is $\bar{k} \in \mathbb{N}$ s.t.

$$\frac{f_i(z_k) - f_i(x^*)}{t_k} = \nabla f_i(x^*)^\mathsf{T} d + \frac{o(t_k)}{t_k} < 0 \qquad \forall\, k > \bar{k}, \; \forall i = 1, .., s.$$

i.e. $f_i(z_k) < f_i(x^*)$ for all $k > \bar{k}$, and every $i = 1, .., s$, which is impossible because x^* is a weak minimum of (P). $\square$

Corollary

If x^* is a weak minimum of (P) and ACQ holds at x^*, then the system

$$\begin{cases} v^\mathsf{T} \nabla f_i(x^*) < 0, i = 1, ..., s \\ v^\mathsf{T} \nabla g_j(x^*) \leq 0, \ j \in \mathcal{A}(x^*), \\ v^\mathsf{T} \nabla h_k(x^*) = 0, \ k = 1, \ldots, p, \\ v \in \mathbb{R}^n \end{cases} \tag{S1}$$

has no solutions.

Proof. It is enough to observe that, if ACQ holds at x^* then

$$T_X(x^*) = D(x^*) = \left\{ v \in \mathbb{R}^n : \begin{array}{ll} v^\mathsf{T} \nabla g_j(x^*) \leq 0 & \forall \ j \in \mathcal{A}(x^*), \\ v^\mathsf{T} \nabla h_k(x^*) = 0 & \forall \ k = 1, \ldots, p \end{array} \right\}$$

□

Finally, by means of a Theorem of the alternative (similarly to the proof of Proposition 2), it is possible to show that the impossibility of system (S1) implies that the system KKT is possible, i.e., there exist $\theta^* \in \mathbb{R}^s$, $\lambda^* \in \mathbb{R}^m$ and $\mu^* \in \mathbb{R}^p$ such that $(x^*, \theta^*, \lambda^*, \mu^*)$ solves system (4).

Sufficient optimality conditions

If (P) is a convex problem then the KKT conditions are also sufficient for optimality.

Theorem

Assume that f_i and g_j are convex, $i = 1, .., s$, $j = 1, .., m$, h_k are affine $k = 1, .., p$.

- If $(x^*, \theta^*, \lambda^*, \mu^*)$ solves the KKT system, then x^* is a weak minimum of (P).
- If $(x^*, \theta^*, \lambda^*, \mu^*)$ solves the KKT system with $\theta^* > 0$, then x^* is a minimum of (P).

Proposition 4

If x^* is the unique global minimum of the function f_k on the set X for some $k \in \{1, ..., s\}$, then x^* is a minimum of (P).

Proof. It is enough to notice that $f_k(x^*) < f_k(x), \forall x \in X, \; x \neq x^*$, and that the previous inequality implies the impossibility of the system:

$$\begin{aligned} &f_i(x^*) \geq f_i(x) &&\text{for any } i = 1, \ldots, s, \\ &f_j(x^*) > f_j(x) &&\text{for some } j \in \{1, \ldots, s\} \\ &x \in X \end{aligned}$$

i.e., x^* is a minimum of (P).

Example 7

Consider the nonlinear multiobjective problem

$$\begin{cases} \min\ (x_1 + x_2,\ -x_1 + x_2) \\ x_1^2 + x_2^2 - 1 \le 0 \end{cases}$$

(a) Find the set of weak minima by solving the KKT system.

(b) Find the set of minima.

(a) We preliminarly note that the given problem is convex and differentiable and ACQ holds at any $x \in X$; then the KKT system provides a necessary and sufficient condition for a weak minimum. KKT system is given by:

$$\begin{cases} \theta_1 - \theta_2 + 2\lambda x_1 = 0 \\ \theta_1 + \theta_2 + 2\lambda x_2 = 0 \\ \lambda(x_1^2 + x_2^2 - 1) = 0 \\ \theta_1, \theta_2 \ge 0,\ \theta_1 + \theta_2 = 1,\ \lambda \ge 0 \\ x_1^2 + x_2^2 - 1 \le 0 \end{cases}$$

Consider the case $\lambda = 0$, then the system becomes:

$$\begin{cases} \theta_1 - \theta_2 = 0 \\ \theta_1 + \theta_2 = 0 \\ \theta_1, \theta_2 \geq 0, \ \theta_1 + \theta_2 = 1, \ \lambda \geq 0 \\ x_1^2 + x_2^2 - 1 \leq 0 \end{cases}$$

which is clearly impossible, since the first two equations imply $\theta_1 = \theta_2 = 0$, which contradicts $\theta_1 + \theta_2 = 1$.

Then $\lambda \neq 0$. The system becomes:

$$\begin{cases} \theta_1 - \theta_2 + 2\lambda x_1 = 0 \\ \theta_1 + \theta_2 + 2\lambda x_2 = 0 \\ x_1^2 + x_2^2 - 1 = 0 \\ \theta_1, \theta_2 \geq 0, \ \theta_1 + \theta_2 = 1, \ \lambda \geq 0 \end{cases}$$

Then

$$x_1 = \frac{\theta_2 - \theta_1}{2\lambda} = \frac{1 - 2\theta_1}{2\lambda}$$

$$x_2 = -\frac{\theta_1 + \theta_2}{2\lambda} = -\frac{1}{2\lambda}$$

Substituting x_1 and x_2 in the third equation yields:

$$(1 - 2\theta_1)^2 + 1 = 4\lambda^2$$

so that

$$\lambda = \frac{1}{2}\sqrt{(1 - 2\theta_1)^2 + 1}, \quad 0 \le \theta_1 \le 1$$

We obtain the following solutions.

Weak minima $=$

$$\left\{ (x_1, x_2) : x_1 = \frac{1 - 2\theta_1}{\sqrt{(1 - 2\theta_1)^2 + 1}}, \ x_2 = -\frac{1}{\sqrt{(1 - 2\theta_1)^2 + 1}}, \quad 0 \le \theta_1 \le 1 \right\}.$$

(b) The subset of weak minima such that $0 < \theta_1 < 1$ is also a set of minima, since $\theta_1, \theta_2 > 0$.

We need to investigate the cases $\theta_1 = 0$, $\theta_1 = 1$ which correspond to the points

$$\bar{x} = (\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}), \quad \hat{x} = (-\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}),$$

We note that in these cases the KKT conditions collapse to the necessary and sufficient optimality conditions for the problems

$$\min_{x \in X}(-x_1 + x_2) \qquad \min_{x \in X}(x_1 + x_2)$$

so that $\bar{x}$ is the unique global minimum point for the first problem and $\hat{x}$ is the unique global minimum point for the second one.

By Proposition 4, we obtain that $\bar{x}$ and $\hat{x}$ are also minima for the given problem.

Consider the vector optimization problem

$$\begin{cases} \min \quad f(x) = (f_1(x), .., f_s(x)) \\ \\ x \in X \end{cases} \tag{P}$$

with the geometric constraint $x \in X$ and define a vector of weights associated to the objectives:

$$\alpha = (\alpha_1, \ldots, \alpha_s) \geq 0 \quad \text{such that} \quad \sum_{i=1}^{s} \alpha_i = 1$$

We associate with (P) the following scalar optimization problem

$$\begin{cases} \min \; \sum_{i=1}^{s} \alpha_i f_i(x) \\ x \in X \end{cases} \tag{P_α}$$

Let S_α be the set of optimal solutions of (P_α).

- $\bigcup_{\alpha \geq 0} S_\alpha \subseteq \{\text{weak minima of (P)}\}$

  α è un vettore!

- $\bigcup_{\alpha > 0} S_\alpha \subseteq \{\text{minima of (P)}\}$

Proof. Consider the function $\psi(\alpha, x) = \sum_{i=1}^{s} \alpha_i f_i(x)$ and let $x^* \in S_\alpha$. Then,

$$\psi(\alpha, x^*) \leq \psi(\alpha, x), \quad \forall x \in X,$$

i.e.,

$$\sum_{i=1}^{s} \alpha_i (f_i(x^*) - f_i(x)) \leq 0, \quad \forall x \in X.$$

As, $\alpha \in \mathbb{R}^s_+$, $\alpha \neq 0$, the system

$$f_i(x^*) - f_i(x) > 0, \quad i = 1, .., s, \quad x \in X,$$

is impossible and x^* is a weak minimum of (P).

Similarly, we can prove that if, additionally, $\alpha > 0$, then x^* is a minimum of (P).

Solving (P_α) for any possible choice of α does not allow finding all the minima and weak minima.

Example 8

Consider the problem
$$\begin{cases} \min \ (x_1, \ x_2) \\ x_1^2 + x_2^2 - 4 \leq 0 \\ -x_1^2 - x_2^2 + 1 \leq 0 \\ x_1 \geq 0, \ x_2 \geq 0 \end{cases}$$

$$\bigcup_{\alpha \geq 0} S_\alpha = \{(0, x_2) : \ x_2 \in [1, 2]\} \cup \{(x_1, 0) : \ x_1 \in [1, 2]\},$$

while

$$\{\text{weak minima of } (P)\} =$$
$$\{(0, x_2) : \ x_2 \in [1, 2]\} \cup \{(x_1, 0) : \ x_1 \in [1, 2]\} \cup \{x \in \mathbb{R}_+^2 : \ x_1^2 + x_2^2 = 1\}.$$

Furthermore,

$$\bigcup_{\alpha > 0} S_\alpha = \{(0, 1), (1, 0)\},$$

while

$$\{\text{minima of } (P)\} = \{x \in \mathbb{R}_+^2 : \ x_1^2 + x_2^2 = 1\}.$$

Scalarization method: the convex case

Theorem ● ● ●

Assume that X is a convex set and that f_i are convex on X for $i = 1, .., s$.
Then {weak minima of (P)} $= \bigcup_{\alpha \geq 0} S_\alpha$

Proof. By the previous theorem, we have only to prove the inclusion

$$\bigcup_{\alpha \geq 0} S_\alpha \supseteq \{\text{weak minima of (P)}\}.$$

Let x^* be a weak minimum of (P). Then, the system

$$f(x^*) - f(x) > 0, \quad x \in X,$$

is impossible, or ,equivalently,

$$(f(x^*) - f(X)) \cap int(\mathbb{R}^s_+) = \emptyset.$$

The previous condition can be proved to be equivalent to the following one:

$$(f(x^*) - (f(X) + \mathbb{R}^s_+)) \cap int(\mathbb{R}^s_+) = \emptyset.$$

Since f is convex and X is convex, then the set $f(X) + \mathbb{R}^s_+$ is proved to be convex and consequently, the set $\Gamma := f(x^*) - (f(X) + \mathbb{R}^s_+)$ is convex.

Since Γ and $int(\mathbb{R}_+^s)$ are disjoint convex sets then there exists an hyperplane of equation $\langle \theta, u \rangle = 0$, $\theta \in \mathbb{R}_+^s$, $\theta \neq 0$, which separates them, i.e.,

$$\langle \theta, u \rangle \leq 0, \quad \forall u \in \Gamma, \quad \langle \theta, u \rangle > 0, \quad \forall u \in int(\mathbb{R}_+^s).$$

In particular, the first inequality implies that

$$\langle \theta, f(x^*) - f(x) \rangle \leq 0, \quad \forall x \in X$$

and setting

$$\alpha = \frac{\theta}{\sum_{i=1}^{s} \theta_i}$$

we obtain that $x^* \in S_\alpha$.

Theorem ● ● ●

Let (P) be linear, i.e., f_i are linear for $i = 1, .., s$ and X is a polyhedron. Then,

- {weak minima of (P)} $= \bigcup\limits_{\alpha \geq 0} S_\alpha$;

- {minima of (P)} $= \bigcup\limits_{\alpha > 0} S_\alpha$.

Proof. The first assertion is a consequence of the previous theorem.

We omit the proof of the second assertion.

Next example shows that the second assertion of the previous theorem does not hold for a nonlinear convex problem.

Example 9

Consider the non linear convex multiobjective problem

$$\begin{cases} \min (x_1 \, , \, x_1^2 + x_2^2 - 4x_1) \\ (x_1, x_2) \in \mathbb{R}^2 \end{cases}$$

The scalarized problem P_α is given by:

$$\begin{cases} \min \ \alpha_1 x_1 + (1 - \alpha_1)(x_1^2 + x_2^2 - 4x_1) =: \psi_\alpha(x) \\ (x_1, x_2) \in \mathbb{R}^2 \end{cases}$$

where $0 \leq \alpha_1 \leq 1$.

ψ_α is convex so that the optimal points coincide with the solutions of the system

$$\nabla \psi_\alpha(x_1, x_2) = \begin{pmatrix} 2x_1(1 - \alpha_1) - 4 + 5\alpha_1 \\ 2x_2(1 - \alpha_1) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

i.e.,

$$(x_1, x_2) = \left(\frac{4 - 5\alpha_1}{2(1 - \alpha_1)}, 0 \right), \quad 0 \leq \alpha_1 < 1$$

We obtain:

- the set of weak minima of (P) $= \{(x_1, x_2) : x_1 \leq 2, x_2 = 0\}$
- the set of minima of (P) $\supseteq \{(x_1, x_2) : x_1 < 2, x_2 = 0\}$ $\quad (0 < \alpha_1 < 1)$

It remains to consider the case where $\alpha_1 = 0$ which corresponds to the point $(2, 0)$.

Notice that $(2, 0)$ is the unique minimum point of the function $f_2(x_1, x_2) = x_1^2 + x_2^2 - 4x_1$. By the previous Proposition 4 we obtain that it is a minimum of (P).

Exercise 1

Consider the linear multiobjective problem

$$\begin{cases} \min \, (x_1 - x_2 \, , \, x_1 + x_2) \\ -2\,x_1 + x_2 \le 0 \\ -x_1 - x_2 \le 0 \\ 5\,x_1 - x_2 \le 6 \end{cases}$$

Find the set of minima and weak minima by means of the scalarization method.

The scalarized problem P_α is given by

$$\begin{cases} \min \, \alpha_1(x_1 - x_2) + \alpha_2(x_1 + x_2) \\ -2\,x_1 + x_2 \le 0 \\ -x_1 - x_2 \le 0 \\ 5\,x_1 - x_2 \le 6 \end{cases}$$

Recalling that $\alpha_1 + \alpha_2 = 1$, by eliminating α_2 we obtain that P_α is equivalent to the problem (P_{α_1})

$$\begin{cases} \min\ \alpha_1(x_1 - x_2) + (1 - \alpha_1)(x_1 + x_2) = x_1 + (1 - 2\alpha_1)x_2 \\ -2\,x_1 + x_2 \leq 0 \\ -x_1 - x_2 \leq 0 \\ 5\,x_1 - x_2 \leq 6 \end{cases}$$

where $0 \leq \alpha_1 \leq 1$.

The previous problem can be solved by the Matlab function "linprog".

For $0 < \alpha_1 < 1$, we have that the optimal solutions of P_{α_1} are the minima of the given problem.

Recall that $\bigcup_{0 < \alpha_1 < 1} Sol(P_{\alpha_1})$ is given by the union of faces of the polyhedron X.

Matlab solution

```
C = [1 -1; 1 1] ;

A =[ -2 1; -1 -1; 5 -1 ];

b = [0 0 6]';
```

% solve the scalarized problem with 0 < alfa1 < 1

```
MINIMA=[ ]; % First column: value of alfa1

LAMBDA=[ ]; % First column: value of alfa1

for alfa1 = 0.01 : 0.01 : 0.99
[x,fval,exitflag,output,lambda] = linprog(alfa1*C(1,:)+(1-alfa1)*C(2,:),A,b) ;
MINIMA=[MINIMA; alfa1, x'];
LAMBDA=[LAMBDA;alfa1,lambda.ineqlin'];
end
% solve the scalarized problem with alfa1 = 0 and alfa1 = 1
alfa1 = 0;
[xalfa0,f0,exitflag,output,lambda0] = linprog(alfa1*C(1,:)+(1-alfa1)*C(2,:),A,b) ;

alfa1 = 1;
[xalfa1,f1,exitflag,output,lambda1] = linprog(alfa1*C(1,:)+(1-alfa1)*C(2,:),A,b) ;
```

For $0 < \alpha_1 < 0.75$ we obtain the optimal solution of P_{α_1}: $x^* = (0,0)$, with nondegenerate dual solution λ^*, so that x^* is the unique optimal solution of P_{α_1}.

For $\alpha_1 = 0.75$, the optimal solution of P_{α_1} is $x^* = (0,0)$ with $\lambda^* = (0.5, 0, 0)$, which is degenerate (i.e., the number of strictly positive components of λ^* is less than the dimension n of the space where the problem is defined, in this case $n = 2$). .

By means of the KKT conditions we have that all the solutions of P_{α_1} solve the system

$$\begin{cases} \lambda_j^*(A_j x - b_j) = 0, \ j = 1, ..., m \\ Ax \leq b \end{cases}$$

where A_j denotes the $j - th$ row of A and λ^* is any dual solution of P_{α_1} which is given by linprog in the vector "lambda.ineqlin".

For $0.75 < \alpha_1 < 1$ we obtain the optimal solution of P_{α_1}: $x^* = (2,4)$, with nondegenerate dual solution λ^*, so that x^* is the unique optimal solution of P_{α_1}. We obtain

$$\text{minima of (P)} = \bigcup_{0 < \alpha_1 < 1} Sol(P_{\alpha_1}) = (x_1, x_2) : \begin{cases} -2\,x_1 + x_2 = 0 \\ -x_1 - x_2 \leq 0 \\ 5\,x_1 - x_2 \leq 6 \end{cases}$$

Considering the further particular cases $\alpha_1 = 0$ and $\alpha_1 = 1$ we have:

- For $\alpha_1 = 0$, the optimal solution of P_{α_1} is $x^* = (0,0)$ with $\lambda^* = (0,1,0)$, which is degenerate.

- For $\alpha_1 = 1$, the optimal solution of P_{α_1} is $x^* = (2,4)$ with $\lambda^* = (1.3333, 0, 0.3333)$, which is non degenerate.

We obtain that:

Weak minima of (P)$= \bigcup_{0 \leq \alpha_1 \leq 1} Sol(P_{\alpha_1})$

$$= (x_1, x_2) : \left\{ \begin{array}{l} -2\,x_1 + x_2 = 0 \\ -x_1 - x_2 \leq 0 \\ 5\,x_1 - x_2 \leq 6 \end{array} \right. \cup \left\{ \begin{array}{l} -2\,x_1 + x_2 \leq 0 \\ -x_1 - x_2 = 0 \\ 5\,x_1 - x_2 \leq 6 \end{array} \right.$$

The next sufficient condition is useful for detecting minima of (P) by means of a scalarized problem.

Proposition

If x^* is the unique global minimum of P_α for some α, then x^* is a minimum of (P).

Proof. Consider the function $L(\alpha, x) = \sum_{i=1}^{s} \alpha_i f_i(x)$ and let $x^* \in S_\alpha$. Then,

$$\sum_{i=1}^{s} \alpha_i (f(x^*) - f_i(x))\rangle < 0, \quad \forall x \in X, \quad x \neq x^*.$$

Ab absurdo, assume that x^* is not a minimum of (P). Then, the system:

$$
\begin{aligned}
f_i(x^*) &\geq f_i(x) && \text{for any } i = 1, \dots, s, \ i \neq j \\
f_j(x^*) &> f_j(x) && \text{for some } j \in \{1, \dots, s\} \\
x &\in X
\end{aligned}
$$

admits a solution $\hat{x} \neq x^*$.
Multiplying the i-th inequality by α_i and summing all the inequalities we obtain:

$$\sum_{i=1}^{s} \alpha_i f_i(x^*) \geq \sum_{i=1}^{s} \alpha_i f_i(\hat{x})$$

which contradicts that $L(\alpha, x^*) < L(\alpha, x), \quad \forall x \in X, \quad x \neq x^*$.
Therefore, x^* is a minimum of (P).

The previous proposition also allows us to obtain existence results for multiobjective optimization problems.

Consider the nonlinear multiobjective problem (P)

$$\begin{cases} \min \ (x_1 \ , \ x_1^2 + x_2^2 - 2x_1) \\ -x_1 \leq 0 \\ x_1 + x_2 \leq 2 \end{cases}$$

a) Does a minimum point exists?

b) Find the set of weak minima by means of the scalarization method.

a) Consider the scalarized problem (P_{α_1}) where $\alpha_1 \neq 1$, i.e.

$$\begin{cases} \min \ \alpha_1 x_1 + (1 - \alpha_1)(x_1^2 + x_2^2 - 2x_1) =: \psi_{\alpha_1}(x) \\ -x_1 \leq 0 \\ x_1 + x_2 \leq 2 \end{cases}$$

with $0 \leq \alpha_1 < 1$.
ψ_{α_1} is strongly convex so that P_{α_1} admits a unique optimal solution which is a minimum of (P).

Exercise 3

Consider the nonlinear multiobjective problem

$$
\begin{cases}
\min \ (x_1^2 + x_2^2 + 2x_1 - 4x_2 \ , \ x_1^2 + x_2^2 - 6x_1 - 4x_2) \\
-x_2 \le 0 \\
-2x_1 + x_2 \le 0 \\
2x_1 + x_2 \le 4
\end{cases}
$$

Find the set of minima and weak minima by means of the scalarization method.

The scalarized problem P_α is

$$
\begin{cases}
\min \ (\alpha_1(x_1^2 + x_2^2 + 2x_1 - 4x_2) + \alpha_2(x_1^2 + x_2^2 - 6x_1 - 4x_2)) \\
-x_2 \le 0 \\
-2x_1 + x_2 \le 0 \\
2x_1 + x_2 \le 4
\end{cases}
$$

We note that the feasible set X is convex and the objective function of P_α is strongly convex for any $\alpha = (\alpha_1, \alpha_2) \in \mathbb{R}^2_+$ with $\alpha_1 + \alpha_2 = 1$ so that the set of minima and weak minima coincide.

Let us express the problem in matrix form.

The objectives are given by: $f_1(x_1, x_2) = \frac{1}{2}x^T Q_1 x + c1^T x$ where

$$Q_1 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \quad c1^T = (2, -4)$$

$f_2(x_1, x_2) = \frac{1}{2}x^T Q_2 x + c2^T x$ where

$$Q_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \quad c2^T = (-6, -4)$$

The constraints are given by $Ax \leq b$ where

$$A = \begin{pmatrix} 0 & -1 \\ -2 & 1 \\ 2 & 1 \end{pmatrix} \quad b = (0, 0, 4)^T$$

The given problem becomes:

$$\begin{cases} \min \left(\frac{1}{2}x^T Q_1 x + c1^T x \, , \, \frac{1}{2}x^T Q_2 x + c2^T x \right) \\ Ax \leq b \end{cases}$$

The scalarized problem P_α becomes:

$$\begin{cases} \min \left(\frac{1}{2}x^T(\alpha_1 Q_1 + \alpha_2 Q_2)x + (\alpha_1 c1^T + \alpha_2 c2^T)x\right) \\ Ax \leq b \end{cases}$$

which can be solved by the Matlab function "quadprog".

Matlab solution

Q1 = [2 0; 0 2] ;

Q2 = [2 0; 0 2] ;

c1=[2;-4]; c2=[-6; -4]; A =[0 -1; -2 1; 2 1];

b = [0 0 4]';

% solve the scalarized problem with $0 \leq alfa1 \leq 1$

MINIMA=[ ]; % First column: value of alfa1

LAMBDA=[ ]; % First column: value of alfa1

for alfa1 = 0 : 0.01 : 1
[x,fval,exitflag,output,lambda] =
quadprog(alfa1*Q1+(1-alfa1)*Q2,alfa1*c1+(1-alfa1)*c2,A,b) ;

MINIMA=[MINIMA; alfa1 x'];
LAMBDA=[LAMBDA;alfa1,lambda.ineqlin'];
end

plot(MINIMA(:,2),MINIMA(:,3))

We obtain:

Minima =Weak Minima= $AB \cup BC$

where
$$A = (0.6, 1.2), \quad B = (1, 2), \quad C = (1.4, 1.2)$$

Exercise 4

Consider the nonlinear multiobjective problem defined in Example 7:

$$\begin{cases} \min \left(x_1 + x_2, \ -x_1 + x_2\right) \\ x_1^2 + x_2^2 - 1 \le 0 \end{cases}$$

(a) Find the set of weak minima by means of the scalarization method.

(a) Find a suitable subset of minima by means of the scalarization method.

The scalarized problem P_α is given by

$$\begin{cases} \min \ \alpha_1(x_1 + x_2) + \alpha_2(-x_1 + x_2) \\ x_1^2 + x_2^2 - 1 \le 0 \end{cases}$$

Since $\alpha_1 + \alpha_2 = 1$, by eliminating α_2 we obtain that P_α is equivalent to the problem (P_{α_1})

$$\begin{cases} \min \ \alpha_1(x_1 + x_2) + (1 - \alpha_1)(-x_1 + x_2) = (2\alpha_1 - 1)x_1 + x_2 \\ x_1^2 + x_2^2 - 1 \le 0 \end{cases}$$

where $0 \le \alpha_1 \le 1$.

The previous problem can be solved by the KKT conditions or by the Matlab function "fmincon".

The function fmincon solves a problem of the form:

$$\begin{cases} \min\ f(x) \\ Ax \leq b \\ D\,x = e \\ l \leq x \leq u \\ c(x) \leq 0 \\ ceq(x) = 0 \end{cases} \tag{5}$$

where x, b, e, l, u are vectors, A, D are matrices, c and ceq are functions that return vectors and f is a scalar function.

The sintax of the function is the following:

```
fun=@(x) ..............

nonlcon=@(x) const(x)
```

```
[x,fval,exitflag,output,lambda]=fmincon(fun,x0,A,b,D,e,l,u,nonlcon)
```

```
function [c,ceq] = const(x)
c=[.........];
ceq= [.........];
end
```

Matlab solution

% solve the scalarized problem with $0 \leq alfa1 \leq 1$

MINIMA=[ ]; % First column: value of alfa1

```
for alfa1 = 0 : 0.01 : 1
fun=@(x) (2*alfa1-1)*x(1)+x(2);
nonlcon= @(x) const(x);
x0=[0,0]';
[x,fval,exitflag,output,lambda] = fmincon(fun,x0,[ ],[ ],[ ],[ ],[ ],[ ],nonlcon) ;

MINIMA=[MINIMA; alfa1, x'];
end

plot(MINIMA(:,2),MINIMA(:,3))

function [C,Ceq]=const(x)
C=x(1)^2 +x(2)^2 -1;
Ceq=[ ];
end
```

Goal method

In the objective space $\mathbb{R}^s$ define the ideal point z as

$$z_i = \min_{x \in X} \ f_i(x), \qquad \forall \ i = 1, \ldots, s.$$

Since very often (P) has no ideal minimum, i.e., $z \notin f(X)$, we want to find the point of $f(X)$ which is as close as possible to z:

$$\begin{cases} \min \ \|f(x) - z\|_q \\ x \in X \end{cases} \qquad \text{with} \ \ q \in [1, +\infty]. \tag{G}$$

Theorem

- If $q \in [1, +\infty)$, then any optimal solution of (G) is a minimum of (P).
- If $q = +\infty$, then any optimal solution of (G) is a weak minimum of (P).

Assume that (P) is a linear multiobjective optimization problem, i.e.,

$$\begin{cases} \min \ Cx \\ Ax \leq b \end{cases} \tag{P}$$

where C is a $s \times n$ matrix, A is a $m \times n$ matrix, $b \in \mathbb{R}^m$.

If $q = 2$, then (G) is equivalent to a quadratic programming problem:

$$\begin{cases} \min \ \frac{1}{2}\|Cx - z\|_2^2 = \frac{1}{2}x^\mathsf{T} C^\mathsf{T} Cx - x^\mathsf{T} C^\mathsf{T} z + \frac{1}{2}z^\mathsf{T} z \\ Ax \leq b \end{cases} \tag{G_2}$$

Matlab solution

| data | ```
C=[.....];
A=[.......];
b=[.......];
s=size(C,1);
``` |
|------|---------|
| Ideal point | ```
z=zeros(s,1);
for i=1:s
[a,z(i)] = linprog(C(i,:)',A,b)
end
``` |

object. funct.	`H=C'*C     f= -C'*z`
Solut. Command	`x=quadprog(H,f, A, b)`

Example 10

Consider the problem

$$\begin{cases} \min \left(x_1 - x_2 \,,\; x_1 + x_2 \right) \\ -2\,x_1 + x_2 \leq 0 \\ -x_1 - x_2 \leq 0 \\ 5\,x_1 - x_2 \leq 6 \end{cases}$$

a) Find the ideal point.

b) Apply the goal method with norm $q = 2$.

Matlab solution

C = [1 -1; 1 1] ;

A =[-2 1; -1 -1; 5 -1];

b = [0 0 6]';

% find the ideal point z

z=[0,0]';
for i = 1:2
[a,z(i)]=linprog(C(i,:)',A,b);
end

% solve the quadratic problem with norm $q = 2$

x = quadprog(C'*C,-C'*z,A,b);

a) The ideal point is $z = (-2, 0)$.

b) The optimal solution of (G_2) is $x^* = (0.2, 0.4)$.

Exercises

Exercise 5

Consider the non linear convex multiobjective problem (defined in Example 9)

$$
\begin{cases}
\min \left(x_1 \ , \ x_1^2 + x_2^2 - 4x_1 \right) \\
(x_1, x_2) \in \mathbb{R}^2
\end{cases}
$$

Find, by making use of Matlab, the sets of weak minima and minima.

Exercise 6

Consider the linear multiobjective problem (defined in Example 5)

$$
\begin{cases}
\min \left(x_1 + 2x_2 - 3x_3 \ , \ -x_1 - x_2 - x_3 \ , \ -4x_1 - 2x_2 + x_3 \right) \\
x_1 + x_2 + x_3 \leq 10 \\
x_3 \leq 5 \\
x_1, x_2, x_3 \geq 0
\end{cases}
$$

Find, by making use of Matlab, the sets of weak minima and minima.

10 - Non-cooperative game theory

G. Mastroeni and M. Passacantando

Optimization Methods and Game Theory
Master of Science in Artificial Intelligence and Data Engineering
University of Pisa – A.Y. 2023/24

Contents

- Non-cooperative games

- Matrix games

- Bimatrix games

- Convex games

Game theory

Game theory is concerned with the analysis of conflictual situations involving various decision makers (called "players") having different aims or objectives.

The decision (called "strategy") of each player has a different cost depending on the strategies chosen by the other players.

Game theory studies the possibility to forecast the strategies that will be chosen by each player in order to minimize his cost.

Definition 1

A non-cooperative game (in normal form) is defined by a set of N players, where each player i has a set X_i of strategies and a cost function $f_i : X_1 \times \cdots \times X_N \to \mathbb{R}$.
The aim of each player i consists in solving the optimization problem

$$\begin{cases} \min \ f_i(x^1, x^2, \ldots, x^{i-1}, x^i, x^{i+1}, \ldots, x^N) \\ x^i \in X_i \end{cases}$$

Nash equilibrium

We will consider non-cooperative games with two players:

$$\text{Player 1:} \quad \begin{cases} \min \ f_1(x,y) \\ x \in X \end{cases} \qquad\qquad \text{Player 2:} \quad \begin{cases} \min \ f_2(x,y) \\ y \in Y \end{cases}$$

Definition 2

In a two-person non-cooperative game, a pair of strategies $(\bar{x}, \bar{y})$ is a **Nash equilibrium** if

$$f_1(\bar{x}, \bar{y}) = \min_{x \in X} \ f_1(x, \bar{y}), \qquad\qquad f_2(\bar{x}, \bar{y}) = \min_{y \in Y} \ f_2(\bar{x}, y).$$

In other words, $(\bar{x}, \bar{y})$ is a **Nash equilibrium** if and only if
- $\bar{x}$ is the best response of player 1 to strategy $\bar{y}$ of player 2
- $\bar{y}$ is the best response of player 2 to strategy $\bar{x}$ of player 1

A **matrix game** is a two-persons non-cooperative game where:

- X and Y are finite sets: $X = \{1, \ldots, m\}$, $Y = \{1, \ldots, n\}$;
- $f_2 = -f_1$ (zero-sum game).

It can be represented by a $m \times n$ matrix C, where $f_1(i,j) = c_{ij}$ is the amount of money player 1 pays to player 2 if player 1 chooses strategy i and player 2 chooses strategy j.

Remark 1

Notice that if a Nash equilibrium $(\bar{i}, \bar{j})$ exists it must be

$$f_1(\bar{i}, \bar{j}) = \min_{i \in X} f_1(i, \bar{j})$$

$$f_2(\bar{i}, \bar{j}) = \min_{j \in Y} f_2(\bar{i}, j) = \min_{j \in Y} -f_1(\bar{i}, j) = -\max_{j \in Y} f_1(\bar{i}, j), \quad i.e.,$$

$$f_1(\bar{i}, \bar{j}) = \max_{j \in Y} f_1(\bar{i}, j)$$

Example 1. Find the Nash equilibria of the matrix game

Player 2

		1	2	3
		1	2	3
Player 1	1	1	−1	0
	2	3	−2	−1
	3	2	3	−2

For player 2, strategy 3 is worse than strategy 1 because his/her profit is less than the one obtained playing strategy 1 for any strategy of player 1. Hence, player 2 will never choose strategy 3, which can be deleted from the game. The game is equivalent to

Player 2

		1	2
		1	2
Player 1	1	1	−1
	2	3	−2
	3	2	3

Now, for player 1 strategy 3 is worse than strategy 1.

The reduced game is

$$
\begin{array}{c}
\textcolor{blue}{\text{Player 2}} \\
\begin{array}{cc|cc}
 & & \textcolor{blue}{1} & \textcolor{blue}{2} \\
\hline
 & \textcolor{red}{1} & 1 & -1 \\
\textcolor{red}{\text{Player 1}} & \textcolor{red}{2} & 3 & -2
\end{array}
\end{array}
$$

For player 2, strategy 2 is worse than strategy 1. Thus, player 2 will always choose strategy 1. The reduced game is

$$
\begin{array}{c}
\textcolor{blue}{\text{Player 2}} \\
\begin{array}{cc|c}
 & & \textcolor{blue}{1} \\
\hline
 & \textcolor{red}{1} & 1 \\
\textcolor{red}{\text{Player 1}} & \textcolor{red}{2} & 3
\end{array}
\end{array}
$$

Finally, for player 1, strategy 2 is worse than strategy 1. Therefore, player 1 will always choose strategy 1.
Hence $(1, 1)$ is a Nash equilibrium.

For a general two-persons game (non necessarily zero-sum) we can give the following definition:

Definition 3 ● ● ●

Given a two-persons non-cooperative game, a strategy $x \in X$ is strictly dominated by $\widetilde{x} \in X$ if

$$f_1(x, y) > f_1(\widetilde{x}, y) \qquad \forall \ y \in Y.$$

Similarly, a strategy $y \in Y$ is strictly dominated by $\widetilde{y} \in Y$ if

$$f_2(x, y) > f_2(x, \widetilde{y}) \qquad \forall \ x \in X.$$

Strictly dominated strategies can be deleted from the game.

a) Find all the Nash equilibria of the following matrix game:

Player 2

	1	2	3	4	5
1	1	−1	1	−2	−3
2	2	−2	3	4	0
3	1	0	1	−3	−4
4	4	−3	2	−1	−1
5	5	−2	4	−3	2

Player 1 (rows 1–5), Player 2 (columns 1–5)

b) Prove that if (i, j) and (p, q) are Nash equilibria of a matrix game, then

- $c_{ij} = c_{pq}$
- (i, q) and (p, j) are Nash equilibria as well.

a) Strategies 2 and 5 of player 2 are dominated by Strategy 1 and can be deleted:

Player 2

	1	3	4
1	1	1	−2
2	2	3	4
3	1	1	−3
4	4	2	−1
5	5	4	−3

Player 1

Strategies 2 and 4 of player 1 are dominated by Strategy 1 (or 3) and can be deleted:

Player 2

	1	3	4
1	1	1	−2
3	1	1	−3
5	5	4	−3

Player 1

Strategy 4 of player 2 is dominated by the remaining ones and consequently Strategy 5 of player 1 is dominated by the remaining ones and can be deleted:

$$
\begin{array}{c|cc}
 & \text{Player 2} & \\
 & 1 & 3 \\
\hline
1 & 1 & 1 \\
3 & 1 & 1 \\
\end{array}
$$

Player 1

Clearly all the remaining strategies form pairs of Nash equilibria:

$$(1,1) \quad (1,3) \quad (3,1) \quad (3,3).$$

Two companies $C1$ and $C2$ want to build a new supermarket in one of the districts $D1$, $D2$ and $D3$ of a town.

$$X = \{1, 2, 3\} \quad Y = \{1, 2, 3\}$$

are the sets of the strategies of $C1$ and $C2$ where strategy i corresponds to the decision of building a supermarket in the district D_i.

The company $C1$ estimates that building a supermarket in the district D_i while the company $C2$ builds a supermarket in the district D_j, implies a loss given by the cost function:

$$c(i, j) = 100 \frac{1}{1 + d_{ij}}$$

where d_{ij} is the (average) distance between D_i and D_j.
Assume that the distances (in minutes) between the districts are:

- 9 min between $D1$ and $D2$;
- 19 min between $D1$ and $D3$;
- 24 min between $D2$ and $D3$.

We set $d_{ii} = 0$, $\quad i = 1, 2, 3$.

We set $f_1(i,j) = c(i,j)$ and we assume that the company $C2$ has a profit equal to the loss of $C1$, i.e.,

$$f_2(i,j) = -f_1(i,j) \quad i = 1,2,3, \quad j = 1,2,3.$$

The matrix of the game is given by

$$C = \begin{pmatrix} 100 & 10 & 5 \\ 10 & 100 & 4 \\ 5 & 4 & 100 \end{pmatrix}$$

Remark

Notice that in this case no Nash equilibria exist.

Mixed strategies

Example 2. (Odds and evens)

		Player 2	
		1 (odd)	2 (even)
	1 (odd)	1	-1
Player 1	2 (even)	-1	1

- Are there strictly dominated strategies?
- Are there Nash equilibria?

In both cases the answer is NO

Definition 4

If C is a $m \times n$ matrix game, then a <u>mixed strategy</u> for player 1 is a m-vector of probabilities and we consider
$X = \{x \in \mathbb{R}^m : x \geq 0, \quad \sum_{i=1}^m x_i = 1\}$ the set of mixed strategies of player 1.
The vertices of X, i.e., $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)$ are <u>pure strategies</u> of player 1.

Similarly, a <u>mixed strategy</u> for player 2 is a n-vector of probabilities and $Y = \{y \in \mathbb{R}^n : y \geq 0, \quad \sum_{j=1}^n y_j = 1\}$ is the set of mixed strategies of player 2.

The expected costs are $f_1(x, y) = x^\mathsf{T} C y$ (player 1), $f_2(x, y) = -x^\mathsf{T} C y$ (player 2).

Note that
$$x^\mathsf{T} C y = \sum_{i=1}^m \sum_{j=1}^n x_i c_{ij} y_j.$$

Definition 5

If C is a $m \times n$ matrix game, then $(\bar{x}, \bar{y}) \in X \times Y$ is a mixed strategies Nash equilibrium if

$$\max_{y \in Y} \bar{x}^\mathsf{T} C y = \bar{x}^\mathsf{T} C \bar{y} = \min_{x \in X} x^\mathsf{T} C \bar{y},$$

or, equivalently,

$$\bar{x}^\mathsf{T} C y \leq \bar{x}^\mathsf{T} C \bar{y} \leq x^\mathsf{T} C \bar{y}, \quad \forall (x, y) \in X \times Y,$$

i.e., $(\bar{x}, \bar{y})$ is a <u>saddle point</u> of the function $f_1(x, y) = x^\mathsf{T} C y$ on $X \times Y$.

We recall the definition of a saddle point for a general function $F : X \times Y \to \mathbb{R}$.

Definition

Let $X \subseteq \mathbb{R}^m$, $Y \subseteq \mathbb{R}^n$.
$(\bar{x}, \bar{y})$ is said to be a saddle point for the function $F : X \times Y \to \mathbb{R}$ if

$$F(\bar{x}, y) \leq F(\bar{x}, \bar{y}) \leq F(x, \bar{y}), \quad \forall (x, y) \in X \times Y. \tag{1}$$

Define

$$\psi(x) := \sup_{y \in Y} F(x, y), \quad x \in X$$

$$\phi(y) := \inf_{x \in X} F(x, y), \quad y \in Y$$

Then,

$$\phi(y) \le F(x, y) \le \psi(x), \quad \forall (x, y) \in X \times Y$$

Theorem 1

$(\bar{x}, \bar{y}) \in X \times Y$ satisfies the saddle point condition (1) if and only if

1. $\bar{x}$ is an optimal solution of problem $\min_{x \in X} \psi(x)$;
2. $\bar{y}$ is an optimal solution of problem $\max_{y \in Y} \phi(y)$;
3. $\psi(\bar{x}) = \phi(\bar{y})$.

Remark

Notice that conditions 1-2-3 are equivalent to:

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

Theorem 2 (Existence of a saddle point)

Let $X \subseteq \mathbb{R}^m$, $Y \subseteq \mathbb{R}^n$ and assume that

- X and Y are nonempty compact convex sets;
- $F(\cdot, y)$ is continuous and quasi convex on X, for every $y \in Y$;
- $F(x, \cdot)$ is continuous and quasi concave on Y, for every $x \in X$.

Then F admits a saddle point on $X \times Y$.

As a consequence of Theorems 1 and 2 , we obtain the following characterization of a mixed strategies Nash equilibrium.

Corollary 1

- Any matrix game has at least a mixed strategies Nash equilibrium.
- $(\bar{x}, \bar{y})$ is a mixed strategies Nash equilibrium if and only if

$$
\begin{cases}
\bar{x} \text{ is an optimal solution of } \min_{x \in X} \max_{y \in Y} x^\mathsf{T} C y \\
\bar{y} \text{ is an optimal solution of } \max_{y \in Y} \min_{x \in X} x^\mathsf{T} C y
\end{cases}
$$

with optimal values both equal to $\bar{x}^T C \bar{y}$.

Theorem 3 ● ● ●

1. The problem $\min\limits_{x \in X} \max\limits_{y \in Y} x^\top C y$ is equivalent to the linear programming problem

$$
\begin{cases}
\min \ v \\
v \geq \sum\limits_{i=1}^{m} c_{ij} x_i \quad \forall \, j = 1, \ldots, n \\
x \geq 0, \quad \sum\limits_{i=1}^{m} x_i = 1
\end{cases}
\tag{P_1}
$$

2. The problem $\max\limits_{y \in Y} \min\limits_{x \in X} x^\top C y$ is equivalent to the linear programming problem

$$
\begin{cases}
\max \ w \\
w \leq \sum\limits_{j=1}^{n} c_{ij} y_j \quad \forall \, i = 1, \ldots, m \\
y \geq 0, \quad \sum\limits_{j=1}^{n} y_j = 1
\end{cases}
\tag{P_2}
$$

Proposition 1

(P_2) is the dual of (P_1).

Remark

Notice that, by strong duality for linear programming it is also possible to prove that any matrix game has at least a mixed strategies Nash equilibrium.

Matlab solution

Let us formulate problem P_1 in matrix form, we obtain:

$$
\begin{cases}
\min \ v \\
(C^\top, -e_n) \begin{pmatrix} x \\ v \end{pmatrix} \leq 0 \\
(e_m^\top, 0) \begin{pmatrix} x \\ v \end{pmatrix} = 1 \\
x \geq 0,
\end{cases}
\tag{P_1}
$$

where $e_n = (1, ..., 1)^\top \in \mathbb{R}^n$, $x \in \mathbb{R}^m$, $v \in \mathbb{R}$.

Matlab solution

```
C=[..........] % Define C

m = size(C,1);

n = size(C,2);

c=[zeros(m,1);1];

A= [C', -ones(n,1)]; b=zeros(n,1);

Aeq=[ones(1,m),0]; beq=1;

lb= [zeros(m,1);-inf]; ub=[ ];

[sol,Val,exitflag,output,lambda] = linprog(c, A,b, Aeq, beq, lb, ub);

x = sol(1:m)

y = lambda.ineqlin
```

Example 3

(Example 2 continued: odds and evens)

	Player 2	
	1 (odd)	2 (even)
Player 1 1 (odd)	1	−1
2 (even)	−1	1

$$(P_1) \begin{cases} \min \ v \\ v \geq x_1 - x_2 \\ v \geq -x_1 + x_2 \\ x \geq 0 \\ x_1 + x_2 = 1 \end{cases} \text{is equivalent to} \begin{cases} \min \ v \\ v \geq 2x_1 - 1 \\ v \geq 1 - 2x_1 \\ 0 \leq x_1 \leq 1 \end{cases} \Rightarrow \bar{x} = (1/2, 1/2)$$

$$(P_2) \begin{cases} \max \ w \\ w \leq y_1 - y_2 \\ w \leq -y_1 + y_2 \\ y \geq 0 \\ y_1 + y_2 = 1 \end{cases} \text{is equivalent to} \begin{cases} \max \ w \\ w \leq 2y_1 - 1 \\ w \leq 1 - 2y_1 \\ 0 \leq y_1 \leq 1 \end{cases} \Rightarrow \bar{y} = (1/2, 1/2)$$

Exercise 2

Consider the following matrix game:

$$C = \begin{pmatrix} 7 & 15 & 2 & 3 \\ 4 & 2 & 3 & 10 \\ 5 & 3 & 4 & 12 \end{pmatrix}$$

a) Are there strictly dominated strategies?

b) Are there pure strategies Nash equilibria?

c) Find a mixed strategies Nash equilibrium.

a) Note that Strategy 3 of Player 1 is dominated by Strategy 2, while Strategy 3 of Player 2 is dominated by Strategy 1.
Therefore the third row and the third column can be deleted, i.e., $x_3 = 0$, $y_3 = 0$.
The reduced matrix results:

$$\begin{array}{ccc} y_1 & y_2 & y_4 \end{array}$$

$$C_R = \begin{pmatrix} 7 & 15 & 3 \\ 4 & 2 & 10 \end{pmatrix} \begin{array}{c} x_1 \\ x_2 \end{array}$$

b) We observe that no pure strategy Nash equilibrium exist for the reduced game C_R. Indeed, not any of the minima evaluated on the columns, (i.e., 4,2,3) coincides with the maximum evaluated on the rows (i.e., 15,10).

c) Let us solve the linear programming problem associated with player 1.

$$(P_1) \quad \begin{cases} \min \ v \\ v \geq 7x_1 + 4x_2 + 5x_3 \\ v \geq 15x_1 + 2x_2 + 3x_3 \\ v \geq 2x_1 + 3x_2 + 4x_3 \\ v \geq 3x_1 + 10x_2 + 12x_3 \\ x_1 + x_2 + x_3 = 1 \\ x_1, x_2, x_3 \geq 0 \end{cases}$$

The previous problem can be solved by the Matlab function "linprog".

Matlab solution

C=[7 15 2 3; 4 2 3 10; 5 3 4 12]

m = 3;

n = 4;

c=[0 0 0 1]';

A= [C', -ones(n,1)]; b=[0;0;0;0];

Aeq=[1 1 1,0]; beq=1;

lb= [0;0;0;-inf]; ub=[ ];

[sol,Val,exitflag,output,lambda] = linprog(c, A,b, Aeq, beq, lb, ub);

x = sol(1:m)

y = lambda.ineqlin

Optimal solution

x = (0.4, 0.6, 0)

y = (0, 0.35, 0, 0.65)

is a mixed strategies Nash equilibrium.

A **bimatrix game** is a two-person non-cooperative game where:

- the sets of pure strategies are finite, hence the sets of mixed strategies are $X = \{x \in \mathbb{R}^m : x \geq 0, \quad \sum_{i=1}^m x_i = 1\}$ and $Y = \{y \in \mathbb{R}^n : y \geq 0, \quad \sum_{j=1}^n y_j = 1\}$;
- $f_2 \neq -f_1$ (non-zero-sum game), the cost functions are $f_1(x,y) = x^\mathsf{T} C_1 y$ and $f_2(x,y) = x^\mathsf{T} C_2 y$, where C_1 and C_2 are $m \times n$ matrices.

Theorem 3 (Nash)

Any bimatrix game has at least a mixed strategies Nash equilibrium.

Two persons have been arrested for the same severe crime and for small robbery. They are known to be guilty in the robbery but police has no evidence for the severe crime. They are interrogated separately.

Each of the two prisoners can choose: to confess (Strategy 1) or to stay quiet (Strategy 2).

If both stay quiet, they have 2 years for small robbery; if they both confess they are convicted to 5 years; if one and only one confesses, he will be convicted to 1 year and used as witness against the other who will spend 10 years in prison.

Bimatrix game associated with the prisoner's dilemma

$$C_1 = \begin{pmatrix} 5 & 1 \\ 10 & 2 \end{pmatrix} \qquad C_2 = \begin{pmatrix} 5 & 10 \\ 1 & 2 \end{pmatrix}$$

Are there strictly dominated strategies?

Example 5

$$C_1 = \begin{pmatrix} -5 & 0 \\ 0 & -1 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -1 & 0 \\ 0 & -5 \end{pmatrix}$$

(a) Are there strictly dominated strategies?

(b) Are there pure strategies Nash equilibria?

(c) Are there mixed strategies Nash equilibria?

(a) No row in C_1 is strictly greater than the other and similarly no column in C_2 is strictly greater than the other.

(b) Let us denote by (a, b) the couple of strategies chosen by the two players.
Consider player 1. By definition of (NE), if possible pure strategies exist, they may be:

$$(1, 1) \quad or \quad (2, 2)$$

since -5 and -1 are the minimum values in columns 1 and 2 of C_1, respectively.

Consider player 2. The cost related to couple (1,1) is -1 which is the minimum on the row 1 in C_2, so (1,1) is a pure strategies Nash equilibrium.

Similarly for the couple $(2,2)$, -5 is the minimum on the row 2 in C_2, so $(2,2)$ is a pure strategies Nash equilibrium.

(c) Are there mixed strategies Nash equilibria? How to compute them?

The considerations made in part (b) lead us to define a procedure to compute mixed strategies Nash equilibria, based on the definition of the best response mappings.

Theorem ● ● ●

If we define the best response mappings $B_1 : Y \to X$ and $B_2 : X \to Y$ as

$$B_1(y) = \left\{ \text{optimal solutions of } \min_{x \in X} \; x^{\mathsf{T}} C_1 y \right\},$$

$$B_2(x) = \left\{ \text{optimal solutions of } \min_{y \in Y} \; x^{\mathsf{T}} C_2 y \right\},$$

then $(\bar{x}, \bar{y})$ is a Nash equilibrium if and only if $\bar{x} \in B_1(\bar{y})$ and $\bar{y} \in B_2(\bar{x})$.

Example 5 (continued) ● ● ●

$$C_1 = \begin{pmatrix} -5 & 0 \\ 0 & -1 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -1 & 0 \\ 0 & -5 \end{pmatrix}$$

Given $y \in Y$ we have to solve the problem

$$\begin{cases} \min \ x^\mathsf{T} C_1 y = -5x_1 y_1 - x_2 y_2 \\ x \in X \end{cases} \equiv \begin{cases} \min \ (1 - 6y_1)x_1 + y_1 - 1 \\ 0 \leq x_1 \leq 1 \end{cases}$$

hence the optimal solution is

$$B_1(y_1) = \begin{cases} 0 & \text{if } y_1 \in [0, 1/6) \\ [0, 1] & \text{if } y_1 = 1/6 \\ 1 & \text{if } y_1 \in (1/6, 1] \end{cases}$$

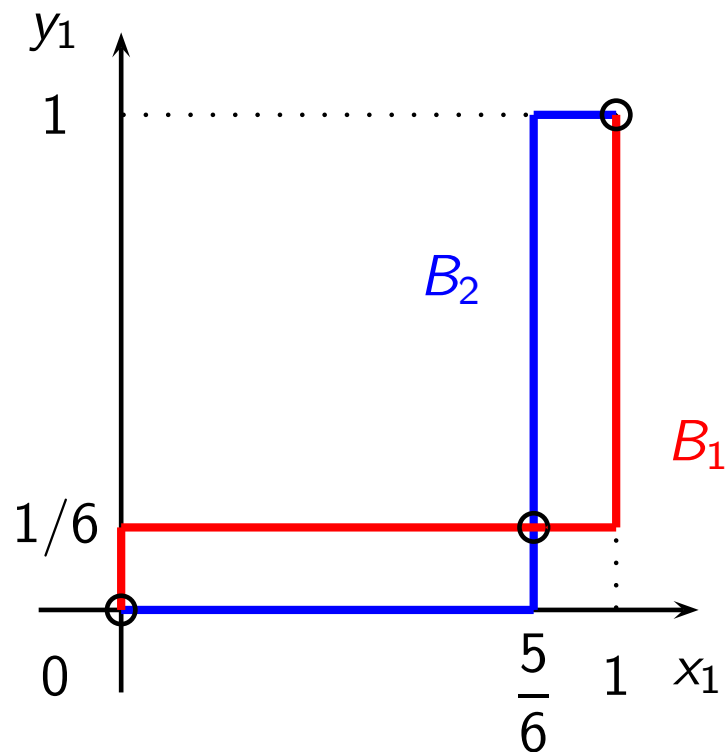Similarly, given $x \in X$ we have to solve the problem

$$\begin{cases} \min \ x^\mathsf{T} C_2 y = -x_1 y_1 - 5x_2 y_2 \\ y \in Y \end{cases} \equiv \begin{cases} \min \ (5 - 6x_1)y_1 + 5x_1 - 5 \\ 0 \leq y_1 \leq 1 \end{cases}$$

hence the optimal solution is

$$B_2(x_1) = \begin{cases} 0 & \text{if } x_1 \in [0, 5/6) \\ [0, 1] & \text{if } x_1 = 5/6 \\ 1 & \text{if } x_1 \in (5/6, 1] \end{cases}$$

Nash equilibria are given by the <u>intersections</u> of the graphs of the best response mappings B_1 and B_2:

There are 3 Nash equilibria:

- $\bar{x} = (0, 1)$, $\bar{y} = (0, 1)$ (pure strategies)
- $\bar{x} = (5/6, 1/6)$, $\bar{y} = (1/6, 5/6)$ (mixed strategies)
- $\bar{x} = (1, 0)$, $\bar{y} = (1, 0)$ (pure strategies)

Consider the optimization problems associated with the two players:

$$P_1(y) : \begin{cases} \min \ x^T C_1 y \\ \sum_{i=1}^{m} x_i = 1 \\ x \geq 0 \end{cases} \qquad P_2(x) : \begin{cases} \min \ x^T C_2 y \\ \sum_{j=1}^{n} y_j = 1 \\ y \geq 0 \end{cases}$$

The KKT conditions for a bimatrix game are obtained by simultaneously considering the single KKT conditions associated with $P_1(y)$ and $P_2(x)$:

$$\begin{cases} C_1 y + \mu_1 e_m \geq 0 \\ x \geq 0, \quad \sum_{i=1}^{m} x_i = 1 \\ x_i (C_1 y + \mu_1 e_m)_i = 0, \quad i = 1, .., m \end{cases} \qquad \begin{cases} C_2^\mathsf{T} x + \mu_2 e_n \geq 0 \\ y \geq 0, \quad \sum_{j=1}^{n} y_j = 1 \\ y_j (C_2^\mathsf{T} x + \mu_2 e_n)_j = 0, \ j = 1, .., n \end{cases}$$

where $e_m = (1, \ldots, 1)^\mathsf{T} \in \mathbb{R}^m$ and $e_n = (1, \ldots, 1)^\mathsf{T} \in \mathbb{R}^n$.

Remark

Notice that $P_1(y)$ and $P_2(x)$ are parametric linear problems so that the KKT conditions are necessary and sufficient for optimality.

Theorem (KKT conditions for bimatrix games)

$(\bar{x}, \bar{y})$ is a Nash equilibrium if and only if there exist $\mu_1, \mu_2 \in \mathbb{R}$ such that

$$
\begin{cases}
C_1 \bar{y} + \mu_1 e_m \geq 0 \\
\bar{x} \geq 0, \quad \sum_{i=1}^{m} \bar{x}_i = 1 \\
\bar{x}_i (C_1 \bar{y} + \mu_1 e_m)_i = 0 \quad \forall\, i = 1, \ldots, m \\
C_2^\mathsf{T} \bar{x} + \mu_2 e_n \geq 0 \\
\bar{y} \geq 0, \quad \sum_{j=1}^{n} \bar{y}_j = 1 \\
\bar{y}_j (C_2^\mathsf{T} \bar{x} + \mu_2 e_n)_j = 0 \quad \forall\, j = 1, \ldots, n
\end{cases}
\tag{KS}
$$

where $e_m = (1, \ldots, 1)^\mathsf{T} \in \mathbb{R}^m$.

Example 5 (continued)

Find all the Nash equilibria of the following bimatrix game by means of the KKT conditions:

$$
C_1 = \begin{pmatrix} -5 & 0 \\ 0 & -1 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -1 & 0 \\ 0 & -5 \end{pmatrix}
$$

The KKT conditions are given by:

$$
\begin{cases}
-5y_1 + \mu_1 \geq 0 \\
-y_2 + \mu_1 \geq 0 \\
x \geq 0, \ x_1 + x_2 = 1 \\
x_1(-5y_1 + \mu_1) = 0 \\
x_2(-y_2 + \mu_1) = 0 \\
-x_1 + \mu_2 \geq 0 \\
-5x_2 + \mu_2 \geq 0 \\
y \geq 0, \quad y_1 + y_2 = 1 \\
y_1(-x_1 + \mu_2) = 0 \\
y_2(-5x_2 + \mu_2) = 0
\end{cases}
$$

Let us simplify the previous system by eliminating y_2 and x_2, i.e.,

$$y_2 = 1 - y_1, \quad x_2 = 1 - x_1. \tag{2}$$

We obtain:

$$\begin{cases} -5y_1 + \mu_1 \geq 0 \\ -(1 - y_1) + \mu_1 \geq 0 \\ x_1(-5y_1 + \mu_1) = 0 \\ (1 - x_1)(-1 + y_1 + \mu_1) = 0 \\ -x_1 + \mu_2 \geq 0 \\ -5(1 - x_1) + \mu_2 \geq 0 \\ y_1(-x_1 + \mu_2) = 0 \\ (1 - y_1)(-5 + 5x_1 + \mu_2) = 0 \\ 0 \leq x_1 \leq 1, \ 0 \leq y_1 \leq 1 \end{cases} \tag{3}$$

We can consider the following three cases:

1. $x_1 = 0$,
2. $x_1 = 1$,
3. $0 < x_1 < 1$.

Case 1: $x_1 = 0$. The previous system becomes:

$$\begin{cases} x_1 = 0 \\ -5y_1 + \mu_1 \geq 0 \\ -(1 - y_1) + \mu_1 \geq 0 \\ -1 + y_1 + \mu_1 = 0 \\ \mu_2 \geq 0 \\ -5 + \mu_2 \geq 0 \\ y_1 \mu_2 = 0 \\ (1 - y_1)(-5 + \mu_2) = 0 \\ 0 \leq y_1 \leq 1 \end{cases}$$

We have the two subcases $\mu_2 = 0$, or $y_1 = 0$. For $\mu_2 = 0$ the system is clearly impossible, while for $y_1 = 0$, taking into account (2), we obtain the solution:

$$\bar{x} = (0, 1), \; \bar{y} = (0, 1), \; \mu_1 = 1, \; \mu_2 = 5,$$

which is a pure strategies Nash equilibrium.

Case 2: $x_1 = 1$. The system (3) becomes:

$$\begin{cases} x_1 = 1 \\ -5y_1 + \mu_1 \geq 0 \\ -(1 - y_1) + \mu_1 \geq 0 \\ -5y_1 + \mu_1 = 0 \\ -1 + \mu_2 \geq 0 \\ y_1(-1 + \mu_2) = 0 \\ (1 - y_1)\mu_2 = 0 \\ 0 \leq y_1 \leq 1 \end{cases}$$

We obtain the solution, taking into account (2):

$$\bar{x} = (1, 0), \ \bar{y} = (1, 0), \ \mu_1 = 5, \ \mu_2 = 1,$$

which is a pure strategies Nash equilibrium.

Case 3: $0 < x_1 < 1$. The system (2) becomes:

$$\begin{cases} 0 < x_1 < 1 \\ -5y_1 + \mu_1 \geq 0 \\ -(1 - y_1) + \mu_1 \geq 0 \\ -5y_1 + \mu_1 = 0 \\ -1 + y_1 + \mu_1 = 0 \\ -x_1 + \mu_2 \geq 0 \\ -5(1 - x_1) + \mu_2 \geq 0 \\ y_1(-x_1 + \mu_2) = 0 \\ (1 - y_1)(-5 + 5x_1 + \mu_2) = 0 \\ 0 \leq y_1 \leq 1 \end{cases}$$

The equations

$$\begin{cases} -5y_1 + \mu_1 = 0 \\ -1 + y_1 + \mu_1 = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} y_1 = 1/6 \\ \mu_1 = 5/6 \end{cases}$$

Then, the previous system becomes:

$$\begin{cases} 0 < x_1 < 1 \\ y_1 = 1/6 \\ \mu_1 = 5/6 \\ -x_1 + \mu_2 = 0 \\ -5 + 5x_1 + \mu_2 = 0 \end{cases} \Rightarrow \begin{cases} y_1 = 1/6 \\ \mu_1 = 5/6 \\ x_1 = 5/6 \\ \mu_2 = 5/6 \end{cases}$$

We obtain the solution:

$$\bar{x} = (5/6, 1/6), \ \bar{y} = (1/6, 5/6), \ \mu_1 = \mu_2 = 5/6,$$

which is a mixed strategies Nash equilibrium.

Exercise 3

Find all the Nash equilibria of the following bimatrix game by means of the KKT conditions:

$$C_1 = \begin{pmatrix} 3 & 3 \\ 4 & 1 \\ 6 & 0 \end{pmatrix} \qquad C_2 = \begin{pmatrix} 3 & 4 \\ 4 & 0 \\ 3 & 5 \end{pmatrix}$$

The KKT conditions are given by:

$$
\begin{cases}
3y_1 + 3y_2 + \mu_1 \geq 0 \\
4y_1 + y_2 + \mu_1 \geq 0 \\
6y_1 + \mu_1 \geq 0 \\
x \geq 0, \ x_1 + x_2 + x_3 = 1 \\
x_1(3y_1 + 3y_2 + \mu_1) = 0 \\
x_2(4y_1 + y_2 + \mu_1) = 0 \\
x_3(6y_1 + \mu_1) = 0 \\
3x_1 + 4x_2 + 3x_3 + \mu_2 \geq 0 \\
4x_1 + 5x_3 + \mu_2 \geq 0 \\
y \geq 0, \quad y_1 + y_2 = 1 \\
y_1(3x_1 + 4x_2 + 3x_3 + \mu_2) = 0 \\
y_2(4x_1 + 5x_3 + \mu_2) = 0
\end{cases}
$$

Let us simplify the previous system by eliminating y_2 and x_1, i.e.,

$$
y_2 = 1 - y_1, \quad x_1 = 1 - x_2 - x_3.
$$

We obtain:

$$
\begin{cases}
3 + \mu_1 \geq 0 \\
3y_1 + 1 + \mu_1 \geq 0 \\
6y_1 + \mu_1 \geq 0 \\
x_2, x_3 \geq 0, \;\; x_2 + x_3 \leq 1 \\
(1 - x_2 - x_3)(3 + \mu_1) = 0 \\
x_2(3y_1 + 1 + \mu_1) = 0 \\
x_3(6y_1 + \mu_1) = 0 \\
3 + x_2 + \mu_2 \geq 0 \\
4 - 4x_2 + x_3 + \mu_2 \geq 0 \\
y_1 \geq 0, \quad y_1 \leq 1 \\
y_1(3 + x_2 + \mu_2) = 0 \\
(1 - y_1)(4 - 4x_2 + x_3 + \mu_2) = 0
\end{cases}
\tag{S}
$$

We can consider the following three cases:

1. $y_1 = 0$,

2. $y_1 = 1$,

3. $0 < y_1 < 1$.

Case 1: $y_1 = 0$. The system becomes:

$$
\begin{cases}
3 + \mu_1 \geq 0 \\
1 + \mu_1 \geq 0 \\
\mu_1 \geq 0 \\
x_2, x_3 \geq 0, \ x_2 + x_3 \leq 1 \\
1 - x_2 - x_3 = 0 \\
x_2 = 0 \\
x_3 \mu_1 = 0 \\
3 + \mu_2 \geq 0 \\
4 - 4x_2 + x_3 + \mu_2 \geq 0 \\
y_1 = 0, \\
4 + x_3 + \mu_2 = 0
\end{cases}
$$

The previous system is clearly impossible. Indeed, $x_3 = 1$ and by the last equation $\mu_2 = -5 \ngeq -3$.

Case 2: $y_1 = 1$. The system (S) becomes:

$$
\begin{cases}
\mu_1 \geq -3 \\
x_2, x_3 \geq 0, \ x_2 + x_3 \leq 1 \\
(1 - x_2 - x_3)(\mu_1 + 3) = 0 \\
x_2 = 0 \\
x_3 = 0 \\
3 + \mu_2 \geq 0 \\
4 + \mu_2 \geq 0 \\
3 + \mu_2 = 0,
\end{cases}
$$

The previous system admits the solution $\mu_1 = \mu_2 = -3$, $x_2 = x_3 = 0$ which leads to the Nash Equilibrium:

$$
\bar{x} = (1, 0, 0) \quad \bar{y} = (1, 0)
$$

Case 3: $0 < y_1 < 1$. The system (S) becomes:

$$
\begin{cases}
3 + \mu_1 \geq 0 \\
3y_1 + 1 + \mu_1 \geq 0 \\
6y_1 + \mu_1 \geq 0 \\
x_2, x_3 \geq 0, \ \ x_2 + x_3 \leq 1 \\
(1 - x_2 - x_3)(3 + \mu_1) = 0 \\
x_2(3y_1 + 1 + \mu_1) = 0 \\
x_3(6y_1 + \mu_1) = 0 \\
3 + x_2 + \mu_2 = 0 \\
4 - 4x_2 + x_3 + \mu_2 = 0 \\
y_1 > 0, \ \ \ y_1 < 1
\end{cases}
\tag{S3}
$$

Note that $x_2 \neq 0$, indeed, otherwise, by the last two equalities

$$
\mu_2 = -3, \quad x_3 = -1
$$

Then system (S3) becomes:

$$\begin{cases} 3 + \mu_1 \geq 0 \\ 6y_1 + \mu_1 \geq 0 \\ x_2 > 0, \ x_3 \geq 0, \ x_2 + x_3 \leq 1 \\ (1 - x_2 - x_3)(3 + \mu_1) = 0 \\ 3y_1 + 1 + \mu_1 = 0 \\ x_3(6y_1 + \mu_1) = 0 \\ 3 + x_2 + \mu_2 = 0 \\ 4 - 4x_2 + x_3 + \mu_2 = 0 \\ y_1 > 0, \quad y_1 < 1 \end{cases}$$

We discuss the cases (a) $x_3 = 0$ and (b) $0 < x_3 \leq 1$.

(a) For $x_3 = 0$, by the last two equalities we obtain:

$$\mu_2 = -\frac{16}{5}, \quad x_2 = \frac{1}{5}$$

Consequently,

$$\mu_1 = -3, \quad y_1 = \frac{2}{3}$$

Therefore

$$\bar{x} = (\frac{4}{5}, \frac{1}{5}, 0) \quad \bar{y} = (\frac{2}{3}, \frac{1}{3}) \quad \text{is a Nash Equilibrium.}$$

(b) $0 < x_3 \leq 1$. The previous system becomes:

$$\begin{cases} 3 + \mu_1 \geq 0 \\ x_2 > 0, \ x_3 > 0, \ x_2 + x_3 \leq 1 \\ (1 - x_2 - x_3)(3 + \mu_1) = 0 \\ 3y_1 + 1 + \mu_1 = 0 \\ 6y_1 + \mu_1 = 0 \\ 3 + x_2 + \mu_2 = 0 \\ 4 - 4x_2 + x_3 + \mu_2 = 0 \\ 0 < y_1 < 1 \end{cases}$$

From the equalities

$$3y_1 + 1 + \mu_1 = 0, \quad 6y_1 + \mu_1 = 0$$

we obtain: $\mu_1 = -2, \quad y_1 = \frac{1}{3}$.

Since $\mu_1 = -2$, by the first equality it follows $x_2 + x_3 = 1$, i.e., $x_3 = 1 - x_2$ and substituting in the last equality, we have:

$$5 - 5x_2 + \mu_2 = 0, \quad 3 + x_2 + \mu_2 = 0,$$

which lead to

$$x_2 = \frac{1}{3}, \quad \mu_2 = -\frac{10}{3} \quad \Rightarrow \quad \bar{x} = (0, \frac{1}{3}, \frac{2}{3}) \quad \bar{y} = (\frac{1}{3}, \frac{2}{3}) \text{ is a Nash Equilibrium.}$$

Let us solve system (KS) by using Matlab. To this aim we trasform it into an equivalent optimization problem defined on the set $X \times Y \times \mathbb{R}^2$.

Note that (KS) can be written as:

$$
\begin{cases}
C_1 \bar{y} + \mu_1 e_m \geq 0 \\
\bar{x} \geq 0, \quad \sum_{i=1}^{m} \bar{x}_i = 1 \\
\bar{x}^T (C_1 \bar{y} + \mu_1 e_m) = 0 \\
C_2^{\mathsf{T}} \bar{x} + \mu_2 e_n \geq 0 \\
\bar{y} \geq 0, \quad \sum_{j=1}^{n} \bar{y}_j = 1 \\
\bar{y}^T (C_2^{\mathsf{T}} \bar{x} + \mu_2 e_n) = 0
\end{cases}
\tag{KS}
$$

where $e_m = (1, \dots, 1)^{\mathsf{T}} \in \mathbb{R}^m$.

Then

Proposition

$(\bar{x}, \bar{y}, \mu_1, \mu_2)$ is a solution of (KS) if and only if it is an optimal solution of the quadratic programming problem

$$
\begin{cases}
\min \psi(x, y, \mu_1, \mu_2) = [(x^T(C_1 y + \mu_1 e_m) + y^T(C_2^\mathsf{T} x + \mu_2 e_n)] \\
C_1 y + \mu_1 e_m \geq 0 \\
x \geq 0, \quad \sum_{i=1}^{m} x_i = 1 \\
C_2^\mathsf{T} x + \mu_2 e_n \geq 0 \\
y \geq 0, \quad \sum_{j=1}^{n} y_j = 1
\end{cases}
\qquad (QP)
$$

and $\psi(\bar{x}, \bar{y}, \mu_1, \mu_2) = 0$.

Remark

We observe that by Theorem 3 it follows that there exists at least one Nash Equilibrium for a bimatrix game so that the optimal value of (QP) is zero.

We have:
$$\nabla\psi(x, y, \mu_1, \mu_2) = \begin{pmatrix} C_1 y + \mu_1 e_m + C_2 y \\ C_1^T x + C_2^T x + \mu_2 e_n \\ e_m^T x \\ e_n^T y \end{pmatrix}$$

The Hessian matrix of ψ is given by:

$$H = \begin{pmatrix} O_{m\times m} & C_1 + C_2 & e_m & O_{m\times 1} \\ C_1^T + C_2^T & O_{n\times n} & O_{n\times 1} & e_n \\ e_m^T & O_{1\times n} & 0 & 0 \\ O_{1\times m} & e_n^T & 0 & 0 \end{pmatrix}$$

Let us write the constraints in the standard matrix form:

$$A_{in} = \begin{pmatrix} -C_2^T & O_{n\times n} & O_{n\times 1} & -e_n \\ O_{m\times m} & -C_1 & -e_m & O_{m\times 1} \end{pmatrix} \quad b_{in} = \begin{pmatrix} O_{n\times 1} \\ O_{m\times 1} \end{pmatrix}$$

$$A_{eq} = \begin{pmatrix} 1 & \cdot & \cdot & 1 & 0 & \cdot & \cdot & 0 & 0 & 0 \\ 0 & \cdot & \cdot & 0 & 1 & \cdot & \cdot & 1 & 0 & 0 \end{pmatrix} \quad b_{eq} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Let
$$w^T = (x^T, y^T) \quad \mu^T = (\mu_1, \mu_2).$$

Problem (QP) can be written in the following matrix form:

$$\begin{cases} \min \psi(w, \mu) = \frac{1}{2}(w^T, \mu^T) H \begin{pmatrix} w \\ \mu \end{pmatrix} \\ A_{in} \begin{pmatrix} w \\ \mu \end{pmatrix} \leq b_{in} \\ A_{eq} \begin{pmatrix} w \\ \mu \end{pmatrix} = b_{eq} \\ w \geq 0, \end{cases} \qquad (QP)$$

Matlab commands

C1=[.........]; C2=[.........];

[m,n] = size(C1);

H=[zeros(m,m),C1+C2,ones(m,1), zeros(m,1);
C1'+C2',zeros(n,n),zeros(n,1),ones(n,1); ones(1,m), zeros(1,n+2);
zeros(1,m),ones(1,n),0,0];

X0=[.............]; % $m + n + 2$ vector

Ain=[-C2', zeros(n,n),zeros(n,1),-ones(n,1);
zeros(m,m), -C1,-ones(m,1),zeros(m,1)]; bin=zeros(n+m,1);

Aeq=[ones(1,m),zeros(1,n+2);zeros(1,m),ones(1,n),0,0]; beq=[1;1];

LB=[zeros(m+n,1);-Inf;-Inf]; UB=[ones(m+n,1);Inf;Inf];

[sol,fval,exitflag,output]=fmincon(@(X) 0.5*X'*H*X, X0, Ain,bin,
Aeq,beq,LB,UB)

x = sol(1:m)

y = sol(m+1:m+n)

Exercise 4

Consider the problem defined in Exercise 3.

(a) Find by Matlab a mixed strategies Nash equilibrium.

(b) Try to find different Nash equilibria by varying the starting point $X0$ (multistart approach).

Exercise 5

Consider the problem defined in Example 5:

$$C_1 = \begin{pmatrix} -5 & 0 \\ 0 & -1 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -1 & 0 \\ 0 & -5 \end{pmatrix}$$

(a) Find by Matlab a mixed strategies Nash equilibrium.

(b) Try to find different Nash equilibria by a multistart approach.

Convex games

Now, we consider a general two-persons non-cooperative game

Player 1: $\begin{cases} \min_x \ f_1(x,y) \\ g_i^1(x) \le 0 \ \ \forall \ i = 1,..,p \end{cases}$ Player 2: $\begin{cases} \min_y \ f_2(x,y) \\ g_j^2(y) \le 0 \ \ \forall \ j = 1,..,q \end{cases}$

where f_1, g^1, f_2 and g^2 are continuously differentiable.
The game is said convex if the optimization problem of each player is convex.

Theorem

If the feasible regions $X = \{x \in \mathbb{R}^m : \ g_i^1(x) \le 0 \ \ i = 1, \ldots, p\}$ and $Y = \{y \in \mathbb{R}^n : \ g_j^2(y) \le 0 \ \ j = 1, \ldots, q\}$ are closed, convex and bounded, the cost function $f_1(\cdot, y)$ is quasiconvex for any $y \in Y$ and $f_2(x, \cdot)$ is quasiconvex for any $x \in X$, then there exists at least a Nash equilibrium.

Remark

The quasiconvexity of the cost functions is crucial. For example, the game defined as $X = Y = [0, 1]$, $f_1(x, y) = -x^2 + 2xy$, $f_2(x, y) = y(1 - 2x)$ has no Nash equilibrium.

Theorem

- If $(\bar{x}, \bar{y})$ is a Nash equilibrium and the Abadie constraints qualification holds both in $\bar{x}$ and $\bar{y}$, then there exist $\lambda^1 \in \mathbb{R}^p$, $\lambda^2 \in \mathbb{R}^q$ such that

$$
\begin{cases}
\nabla_x f_1(\bar{x}, \bar{y}) + \sum_{i=1}^{p} \lambda_i^1 \nabla g_i^1(\bar{x}) = 0 \\
\lambda^1 \geq 0, \qquad g^1(\bar{x}) \leq 0 \\
\lambda_i^1 g_i^1(\bar{x}) = 0, \quad i = 1, \ldots, p \\
\nabla_y f_2(\bar{x}, \bar{y}) + \sum_{j=1}^{q} \lambda_j^2 \nabla g_j^2(\bar{y}) = 0 \\
\lambda^2 \geq 0, \qquad g^2(\bar{y}) \leq 0 \\
\lambda_j^2 g_j^2(\bar{y}) = 0, \quad j = 1, \ldots, q
\end{cases}
$$

- If $(\bar{x}, \bar{y}, \lambda^1, \lambda^2)$ solves the above system and the game is convex, then $(\bar{x}, \bar{y})$ is a Nash equilibrium.

Exercise 6

Consider the following convex game:

Player 1: $\begin{cases} \min\limits_{x} x^2 - x(2y+2) \\ -3 \le x \le 2 \end{cases}$ Player 2: $\begin{cases} \min\limits_{y} (x+2)(1-y) \\ -1 \le y \le 3 \end{cases}$

(a) Find the Nash equilibria by using KKT conditions.

(b) Find the Nash equilibria by using the best response mappings.

(a) The KKT conditions are:

$$\begin{cases} 2x - 2y - 2 - \lambda_1^1 + \lambda_2^1 = 0 \\ \lambda_1^1(-x-3) = \lambda_2^1(x-2) = 0 \\ \lambda^1 \ge 0, \;\; -3 \le x \le 2 \\ -x - 2 - \lambda_1^2 + \lambda_2^2 = 0 \\ \lambda_1^2(-1-y) = \lambda_2^2(y-3) = 0 \\ \lambda^2 \ge 0, \;\; -1 \le y \le 3 \end{cases} \qquad (KKT)$$

where $\lambda^1 = (\lambda_1^1, \lambda_2^1), \quad \lambda^2 = (\lambda_1^2, \lambda_2^2)$.

Consider the variable x; we have the following cases:

I) $-3 < x < 2$;

II) $x = -3$;

III) $x = 2$.

Case I) System (KKT) becomes:

$$\begin{cases} 2x - 2y - 2 = 0 \\ \lambda^1 = 0, -3 < x < 2 \\ -x - 2 - \lambda_1^2 + \lambda_2^2 = 0 \\ \lambda_1^2(-1 - y) = \lambda_2^2(y - 3) = 0 \\ \lambda^2 \geq 0, \ -1 \leq y \leq 3 \end{cases} \qquad (KKT1)$$

By the first equation $x = y + 1$ and substituting in the other relations:

$$\begin{cases} x = y + 1 \\ \lambda^1 = 0, -4 < y < 1 \\ -y - 3 - \lambda_1^2 + \lambda_2^2 = 0 \\ \lambda_1^2(-1 - y) = \lambda_2^2(y - 3) = 0 \\ \lambda^2 \geq 0, \ -1 \leq y \leq 3 \end{cases}$$

Notice that $y < 1 \quad \Rightarrow \lambda_2^2 = 0$, so that the system becomes:

$$
\begin{cases}
x = y + 1 \\
\lambda^1 = 0, \\
-y - 3 - \lambda_1^2 = 0 \\
\lambda_1^2(-1 - y) = 0 \\
\lambda_1^2 \geq 0, \lambda_2^2 = 0 \quad -1 \leq y < 1
\end{cases}
$$

which turns out to be impossible as it can be easily checked (consider that $\lambda_1^2 = -y - 3$).

Case II) $x = -3$. System (KKT) becomes:

$$
\begin{cases}
-6 - 2y - 2 - \lambda_1^1 = 0, \\
\lambda_1^1 \geq 0, \lambda_2^1 = 0, \quad x = -3 \\
1 - \lambda_1^2 + \lambda_2^2 = 0 \\
\lambda_1^2(-1 - y) = \lambda_2^2(y - 3) = 0 \\
\lambda^2 \geq 0, \quad -1 \leq y \leq 3
\end{cases}
\qquad (KKT2)
$$

The previous system is impossible, indeed by the first equation

$$-2y - 8 = \lambda_1^1 \geq 0 \Rightarrow y \leq -4$$

which contradicts $y \geq -1$.

Case III) $x = 2$. System (KKT) becomes:

$$\begin{cases} 4 - 2y - 2 + \lambda_2^1 = 0, \\ \lambda_1^1 = 0, \lambda_2^1 \geq 0, \quad x = 2 \\ -4 - \lambda_1^2 + \lambda_2^2 = 0 \\ \lambda_1^2(-1 - y) = \lambda_2^2(y - 3) = 0 \\ \lambda^2 \geq 0, \ -1 \leq y \leq 3 \end{cases} \qquad (KKT3)$$

Clearly λ_1^2 and λ_2^2 cannot be simultaneously 0 (so we have the two possibilities $y = -1$ and $y = 3$). By the first equation

$$2y - 2 = \lambda_2^1 \geq 0 \Rightarrow y \geq 1$$

so that we have the solution $y = 3$, $x = 2$ with $\lambda_1^1 = \lambda_1^2 = 0$, $\lambda_2^1 = \lambda_2^2 = 4$.

Therefore $(\bar{x}, \bar{y}) = (2, 3)$ is a Nash equilibrium.

(b) Let us solve the problem by means of the best response mappings $B_1(y)$ and $B_2(x)$.

In order to find $B_1(y)$, given $y \in Y$ we have to solve the problem

$$P_1(y) : \begin{cases} \min_x x^2 - x(2y + 2) \\ -3 \le x \le 2 \end{cases}$$

Notice that the unconstrained minimum of $P_1(y)$ is in the point $x(y) = y + 1$. Then $x(y)$ is the global minimum of $P_1(y)$ if

$$-3 \le y + 1 \le 2, \quad i.e., \quad -4 \le y \le 1.$$

Similarly, the global minimum point of $P_1(y)$ is

- $x = -3$, for $y + 1 < -3$, $\quad i.e., \quad y < -4$;
- $x = 2$, $\quad$ for $y + 1 > 2$, $\quad i.e., \quad y > 1$.

Hence the optimal solutions of $P_1(y)$ are

$$B_1(y) = \begin{cases} y + 1 & \text{if } y \in [-1, 1] \\ 2 & \text{if } y \in [1, 3] \end{cases}$$

In order to find $B_2(x)$, given $x \in X$ we have to solve the problem

$$P_2(x) : \begin{cases} \min_{y} \ (x+2)(1-y) \\ -1 \leq y \leq 3 \end{cases}$$

It is easy to see that the optimal solutions of $P_2(x)$ are:

- $y = 3$, for $x + 2 > 0$,
- $y \in [-1, 3]$ for $x = -2$,
- $y = -1$ for $x + 2 < 0$.

Hence,

$$B_2(x) = \begin{cases} -1 & \text{if } x \in [-3, -2) \\ [-1, 3] & \text{if } x = -2 \\ 3 & \text{if } x \in (-2, 2] \end{cases}$$

By drawing the respective graphs of B_1 and B_2, it can be checked that the only couple $(\bar{x}, \bar{y})$ such that $\bar{x} \in B_1(\bar{y})$, $\bar{y} \in B_2(\bar{x})$ is $(\bar{x}, \bar{y}) = (2, 3)$.

Exercise 7 (Exam 6/26/2023)

Consider the following matrix game:

$$C = \begin{pmatrix} 5 & 4 & 3 & 5 \\ 6 & 7 & 8 & 2 \\ 5 & 3 & 4 & 4 \end{pmatrix}$$

(a) Find the set of pure strategies Nash equilibria, if any. Alternatively, show that no pure strategy Nash equilibrium exists.

(b) Find a mixed strategy Nash equilibrium which is not a pure strategy Nash equilibrium, if any. Alternatively, show that no Nash equilibrium of such kind exists.

SOLUTION (a) Considering Player 1, the possible couples of pure strategies Nash equilibria could be $(1,1)$, $(3,1)$, $(3,2)$, $(1,3)$ and $(2,4)$ (minimal components on the columns), while considering Player 2 the pure strategies Nash equilibria could be $(1,1)$, $(1,4)$, $(2,3)$ and $(3,1)$ (maximal components on the rows). The common couples $(1,1)$ and $(3,1)$ are pure strategies Nash equilibria.

(b) Consider the linear optimization problem associated with Player 1:

$$\begin{cases} \min & v \\ 5x_1 + 6x_2 + 5x_3 \le v \\ 4x_1 + 7x_2 + 3x_3 \le v \\ 3x_1 + 8x_2 + 4x_3 \le v \\ 5x_1 + 2x_2 + 4x_3 \le v \\ x_1 + x_2 + x_3 = 1 \\ x \ge 0 \end{cases} \tag{4}$$

Pure strategies for Player 1 correspond to the solutions $(x^1, v^1) = (1, 0, 0, 5)$ and $(x^2, v^2) = (0, 0, 1, 5)$ and $y = (1, 0, 0, 0, 5)$ is a dual solution of (4) associated with the pure strategy $(1, 0, 0, 0)$ of Player 2. Since the problem is linear then any convex combination

$$\alpha(x^1, v^1) + (1 - \alpha)(x^2, v^2), \quad \alpha \in [0, 1]$$

is an optimal solution of (4).
For example, for $\alpha = \frac{1}{2}$ we obtain the solution $\hat{x} = (\frac{1}{2}, 0, \frac{1}{2}, 5)$ so that

$$\hat{x} = (\frac{1}{2}, 0, \frac{1}{2}), \quad \hat{y} = (1, 0, 0, 0)$$

is a mixed-strategies Nash equilibrium.

For further exercises see the Microsoft Teams platform of the course and the web page of prof. Mauro Passacantando:

https://people.unipi.it/mauro_passacantando/wp-content/uploads/sites/208/2020/05/exercises_games.pdf

Answer the questions from points (a) to (c) and (e).