Diagrams of

OPTIMIZATION METHODS AND GAME THEORY

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Preface

This collection of diagrams / schematizations was done after having followed the “**Optimization Methods and Game Theory**” course held by ***prof. Mauro Passacantando*** in the academic year 2020/21. The present work doesn’t in any way try to replace the material of the professor, but instead must be considered as an auxiliary material for better generalizing the concepts studied during the course when repeating theory for the oral exam. You’ll obtain the maximum from these diagrams if you’ll follow prof. Passacantando’s lectures, study from his slides and the advised additional books, and then and only then come here to repeat at a fast pace every concept of the course.

As a **disclaimer**, I’ll just say that any material done by a student isn’t error-free and, if you will spot an error, please send a message about it in one of the AIDE course’s Telegram groups with the tag “[OMGT-DIAGRAMS]” and afterwards you’ll be gladly included in the **Thanking section**.

I will conclude this preface by wishing you the best of luck for your exam.

Luigi Gjoni

Thanking section

Here I’ll list whoever has given its contribution in improving the current material.

Legenda

- “w/” = “with”
- “w/o” = “without”
- “w.r.t.” = “with respect to”
- “s.t.” = “such that”
- Mathematical symbols :
    - “ $\forall$ ” = “for each” or “for all”.
    - “ $\exists$ ” = “there exists (at least) one element”
    - “ $\nexists$ ” = “there doesn’t exist any element”
    - “ $\exists!$ ” = “there exists only one element”
    - “ $x\uparrow \Rightarrow y\uparrow$ ” = “there exists a direct proportion relationship between x and y”
    - “ $x\uparrow \Rightarrow y\downarrow$ ” = “there exists an inverse proportion relationship between x and y”

SUBLEVEL SETS

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

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

is called **α-sublevel** set of f.
TH : if f is convex $\implies$ $S_\alpha(f)$ is a convex set $\forall \alpha \in \mathbb{R}$.
Is the opposite of this TH(eorem) true, i.e. if we start from a convex set $S_\alpha(f)$, can we say that f(x) is convex? No, think about functions like $x^3, log(x), etc$

QUASICONVEX FUNCTIONS

- Given a convex set $C \subseteq \mathbb{R}^n$, a function $f : C \to \mathbb{R}$ is **quasiconvex** if the α-sublevel sets are convex $\forall \alpha \in \mathbb{R}$.
- f is said **quasiconcave** if <u>-f is quasiconvex</u>.
- e.g.
  - $f(x) = \sqrt{x}$ 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
  - $f(x) = ceil(x) = = inf\{z \in \mathbb{Z} : z \ge x\}$ is quasiconvex and quasiconcave.

OPERATIONS THAT PRESERVE CONVEXITY

- <u>**sum** (or difference) of convex sets is convex</u>: this operation must be intended as vector sum of any two points, one of C_1 and the other belonging to C_2, i.e.

$$C_1 + C_2 := \{x + y : x \in C_1, y \in C_2\}$$

- <u>**intersection** of convex sets is convex as well</u>.
- <u>**union**</u> : if I have two separated convex sets of points and I unite these sets, I may not get a convex set $\implies$ <u>no convexity guarantee</u>
- <u>**Interior**</u> **set** : it is the set of all points s.t., chosen an arbitrarily small ϵ and a point $\notin$ border of the set, the circle pictured around one of these points includes only points of the set. In other word, it is the <u>set w/o the border points</u>. If C is convex $\implies$ <u>interior(C) is convex as well</u>.
- <u>**Closure**</u> **set** : <u>for closed sets (!!!), the closure coincides with the set itself</u>, thus if C is convex $\implies$ <u>closure(C) is convex as well</u>.

- **Affine functions** :
  - if $C \subseteq \mathbb{R}^n$ is convex $\implies$ $f(C) = \{f(x) : x \in C\}$
  - if $C \subseteq \mathbb{R}^m$ is convex $\implies$ $f^{-1}(C) = \{x \in \mathbb{R}^n : f(x) \in C\}$
  - e.g. :
    - **scaling** : $f(x) = a\,x,\ with\ a > 0$
    - **translation** : $f(x) = x + b,\ with\ b \in \mathbb{R}^n$
    - **rotation** : $f(x) = \begin{pmatrix} cos\theta & -sin\theta \\ sin\theta & cos\theta \end{pmatrix} x,$ with $\theta \in [0, 2\pi]$
- THEOREMs :
  1. $f(x)$ convex and $\alpha > 0 \implies \alpha f(x)$ convex
  2. $f_1(x), f_2(x)$ convex functions $\implies f_1 + f_2$ convex
  3. $f(x)$ convex $\implies f(Ax + b)$ convex

  e.g. :
  - **Log barrier for linear inequalities** :

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

  - **Norm of affine function** :

$$f(x) = ||Ax + b||$$

- **Pointwise maximum** :
  - Given the convex functions $f_1, \dots, f_m$, we have that $f(x) = max\{f_1(x), \dots, f_m(x)\}$ is convex.
  - If $\{f_i\}_{i \in I}$ is a family of convex functions $\implies$ $f(x) = \sup_{i \in I} f_i(x) is convex$
- **Composition of functions** $f : \mathbb{R}^n \to \mathbb{R}, g : \mathbb{R} \to \mathbb{R}$:
  - THEOREMs :
    - f convex and g convex and nondecreasing $\implies g \circ f$ convex
    - f concave and g convex and nonincreasing $\implies g \circ f$ convex
    - f concave and g concave and nondecreasing $\implies$ $g \circ f$ concave
    - f convex and g concave and nonincreasing $\implies g \circ f$ concave
    - e.g. :
      - f convex $\implies$ $e^{f(x)}$ convex
      - f concave and positive $\implies$ $log(f(x))$ concave

2nd ORDER CONDITIONs

- Assume that :
  - $C \subseteq \mathbb{R}^n$ is **open** and **convex**
  - $f : C \to \mathbb{R}$ is <u>**twice**</u> **continuosly differentiable**.

- THEOREM : f is convex $\iff$ $\forall x \in C$, the **hessian matrix** $\nabla^2 f(x)$ is <u>**positive semidefinite**</u>, i.e.

$$v^T \nabla^2 f(x) v \ge 0, \forall v \ne 0$$

or, equivalently, the eigenvalues of $\nabla^2 f(x)$ are all ≥ 0

- THEOREM : if $\nabla^2 f(x)$ is <u>**positive definite**</u>, i.e.

$$v^T \nabla^2 f(x) v > 0, \forall v \ne 0$$

$\forall x \in C$, then f(x) is **strictly convex**. Equivalently, f(x) is strictly convex if the eigenvalue of its hessian matrix are all > 0.
- THEOREM : f is **strongly convex** $\iff$ $\exists \tau > 0$ s.t. $\nabla^2 f(x) - \tau I$ is positive semidefinite $\forall x \in C$, i.e.

$$v^T \nabla^2 f(x) v \ge \tau ||v||_2^2, \forall v \ne 0$$

Equivalently, the eigenvalues of the hessian matrix of f(x) should all be $\ge \tau$

1st ORDER CONDITIONS

- Assume that :
  - $C \subseteq \mathbb{R}^n$ is **open** and **convex**
  - $f : C \to \mathbb{R}$ is **continuosly differentiable**.

- THEOREM : f is convex $\iff$

$$f(y) \ge f(x) + (y - x)^T \nabla f(x), \forall x, y \in C$$

- First-order approximation of f is a **global underestimator**.
- THEOREM : f is **strictly convex** $\iff$

$$f(y) > f(x) + (y - x)^T \nabla f(x), \forall x, y \in C$$

- THEOREM : f is **strongly convex** $\iff$ $\exists \tau > 0$ s.t.

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

1. CONVEXITY

- Convex functions are quite important in the OPTIMIZATION branch of math.
- <u>Optimizing convex functions is "easy"</u> (even if, the easiness / hardness of every problem depends also on constraints and other factors).

Examples :

- $f(x) = c^T x$ is both convex and concave
- $f(x) = \frac{1}{2} x^T Q x + c^T x$, where $Q = \nabla^2 f(x)$ is :
  - convex (concave) $\iff$ Q is positive (negative) semidefinite
  - strongly convex (concave) $\iff$ Q is positive (negative) definite
- $f(x) = e^{ax}, \forall a \in \mathbb{R}$ is strictly convex, but not strongly convex. Dually, $f(x) = log(x)$ is strictly concave but not strongly concave.
- $f(x) = x^a, x > 0$ is :
  - strictly (not "strongly" because we cannot find a lower threshold τ that the $f''(x)$ function does not "touch") convex for $a < 0$ and for $a > 1$.
  - strictly concave for $0 < a < 1$
- $f(x) = ||x||$ is convex but not strictly convex.

GEOMETRIC TOOLS

CONVEX FUNCTIONs

TH

TH : f is strongly convex $\iff$ $\exists \tau > 0$ s.t.

$$f(x) - \frac{\tau}{2}||x||_2^2$$

is convex.

STRONG CONVEX FUNCTION

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

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

- if f is Strongly convex $\implies$ f is strictly convex $\implies$ f is convex

STRICT CONVEX FUNCTION

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

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

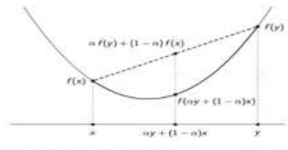
- General formula (for convex combinations of k points) :

$$f\Big(\sum_{i=1}^{k} \alpha_i\, x_i\Big) < \sum_{i=1}^{k} \alpha_i\, f(x_i), \sum_{i=1}^{k} \alpha_i = 1$$

CONVEX FUNCTION

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

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



- **General formula** (k points) with $x_1, \dots, x_k \in C$, and $\alpha_1, \dots, \alpha_k$ s.t. $\sum_{i=1}^{k} \alpha_i = 1$:

$$f\Big(\sum_{i=1}^{k} \alpha_i\, x_i\Big) \le \sum_{i=1}^{k} \alpha_i\, f(x_i)$$

- f is said **concave** if $-f$ is convex

LINEAR COMBINATION

Given the points $x, y \in \mathbb{R}^n$, a **linear combination** of x and y is a point z s.t.

$$z = ax + by, \quad a, b \in \mathbb{R}$$

SUBSPACE

A set $C \subseteq \mathbb{R}^n$ is a **subspace** if it contains all the linear combinations of any two points $x, y \in C$
E.g. :

- {0}
- Any line passing through the origin

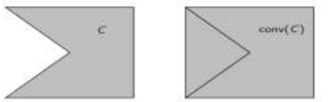
- The **solution set of a <u>homogenous</u> system of <u>linear</u> <u>equations</u>**

$$C = \{x \in \mathbb{R}^n : Ax = 0\}, \quad A \in \mathbb{R}^{m \times n}$$

with the subspace C having a dimension equal to $n - rank(A)$

CONVEX HULL

The <u>convex hull **conv(C)**</u> of a set C is the <u>smallest convex set containing C</u>.



AFFINE COMBINATION

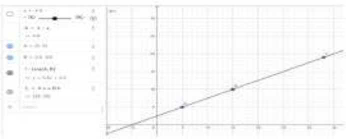
Given the points $x, y \in \mathbb{R}^n$, an **affine combination** of x and y is a point z s.t.

$$z = ax + by, \quad a, b, \in \mathbb{R}, \ a + b = 1$$

AFFINE SET

A set $C \subseteq \mathbb{R}^n$ is an **affine set** if it contains <u>all the affine combinations</u> of <u>any two points</u> $x, y \in C$
E.g. :

- any single point {x}
- any line



- The **solution set of a system of <u>linear</u> <u>equations</u>**

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

- any **subspace**

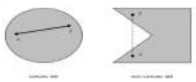
CONVEX COMBINATION

Given the points $x, y \in \mathbb{R}^n$, a **convex combination** of x and y is a point z s.t.

$$z = ax + by, \quad a, b, \in \mathbb{R}, \ a + b = 1, \ a \ge 0, b \ge 0$$

CONVEX SET

A set $C \subseteq \mathbb{R}^n$ is **convex** if it contains <u>all the convex combinations</u> of <u>any two points</u> $x, y \in C$

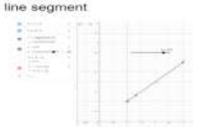


Note :

- conv(C) = {all convex combinations of points in C}
- C is convex $\iff$ C = conv(C)

E.g. :

- subspace
- affine set
- line segment



- **halfspace**

$$\{x \in \mathbb{R}^n : a^T x \le b\}$$

- **polyhedron**

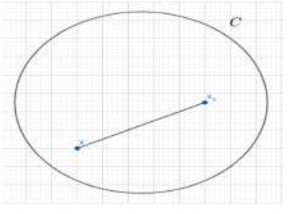
$$P = \{x \in \mathbb{R}^n : Ax \le b\}$$

solution set of a system of <u>linear inequalities</u>.

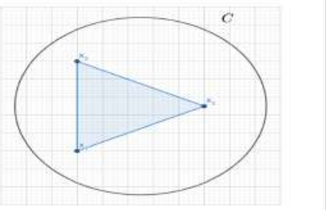
- **ball B(x,r)** = $\{y \in \mathbb{R}^n : ||y - x|| < r\}$, where the operator $|| \cdot ||$ is the norm operator (see "NORM" box for more info)

TH.

- HP :
  - $C \subseteq \mathbb{R}^n$ is convex
  - $x_1, \dots, x_k \in C$
  - $a_1, \dots, a_k \in [0, 1]$
  - $\sum_{i=1}^{k} a_i = 1$
- TH :
  $z = a_1 x_1 + \ldots + a_k x_k = = \sum_{i=1}^{k} a_i x_i \in C$
- PROOF : For simplicity, let's imagine that $C \subseteq \mathbb{R}^2$. We may further prove for n > 3.
  If C is convex, it contains all convex combinations of any two points $x_1, x_2 \in C$



If we had to take into account another point $x_3 \notin \overline{x_1\ x_2}$, the convex combination of x_1, x_2, x_3 would be the set of points inside the triangle $x_1\ x_2\ x_3$ comprehensive of the lines $\overline{x_1\ x_2}$, $\overline{x_1\ x_3}$, $\overline{x_2\ x_3}$



We can go on like this considering another point $x_4 \notin$ triangle $x_1 x_2 x_3$ and so on, generalizing up to the k-th point x_k
Same considerations may be done for $n > 2$.

C is convex $\iff$ C = conv(C)

PROOF (by contradiction) :
Let's suppose that $C \ne conv(C)$. Then, given the cardinality operator $|\cdot|$, we'd have

$$|conv(C)| > |C| \implies$$

$$\implies \exists x\ s.t.\ x \in conv(C) \wedge x \notin C,$$

where

$$x = \sum_{i=1}^{k} a_i x_i, x_i \in C\ for\ i = 1, .., k$$

$\implies$ C is not convex.
CONTRADICTION! C must be convex $\implies$

$$C \text{ is convex} \iff C = conv(C)$$

CONE

A set $C \subseteq \mathbb{R}^n$ is a cone if $a\,x \in C$ for any $x \in C$ and $a \ge 0$
E.g. :

- $\mathbb{R}^n_+$
- $\{x \in \mathbb{R}^2 : x_1 x_2 = 0\}$ is a non convex cone, because it consists essentially of the two main axes x_1, x_2, and any point on x_1 cannot be linked directly to any point of x_2, unless one of the two points is (0,0), which is the common point between the two axes. All other cases excluding the (0,0) point don't allow us to directly link points of the cone without "touching" other points $\notin C$
- Given a polyhedron $P = \{x : Ax \le b\}$, the **recession cone of P** is defined as

$$rec(P) = \{d : x + a\,d \in P, \quad \forall x \in P, a \ge 0$$

NOTE : it's easy to prove that

$$rec(P) = \{x : A\,x \le 0\},$$

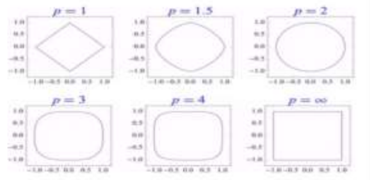
thus it is a polyhedral cone.
- $x \in \mathbb{R}^3 : x_3 \ge \sqrt{x_1^2 + x_2^2}$ is a non-polyhedral (due to the quadratic inequality) cone.

NORM

- General **p-norm** : $||x||_p = \sqrt[p]{\sum_{i=1}^{n} |x_i|^p}$, with $1 \le p < \infty$

Here is a geometrical interpretation of these different p-norms when we want to obtain a Ball

$$B(x, r) = \{y \in \mathbb{R}^n : ||y - x|| \le r\}$$



- **Manhattan** distance $(p = 1) : ||x||_1 = \sum_{i=1}^{n} |x_i|$
- **Euclidean** distance $(p = 2) : ||x||_2 = \sqrt{\sum_{i=1}^{n} |x_i|^2}$
- **Chebyshev** norm $(p = \infty) : \max_{i=1,\dots,n} |x_i|$
- **Matrix** norm : $||x||_A = \sqrt{x^T A x}$, where A is symmetric and a positive definite matrix (i.e. $x^T A x > 0$)

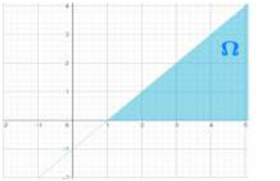
e.g. Suppose we have this problem :

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

We have to prove that this problem has a global optimum.

First, let's see the objective function $f(x_1, x_2)$: obtaining $\nabla^2 f(x_1, x_2) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ which is a diagonal matrix with at least a negative eigenvalue $\implies$ $f(x_1, x_2)$ is non-convex.

We can see that Ω is unbounded :



We may use Eaves' theorem : we first start by finding the recession directions that guarantee us that $A\,d \leq 0$.

$$rec(\Omega) = \{d \in \mathbb{R}^2 : \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} \leq 0\} \rightarrow$$

$$\rightarrow \begin{cases} d_1 \geq d_2 \\ d_2 \geq 0 \end{cases}$$

1

1ST Eaves condition :

$$d^T Q d \geq 0 \rightarrow$$

$$\rightarrow (d_1 \quad d_2) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = d_1^2 - d_2^2 =$$

$$= (d_1 - d_2)(d_1 + d_2) \geq 0$$

$d_1 \geq d_2$ and $d_2 \geq 0$ thus the whole thing inside brackets is ≥ 0

Since the 1ST condition is respected, let's test the 2ND condition : $d^T(Qx + c) \geq 0$

First let's find a recession direction d s.t. $d^T Q d = 0$. We have two options :

- $d_1 = -d_2$, not acceptable, since $d_2 \geq 0$ and $d_1 \geq d_2$
- $d_1 = d_2$, acceptable $\implies$ any vector with two equal x_1 and x_2 components is valid.

$$d^T(Qx + c) = k(1 \quad 1)\left(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} 1 \\ -2 \end{pmatrix}\right) =$$

$$= x_1 - x_2 - 1 \geq 0,$$

which is already a condition satisfied by all $x \in \Omega$, thus also 2ND condition is respected $\implies$ the problem at hand has a global optimum.

FEASIBLE REGION Ω

$\Omega = \{x \in D : g(x) \leq 0,\ h(x) = 0\}$

DOMAIN D

$D = dom(f) \cap \bigcap_{i=1}^{m} dom(g_i) \cap \bigcap_{j=1}^{p} dom(h_i)$

2. CONVEX OPTIMIZATION PROBLEMS

- Optimization problem in **standard form** :

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

  where :
  - $\boldsymbol{f} : \mathbb{R}^n \rightarrow \mathbb{R}$ is the **objective function.**
  - $g(x) = (g_1(x), .., g_m(x))$ represents a set of functions $\boldsymbol{g_i} : \mathbb{R}^n \rightarrow \mathbb{R},\ i = 1, .., m$ called **inequality constraints functions.**
  - $h(x) = (h_1(x), .., h_p(x))$ represents a set of functions $\boldsymbol{h_j} : \mathbb{R}^n \rightarrow \mathbb{R},\ j = 1, .., p$ called **equality constraints functions.**
- **Implicit constraint** : $x \in D$
- **Explicit constraints** : $g(x) \leq 0, h(x) = 0$
- An optimization problem is called convex $\iff$ 3 conditions are satisfied :
  - f is **convex**.
  - $g_i, i = 1, .., m$ are **convex**.
  - $h_j, j = 1, .., p$ are **affine** (i.e. $h_j(x) = c^T x + d$).
- We can convert maximization problems to minimization ones and viceversa in the following way : $max\{f(x) : x \in \Omega\} = -min\{-f(x) : x \in \Omega\}$

THEOREM OF EAVES

- Given a **quadratic programming problem**

$$\begin{cases} min\ \frac{1}{2}x^T Q x + c^T x \\ Ax \leq b \end{cases},$$

  we have to take into consideration the recession cone of Ω, $\boldsymbol{rec(\Omega)}$.
- The theorem says that a problem like this has a global optimum $\iff$ following conditions relative to $rec(\Omega)$ hold :
  - Q is positive semidefinite only taking into account the recession directions, i.e. $d^T Q d \geq 0, \forall d \in rec(\Omega)$
  - $\forall x \in \Omega$, $\forall d \in rec(\Omega)$ s.t. $d^T Q d = 0$ (i.e. recession directions d in which the objective function f is not strongly convex), we have that $d^T(Qx + c) \geq 0$. NOTE : $Qx + c$ is the gradient of the objective function.
- Special cases :
  - $Q = 0$ (i.e. linear programming), then the problem has a global optimum $\iff$ $d^T c \geq 0, \forall d \in rec(\Omega)$
  - Q positive definite $\implies$ both necessary and sufficient conditions are satisfied
  - Ω is bounded $\implies$ no recession cone exists $\implies$ only possible recession direction is the 0 vector $\implies$ both necessary and sufficient conditions are satisfied.

THEOREM of WEIERSTRASS

- **HP** :
  - objective function f is continuous
  - feasible region Ω is closed and bounded
- **TH** : $\exists x^* \in \Omega$ s.t. $f(x^*) \leq f(x), \forall x \in \Omega$, i.e. there exists a global optimum.
- **PROOF** :
  1. $v^* = \inf_{x \in \Omega} f(x)$
  2. Define a minimizing sequence $\{x^k\} \subseteq \Omega$ s.t. $f(x^k) \rightarrow v^*$
  3. Since $\{x^k\}$ is bounded, the Bolzano-Weierstrass theorem guarantees that $\exists$ subsequence $\{x^{k_p}\}$ converging to some point x^*
  4. Since Ω is closed, we get $x^* \in \Omega$
  5. Finally, $f(x^{k_p}) \rightarrow f(x^*)$ since f is continuous. Therefore,

$$f(x^*) = v^*,$$

  i.e. x^* is a global optimum.

COROLLARY 1

- **HP** :
  - functions f, g_i, h_j are continuous.
  - Domain D is closed.
  - Feasible region Ω is bounded
- **TH** : $\exists x^* \in \Omega$ s.t. $f(x^*) \leq f(x), \forall x \in \Omega$, i.e. there exists a global optimum.

COROLLARY 2

- **HP** :
  - function f is continuous.
  - Feasible region Ω is closed.
  - $\exists \alpha \in \mathbb{R}$ s.t. the α-sublevel set (see "SUBLEVEL SETS" in the schema "1. CONVEXITY") is nonempty and bounded.
- **TH** : $\exists x^* \in \Omega$ s.t. $f(x^*) \leq f(x), \forall x \in \Omega$, i.e. there exists a global optimum.
- **PROOF** : minimizing f on Ω is equivalent to minimizing f on $S_\alpha(f)$

COROLLARY 3

- **HP** :
  - function f is continuous and coercive, i.e.

$$\lim_{||x|| \rightarrow \infty} f(x) = +\infty$$

  - Feasible region Ω is closed.
- **TH** : $\exists x^* \in \Omega$ s.t. $f(x^*) \leq f(x), \forall x \in \Omega$, i.e. there exists a global optimum.
- **PROOF** : any sublevel set of f is bounded $\implies$ use COROLLARY 2.

COROLLARY 4

- If f is strongly convex and Ω is closed $\implies$ there exists a global optimum.
- If f is strongly convex and Ω is closed and convex $\implies$ $\exists$ **unique** global optimum.
- **PROOF** : any strongly convex function is coercive $\implies$ use COROLLARY 3.
- e.g. : any quadratic programming problem

$$\begin{cases} min\ \frac{1}{2}x^T Q x + c^T x \\ Ax \leq b \end{cases}$$

  where Q is a positive definite matrix, has a unique global optimum. What would happen if Q is positive semidefinite (i.e. some eigenvalues may be ≥ 0) or indefinite (eigenvalues $\lesseqgtr 0$) ? We wouldn't have the guarantee that our objective function is bounded from below.

THEOREM 1 (convex Ω)

- **HP** : optimization problem is convex
- **TH** : feasible region of the optimization problem is a convex set.

THEOREM 2 (Local vs Global optimum in convex optimiz. problem)

- **HP** : optimization problem is convex
- **TH** : any local optimum is a global optimum.
- **PROOF** (by contradiction) :
  1. Let x^* be a local optimum
  2. By contradiction, assume that x^* is not a global optimum, i.e. $\exists\ y\ \in \Omega s.t.$ $f(y) < f(x^*)$
  3. Take $\alpha \in [0, 1]$ s.t. $\alpha\ x^* + (1 - \alpha)y \in B(x^*, R), R > 0.$
  4. Then we have

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

  which is impossible $\implies$ x^* is also a global optimum.

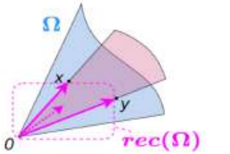
RECESSION CONE of Ω

- Given the feasible region Ω defined as

$$A\,x \leq b,$$

  the set of directions $rec(\Omega)$ is s.t. $\forall x \in \Omega$ we have

$$x + \alpha d \in \Omega, \alpha \geq 0$$



- **d** is called **recession direction**.
- We may obtain the recession cone as

$$rec(\Omega) = \{d : Ad \leq 0\}$$

OPTIMAL VALUE v^*

- Given a minimization problem

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

  the optimal value for the solution of that problem is

$$v^* = inf\{f(x) : x \in \Omega\}$$

- In some cases we may get precise values of v^* and in other cases we may not find finite optimal solutions :
  - $v^* \in \mathbb{R}$ if the problem is bounded below
  - $v^* = -\infty$ if the problem is unbounded below
  - $v^* = +\infty$ if the problem is unfeasible (i.e. $\Omega = \emptyset$)
- **Global optimal solution** : a feasible point $x^* \in \Omega$ s.t. $\forall x \in \Omega$ we have $f(x^*) \leq f(x)$
- **Local optimal solution** : a feasible point $x^* \in \Omega$ s.t. $\forall x \in \Omega \cap B(x^*, R), R > 0$ we have $f(x^*) \leq f(x)$

convex optimization problem

non-convex optimization problem

1ST ORDER OPTIMALITY CONDITIONS

UNCONSTRAINED PROBLEM

CONSTRAINED PROBLEM

TH

- **HP** : x^* is a local optimum.
- **TH** : $d^T \nabla f(x^*) \geq 0, \quad \forall d \in T_\Omega(x^*)$. i.e. every direction d in $T_\Omega(x^*)$ is not a descent direction ($d^T \nabla f(x^*) < 0$) for $f(x^*)$
- **PROOF** (by contradiction) :
  1. assume that, by contradiction, $\exists d \in T_\Omega(x^*)$ s.t.

$$d^T \nabla f(x^*) < 0$$

  2. take the sequences $\{z_k\}$ and $\{t_k\}$ s.t.

$$\lim_{k \rightarrow \infty} \frac{z_k - x^*}{t_k} = d$$

  3. Then $z_k = x^* + t_k\, d + o(t_k)$, where $\frac{o(t_k)}{t_k} \rightarrow 0$
  4. The first order approximation of f gives

$$f(z_k) = f(x^*) + t_k d^T \nabla f(x^*) + o(t_k),$$

  thus $\exists k^* \in \mathbb{N}$ s.t.

$$\frac{f(z_k) - f(x^*)}{t_k} = d^T \nabla f(x^*) + \frac{o(t_k)}{t_k} < 0, \\ \forall k > k^*$$

  i.e. $f(z_k) < f(x^*) \forall k > k^*$, which is impossible because x^* is a local optimum.

TH (NECESSARY OPTIMALITY CONDITION)

- **HP** : considering an unconstrained problem

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

  we have a local optimum x^*
- **TH** : $\nabla f(x^*) = 0$
- **PROOF** (by contradiction) : Assume that $\nabla f(x^*) \neq 0$. Choose direction $d = -\nabla f(x^*)$, define $\varphi(t) = f(x^* + t\,d)$:

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

  thus $f(x^* + t\,d) < f(x^*)$ for any t small enough, but x^* is a local optimum $\implies$ CONTRADICTION!
- Optimality condition for unconstrained convex problems : if f is convex, then x^* is a global optimum $\iff$ $\nabla f(x^*) = 0$

TANGENT CONE $T_\Omega(x)$

- Given $x \in \Omega$, the set

$$T_\Omega(x) = \left\{ d \in \mathbb{R}^n : \begin{array}{l} \exists\{z_k\} \subset \Omega, \\ z_k \rightarrow x, \\ \exists\{t_k\} > 0, \\ t_k \rightarrow 0 \\ \lim_{k \rightarrow \infty} \frac{z_k - x}{t_k} = d \end{array} \right\}$$

  z_k is a sequence of points $\in \Omega$ that get closer and closer to x

  t_k is a sequence of positive numbers that tend to 0

  is called tangent cone to Ω at x
- What would $T_\Omega(x^*)$ be?

PROPERTIES of $T_\Omega(x)$

1ST ORDER FEASIBLE DIRECTION CONE

- $T_\Omega(x)$ is related to **geometric** properties of $Omega$. Recalling the standard form of an optimization problem

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

  we define :
  - set $\boldsymbol{A(x)} = \{i : g_i(x) = 0\}$, i.e. the set of inequality contraints which are **active** at x.
  - set $\boldsymbol{D(x)} = \left\{ d \in \mathbb{R}^n : \begin{array}{l} d^T \nabla g_i(x) \leq 0 \quad \forall i \in A(x), \\ d^T \nabla h_j(x) = 0 \quad \forall j = 1, .., p \end{array} \right\}$

    called first-order feasible direction cone at x

TH

$T_\Omega(x) \subseteq D(x) \quad \forall x \in \Omega$

ABADIE CONSTRAINTS QUALIFICATION (ACQ)

If $T_\Omega(x) = D(x) \implies$ ACQ holds at point x. However we cannot "simply" verify this condition in real life applications with many dimensions, because we are comparing a set ($\boldsymbol{T_\Omega(x)}$) that is geometrically defined w.r.t. Ω with another set that has been defined in an algebric way ($\boldsymbol{D(x)}$).

NOTE : in general, ACQ doesn't hold at any $x \in \Omega$

TH : SUFFICIENT CONDITIONS FOR ACQ

ACQ holds at $\hat{x} \in \Omega$ for any of the following three conditions :

- **Affine constraints**
  - g_i are affine $\forall i = 1, .., m$
  - h_j are affine $\forall j = 1, .., p$
- **Slater condition**
  - g_i are convex $\forall i = 1, .., m$
  - h_j are affine $\forall j = 1, .., p$
  - $\exists \hat{x} \in int(D)$ s.t. $g(\hat{x}) < 0$ (i.e. no inequality constraint is active at the point $\hat{x}$) and $h(\hat{x}) = 0$, with $int(D)$ being the interior set of the domain D.
- **Linear independence of the gradients of active constraints** $\hat{x} \in \Omega$ and the vectors

$$\begin{cases} \nabla g_i(\hat{x}) & i \in A(\hat{x}) \\ \nabla h_j(\hat{x}) & j = 1, .., p \end{cases}$$

  are linearly independent.

KARUSH-KUHN-TUCKER (KKT) THEOREM

- **HP** :
  - x^* is a local optimum
  - ACQ holds at x^*
- **TH** : $\exists \lambda^* \in \mathbb{R}^m$ and $\exists \mu^* \in \mathbb{R}^p$ s.t. (x^*, λ^*, μ^*) satisfies the KKT system

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

- NOTE : ACQ assumption is crucial in the KKT theorem.
- KKT Theorem gives necessary optimality conditions but not sufficient ones.

KKT TH for CONVEX PROBLEMS

- **HP** :
  - optimization problem is convex.
  - (x^*, λ^*, μ^*) solves KKT system
- **TH** : x^* is a global optimum.

TH (NECESSARY OPTIMALITY CONDITION)

- **HP** : Ω is convex.
- **TH** : $\Omega \subseteq T_\Omega(x) + x, \forall x \in \Omega$
- Optimality condition for constrained convex problems : x^* is a global optimum $\iff$

$$\iff (y - x^*)^T \nabla f(x^*) \geq 0, \quad \forall y \in \Omega$$

2ND ORDER OPTIMALITY CONDITIONS

LAGRANGIAN FUNCTION

- Definition :

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

- **Necessary condition** :
  - **HP** :
    - (x^*, λ^*, μ^*) solves KKT system
    - gradients of active constraints are linearly independent
    - x^* is a local optimum
  - **TH** : $d^T \nabla_{XX}^2 L(x^*, \lambda^*, \mu^*) \geq 0$ $\forall d \in C(x^*, \lambda^*, \mu^*)$ where $\nabla_{XX}^2 L(x^*, \lambda^*, \mu^*)$ = hessian matrix of $L(\cdot, \lambda^*, \mu^*)$ at x^*
  - Special case of unconstrained problems : if x^* is a local optimum, then $\nabla^2 f(x^*)$ is positive semidefinite.
- **Sufficient condition** :
  - **HP** :
    - x^*, λ^*, μ^* solves KKT system
    - $d^T \nabla_{XX}^2 L(x^*, \lambda^*, \mu^*) d > 0$ $\forall d \in C(x^*, \lambda^*, \mu^*), d \neq 0$
  - **TH** : x^* is a local optimum
  - Special case of unconstrained problems : if $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite, then x^* is a local optimum.

CRITICAL CONE

- If (x^*, λ^*, μ^*) solves the KKT system, then the **critical cone** is defined as

$$\boldsymbol{C(x^*, \lambda^*, \mu^*)} \begin{cases} d \in \mathbb{R}^n : \\ d^T \nabla g_i(x^*) = 0 \quad \forall i \in A(x^*), \lambda_i^* > 0, \\ d^T \nabla g_i(x^*) \leq 0 \quad \forall i \in A(x^*), \lambda_i^* = 0, \\ d^T \nabla h_j(x^*) = 0 \quad \forall j = 1, .., p \end{cases}$$

- Equivalent definition :

$$\boldsymbol{C(x^*, \lambda^*, \mu^*)} = \{d \in D(x^*) : d^T \nabla f(x^*) = 0\}$$

3. LAGRANGIAN DUALITY

- Given the following general optimization problem P

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

where $x \in D$ and the optimal value is $v(P)$, the **Lagrangian dual problem of (P)** is

$$\begin{cases} max\ \varphi(\lambda, \mu) \\ \lambda \geq 0 \end{cases} \qquad \text{(D)}$$

- Dual problem consists in <u>finding the best lower bound</u> of $v(P)$
- **PRO** :
  - Dual problem is an <u>always convex</u> problem, independently from the convexity (or not) of (P)

LAGRANGIAN RELAXATION OF (P)

- The Lagrangian function $L : D \times \mathbb{R}^n \times \mathbb{R}^p \rightarrow \mathbb{R}$ of (P) is

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

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

$$\begin{cases} min\ L(x, \lambda, \mu) \\ x \in D \end{cases} \quad \text{(Lagr. relaxat. of P)}$$

is called **Lagrangian relaxation of P**. Why relaxation of (P) ? When we solve the lagrangian relaxation of (P), we are actually finding a lower bound for the optimal value $v(P)$ of the primal problem (P).

LAGRANGIAN DUAL FUNCTION

- $$\boldsymbol{\varphi(\lambda, \mu)} = \inf_{x \in D} L(\lambda, \mu) \quad \text{(Lagr. dual function)}$$

  is called the **Lagrangian dual function**.
- Dual function $\boldsymbol{\varphi}$
  - is **concave** because of inf of linear functions w.r.t. λ, μ
  - it can be $-\infty$ at some point.
  - may not be differentiable at some point.

TH

- **HP** :
  - $\lambda \geq 0$
  - $\mu \in \mathbb{R}^p$
- **TH** : $\varphi(\lambda, \mu) \leq v(P)$
- **PROOF** : if $x \in \Omega$, i.e. $g(x) \leq 0$, $h(x) = 0$, then

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

therefore

$$\varphi(\lambda, \mu) = \min_{x \in D} L(x, \lambda, \mu) \leq$$
$$\leq \min_{x \in \Omega} L(x, \lambda, \mu) \leq$$
$$\leq \min_{x \in \Omega} f(x) =$$
$$\leq v(P)$$

TH - WEAK DUALITY

- **TH** : $\forall$ optimization problem (P) we have that $v(D) < v(P)$

TH - STRONG DUALITY

- $$v(D) = v(P)$$

  Note : strong duality doesn't hold, in general.
- **HP** :
  - Optimization problem (P)

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

  is <u>convex</u>.
- **TH** : $\exists x^*$ and ACQ holds at x^*, then :
  - KKT multipliers (λ^*, μ^*) associated to x^* are a global optimum of the dual problem
  - $v(D) = v(P)$
- **PROOF** : $L(x, \lambda, \mu)$ is convex w.r.t. x, thus

$$v(D) \geq \varphi(\lambda^*, \mu^*) = \min_x L(x, \lambda^*, \mu^*) =$$
$$= L(x^*, \lambda^*, \mu^*) =$$
$$= f(x^*) =$$
$$= v(P) \geq$$
$$\geq v(D) \implies$$
$$\implies v(D) = v(P)$$

- Note : strong duality can hold also for some non-convex problems.

4. SUPERVISED PATTERN CLASSIFICATION

- Given a set of objects partitioned in several classes with **known labels**, we want to **predict** the class of any new future object with **unknown label**.
  E.g. : spam filtering, credit card fraud detection, marketing, medical diagnosis, etc.
- Commonly used methods :
  - **Decision trees**
  - **Artificial Neural Networks**
  - **SVMs** (Support Vector Machines)

SVM (Support Vector Machine)

Supervised learning model with associated learning algorithms that analyze data for both **classification** and **regression analysis**.

TYPES OF SVMs

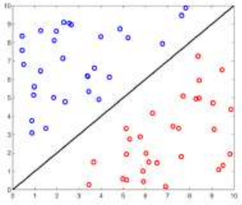
Linear SVM

- **Binary classification** :
  - given two sets $A, B \subset \mathbb{R}^n$ (**training set**), assume that A and B are linearly separable, i.e. there's an hyperplane

$$H = \{x \in \mathbb{R}^n : w^T x + b = 0\}$$

s.t.

$$\begin{aligned} w^T x_{A,i} + b > 0, \qquad \forall x_{A,i} \in A \\ w^T x_{B,j} + b < 0, \qquad \forall x_{B,j} \in B \end{aligned}$$



  - How to classify new data : use the decision function

$$f(x) = sign(w^T x + b) = \\ = \begin{cases} 1 & w^T x + b > 0 \\ -1 & w^T x + b < 0 \end{cases}$$

  - **Linear SVM** for binary classification problem : let $l = |A \cup B|$. $\forall x_i \in A \cup B$, define a label y_i s.t.

$$y_i = \begin{cases} 1 & x_i \in A \\ -1 & x_i \in B \end{cases}$$

  - Then, the **problem** (1) in "TH (MAX MARGIN)" becomes equivalent to

$$\begin{cases} \min\limits_{w,b} \frac{1}{2}||w||^2 & \qquad \boldsymbol{(Linear\ SVM)} \\ 1 - y_i(w^T x_i + b) \leq 0 & i = 1, .., l \end{cases}$$

  - Details on dual problem of $(Linear\ SVM)$:
    - it's a **convex** quadratic programming problem.
    - Dual constraints (lower bound 0 on variables and just one equality constraint) are **simpler** than primal constraints.
    - Dual problem **has optimal solution**(s) : each KKT multiplier λ^* associated to the primal optimum (w^*, b^*) is a dual optimum.
    - If $\exists i\ s.t.\ \lambda_i^* > 0 \implies x_i$ is called **support vector**.
    - If λ^* is a dual optimum $\implies$

$$\implies w^* = \sum_{i=1}^{l} \lambda_i^* y_i x_i$$

    - b^* is obtained by using the complementarity conditions :

$$\lambda_i^* \Big(1 - y_i\big((w^*)^T x_i\big)\Big) = 0$$

      Indeed, if i is s.t. $\lambda_i^* > 0$, then $b^* = \frac{1}{y_i} - (w^*)^T x_i$
    - Finally, the decision function'd be

$$f(x) = sign\big((w^*)^T x + b^*\big)$$

  - What if A, B are not linearly separable? Use **Linear SVM with soft margins**! The linear system

$$1 - y_i(w^T x_i + b) \leq 0 \quad i = 1, .., l$$

    has no solutions, thus we introduce the **slack variables** $\boldsymbol{\xi_i} \geq 0$ and consider the (relaxed) system

$$\begin{aligned} 1 - y_i(w^T x_i + b) \leq \xi_i \quad & i = 1, .., l \\ \xi_i \geq 0 \quad & i = 1, .., l \end{aligned}$$

    If x_i is misclassified $\implies \xi_i > 1 \implies \sum_{i=1}^{l} \xi_i$ is an upper bound of the number of misclassified points.
    Here's the **Linear SVM problem with soft margins** :

$$\begin{cases} \min\limits_{w,b,\xi} \frac{1}{2}||w||^2 + C\sum_{i=1}^{l} \xi_i & \begin{pmatrix} \boldsymbol{Linear\ SVM} \\ \boldsymbol{with\ soft\ margins} \end{pmatrix} \\ 1 - y_i(w^T x_i + b) \leq \xi_i & i = 1, .., l \\ \xi_i \geq 0 & i = 1, .., l \end{cases}$$

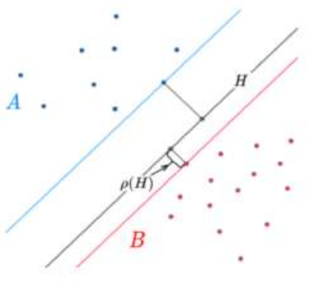
    and here's its dual problem :

$$\begin{cases} \max\limits_{\lambda} -\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} y_i y_j (x_i)^T x_j \lambda_i \lambda_j + \sum_{i=1}^{l} \lambda_i \\ \sum_{i=1}^{l} \lambda_i y_i = 0 & \begin{pmatrix} \boldsymbol{Dual\ of\ Linear\ SVM} \\ \boldsymbol{with\ soft\ margins} \end{pmatrix} \\ 0 \leq \lambda_i \leq C & i = 1, \ldots, l \end{cases}$$

MARGIN OF SEPARATION (of an hyperplane)

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

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



TH (MAX MARGIN)

- Summary : we have to look for the separating hyperplane with the max margin of separation.
- NOTE : it can be further proved that the following problem (1) has a **unique** solution (w^*, b^*)
- **TH** : finding the separating hyperplane with max margin of separation is equivalent to solving the following convex quadratic problem

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

- **PROOF** : If $H = \{w^T x + b = 0\}$ is a separating hyperplane, then there $\exists\ \alpha > 0, \beta > 0$ s.t.

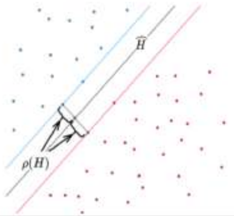
$$\begin{aligned} w^T x_{A,i} + b \geq \ \ \alpha \qquad & \forall x_{A,i} \in A \\ w^T x_{B,j} + b \leq -\beta \qquad & \forall x_{B,j} \in B \end{aligned}$$

  Then, the hyperplane $\widehat{H} = \{\widehat{w}^T x + \hat{b} = 0\}$, with
  - $\widehat{w} = \dfrac{2\,w}{\alpha + \beta}$,
  - $\hat{b} = \dfrac{2\,b - \alpha + \beta}{\alpha + \beta}$,

  is another separating hyperplane, parallel to H, s.t.

$$\begin{aligned} \widehat{w}^T x_{A,i} + \hat{b} \geq \ \ 1 \qquad & \forall x_{A,i} \in A, \\ \widehat{w}^T x_{B,j} + \hat{b} \leq -1 \qquad & \forall x_{B,j} \in B, \end{aligned}$$

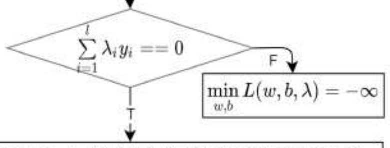
$$\rho(H) \leq \rho(\widehat{H}) = \frac{1}{||\widehat{w}||}$$



Dual of Linear SVM

- **Lagrangian** function :

$$L(w, b, \lambda) = \frac{1}{2}||w||^2 + \sum_{i=1}^{l} \lambda_i \big(1 - y_i(w^T x_i + b)\big) = \\ = \frac{1}{2}||w||^2 - \sum_{i=1}^{l} \lambda_i y_i w^T x_i - b\sum_{i=1}^{l} \lambda_i y_i + \sum_{i=1}^{l} \lambda_i$$



$$\sum_{i=1}^{l} \lambda_i y_i == 0$$

F

$$\boxed{\min_{w,b} L(w, b, \lambda) = -\infty}$$

T

L doesn't depend on $b \implies$ (1) L is strongly convex w.r.t. w and (2) $arg \min\limits_{w} L(w, b, \lambda)$ is given by the unique stationary point

$$\nabla_w L(w, b, \lambda) = w - \sum_{i=1}^{l} \lambda_i y_i x_i = 0$$

- Dual function of the Linear SVM function :

$$\varphi(\lambda) = \begin{cases} -\infty & \sum_{i=1}^{l} \lambda_i y_i \neq 0 \\ -\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} y_i y_j (x_i)^T x_j \lambda_i \lambda_j + \sum_{i=1}^{l} \lambda_i & \sum_{i=1}^{l} \lambda_i y_i = 0 \end{cases}$$

- **Dual function** of the Linear SVM function :

$$\varphi(\lambda) = \begin{cases} -\infty & \sum_{i=1}^{l} \lambda_i y_i \neq 0 \\ -\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} y_i y_j (x_i)^T x_j \lambda_i \lambda_j + \sum_{i=1}^{l} \lambda_i & \sum_{i=1}^{l} \lambda_i y_i = 0 \end{cases}$$

- **Dual problem** of $(Linear\ SVM)$ is

$$\begin{cases} \max\limits_{\lambda} -\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} y_i y_j (x_i)^T x_j \lambda_i \lambda_j + \sum_{i=1}^{l} \lambda_i \\ \sum_{i=1}^{l} \lambda_i y_i = 0 & \begin{pmatrix} \text{Dual of Linear} \\ \text{SVM Problem} \end{pmatrix} \\ \lambda \geq 0 \end{cases}$$

or, in another form,

$$\begin{cases} \max\limits_{\lambda} -\frac{1}{2}\lambda^T X^T X \lambda + e^T \lambda \\ \sum_{i=1}^{l} \lambda_i y_i = 0 & \begin{pmatrix} \text{Dual of Linear} \\ \text{SVM Problem} \end{pmatrix} \\ \lambda \geq 0 \end{cases}$$

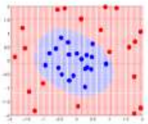
where :
  - $X \in \mathbb{R}^{n \times l}$ is

$$X = \begin{pmatrix} \overset{y_1 \boldsymbol{x_1}}{\uparrow} & & & \\ y_1 x_{1,1} & y_2 x_{2,1} & \ldots & y_l x_{l,1} \\ y_1 x_{1,2} & y_2 x_{2,2} & \ldots & y_l x_{l,2} \\ \ldots & \ldots & \ldots & \ldots \\ y_1 x_{1,n} & y_2 x_{2,n} & \ldots & y_l x_{l,n} \end{pmatrix}$$

  - $e^T = (1\ 1\ \ldots\ 1)$

Non-Linear SVM

- The sets A, B are not linearly separable $\implies$ can't use here neither Linear SVM, nor the one with soft margins, that was used for not "perfectly" separable sets that could still be linearly separated with an acceptable degree of classification error.



- How can we separate A and B? We use the **kernel trick**, i.e. we map the SVM's inputs to a high-dimensional feature space, by using the mapping function $\phi : \mathbb{R}^n \to \mathcal{H}$, with $\mathcal{H}$, the **feature space**, being the higher-dimensional (potentially infinite) space. We try to linearly separate not the various x_i points but their images $\phi(x_i), i = 1, .., l$ in $\mathcal{H}$.

- **Primal problem** :

$$\begin{cases} \min\limits_{w,b,\xi} \frac{1}{2}||w||^2 + C\sum_{i=1}^{l} \xi_i \\ 1 - y_i(w^T \phi(x_i) + b) \leq \xi_i & i = 1, .., l \\ \xi_i \geq 0 & i = 1, .., l \end{cases}$$

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

- **Dual problem** :

$$\begin{cases} \max\limits_{y} -\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} y_i y_j \phi(x_i)^T \phi(x_j) \lambda_i \lambda_j + \sum_{i=1}^{l} \lambda_i \\ \sum_{i=1}^{l} \lambda_i y_i = 0 \\ 0 \leq \lambda_i \leq C & i = 1, .., l \end{cases}$$

Suppose you've solved the dual problem and find λ^*. You can then :
  - compute $w^* = \sum_{i=1}^{l} \lambda_i^* y_i \phi(x_i)$.
  - Use any λ_i^* s.t. $0 < \lambda_i^* < C$ to find b^* :

$$y_i\left(\sum_{j=1}^{l} \lambda_j^* y_j \phi(x_j)^T \phi(x_i) + b^*\right) - 1 = 0$$

$$k(x_i, x_j)$$

  - **Decision function** :

$$f(x) = sign\big((w^*)^T \phi(x) + b^*\big) = \\ = sign\left(\sum_{i=1}^{l} \lambda_i^* y_i \phi(x_i)^T \phi(x) + b^*\right)$$

  depends on :
    - λ^*, that depends on the scalar product $\phi(x_i)^T \phi(x_j)$
    - $\phi(x_i)^T \phi(x)$
    - b^*, that depends on the scalar products $\phi(x_i)^T \phi(x_j)$

  thus, we don't have to explicitly know the single mapping $\phi(x)$ of a point x, but we need only the product of the mappings of two points x_i, x_j, i.e. $\phi(x_i)^T \phi(x_j)$

- **Kernel function** : a function $k : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is called **kernel** if $\exists$ map $\phi : \mathbb{R}^n \to \mathcal{H}$ s.t.

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

  where $\langle\cdot,\cdot\rangle$ is a scalar product in $\mathcal{H}$.
  e.g. of kernel functions :
  - $x^T y$
  - $(x^T y + 1)^p, p \geq 1$ (*polynomial*)
  - $e^{-\gamma||x-y||^2}$ (*gaussian*)
- **THEOREM** :
  HP :
  - $k : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a kernel
  - $x_1, .., x_l \in \mathbb{R}^n$

  TH : matrix K defines as

$$K_i j = k(x_i, x_j)$$

  is positive semidefinite.

REGRESSION with LINEAR SVM and SLACK VARIABLES

- If ε is too small, the model $(Linear\ SVM)$ cannot be feasible $\implies$ we've got to relax the constraints of the problem $Linear\ SVM$ by introducing the **slack variables** ξ^+, ξ^-. This is the **Linear SVM with Slack variables** **primal** :

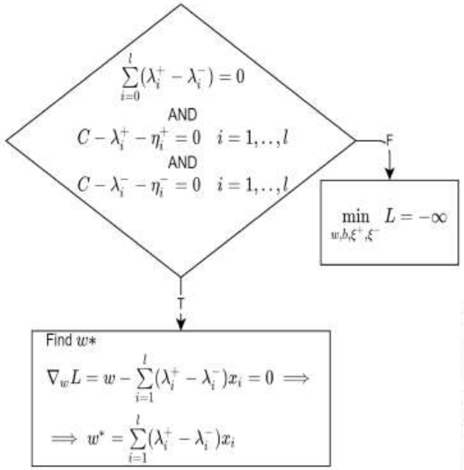
$$\begin{cases} \min\limits_{w,b,\xi^+,\xi^-} \frac{1}{2}||w||^2 + C\sum\limits_{i=1}^{l}(\xi_i^+ + \xi_i^-) \\ y_i \le w^T x_i + b + \varepsilon + \xi_i^+ \quad i = 1,..,l \\ y_i \ge w^T x_i + b - \varepsilon - \xi_i^- \quad i = 1,..,l \\ \xi_i^+ \ge 0 \quad i = 1,..,l \\ \xi_i^- \ge 0 \quad i = 1,..,l \end{cases} \begin{pmatrix}\text{Primal of Linear} \\ \text{SVM w/ Slack} \\ \text{Variables}\end{pmatrix}$$

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

- **Linear SVM with Slack variables** **dual** : let's start from the **Lagrangian function**

primal var.s *dual var.s*

$$L(w, b, \xi^+, \xi^-, \ \lambda^+, \lambda^-, \eta^+, \eta^-) =$$
$$= \frac{1}{2}||w||^2 - w^T\left[\sum_{i=1}^{l}(\lambda_i^+ - \lambda_i^-)x_i\right] +$$
$$- b\sum_{i=1}^{l}\left(\lambda_i^+ - \lambda_i^-\right) + \sum_{i=1}^{l}\xi_i^+(C - \lambda_i^+ - \eta_i^+) +$$
$$+ \sum_{i=1}^{l}\xi_i^-(C - \lambda_i^- - \eta_i^-)$$



$$\sum_{i=0}^{l}(\lambda_i^+ - \lambda_i^-) = 0$$

AND

$$C - \lambda_i^+ - \eta_i^+ = 0 \quad i = 1,..,l$$

AND

$$C - \lambda_i^- - \eta_i^- = 0 \quad i = 1,..,l$$

F

$$\min_{w,b,\xi^+,\xi^-} L = -\infty$$

T

Find $w*$

$$\nabla_w L = w - \sum_{i=1}^{l}(\lambda_i^+ - \lambda_i^-)x_i = 0 \implies$$
$$\implies w^* = \sum_{i=1}^{l}(\lambda_i^+ - \lambda_i^-)x_i$$

Here's the **dual problem** :

$$\begin{cases} \max\limits_{\lambda^+,\lambda^-} -\frac{1}{2}\sum\limits_{i=1}^{l}\sum\limits_{j=1}^{l}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)(x_i)^T x_j + \\ \qquad - \varepsilon\sum\limits_{i=1}^{l}(\lambda_i^+ + \lambda_i^-) + \sum\limits_{i=1}^{l}y_i(\lambda_i^+ - \lambda_i^-) \\ \sum\limits_{i=1}^{l}(\lambda_i^+ - \lambda_i^-) = 0 \\ \lambda_i^+ \in [0, C] \qquad i = 1,..,l \\ \lambda_i^- \in [0, C] \qquad i = 1,..,l \end{cases}$$

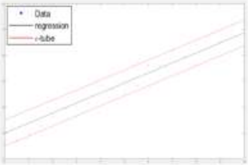
REGRESSION with LINEAR SVM

- Consider an affine function

$$f(x) = w^T x + b$$

and set a tolerance parameter ε.

- Since we want to achieve maximum flatness, we want to minimize w,



thus our problem is in the form

$$\begin{cases} \min\limits_{w,b} \frac{1}{2}||w||^2 \\ y_i \le w^T x_i + b + \varepsilon \quad i = 1,..,l \\ y_i \ge w^T x_i + b - \varepsilon \quad i = 1,..,l \end{cases} \text{(Linear SVM)}$$

$\varepsilon - SV$ REGRESSION

- Having a set of training data $\{(x_1, y_1), (x_2, y_2), \ldots, (x_l, y_l)\}$, with $x_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$, we want to find a function f that :
  - has at most ε deviation from the targets y_i $\forall$ training data
  - is as flat as possible $\left(flatness \uparrow \implies generalization\ capability \uparrow\right)$

Properties of the dual problem :

- it is a **convex** **quadratic** **programming problem**.
- Dual constraints are simpler than primal constraints.
- If either $\lambda_i^+ > 0$ or $\lambda_i^- > 0 \implies x_i$ is a **support vector**.
- If (λ^+, λ^-) is a dual optimum, then

$$w = \sum_{i=1}^{l}(\lambda_i^+ - \lambda_i^-)x_i$$

b is obtained by using the complementarity conditions

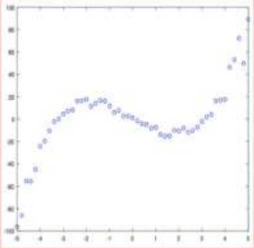
$$\lambda_i^+[\varepsilon + \xi_i^+ - y_i + w^T x_i + b] = 0$$
$$\lambda_i^-[\varepsilon - \xi_i^+ + y_i - w^T x_i - b] = 0$$
$$\xi_i^+(C - \lambda_i^+) = 0$$
$$\xi_i^+(C - \lambda_i^-) = 0$$

Hence :

- if $\exists i$ s.t. $0 < \lambda_i^+ < C \implies b = y_i - w^T x_i - \varepsilon$
- if $\exists i$ s.t. $0 < \lambda_i^- < C \implies b = y_i - w^T x_i + \varepsilon$

5. REGRESSION

- We've got l experimental data $y_1, \ldots, y_l \in \mathbb{R}$ corresponding to the **observations** made on **points** $x_1, .., x_l \in \mathbb{R}$ and we want to fit a line as close as possible (w/o overfitting) to our data.



We may proceed in various ways, but we'll see two ways of fitting a line to some data :

- polynomial regression
- regression by using SVM

POL. REGR. MODEL with $||\cdot||_\infty$

- Norm $||\cdot||_\infty \rightarrow$ linear programming problem :

$$\begin{cases} min\,||Az - y||_\infty = \\ \qquad = \max\limits_{i=1,..,l}|A_i z - y_i| \\ z \in \mathbb{R}^n \end{cases}$$

is equivalent to...

... this problem

$$\begin{cases} min\,u \\ u = \max\limits_{i=1,..,l}|A_i z - y_i| \end{cases} \rightarrow$$

$$\rightarrow \begin{cases} \min\limits_{z,u} u \\ u \ge A_i z - y_i \quad i = 1,..,l \\ u \ge y_i - A_i z \quad i = 1,..,l \end{cases}$$

POL. REGR. MODEL with $||\cdot||_1$

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

$$\begin{cases} min\,||Az - y||_1 = \\ \qquad = \sum\limits_{i=1}^{l}|A_i z - y_i| \\ z \in \mathbb{R}^n \end{cases}$$

is equivalent to...

... this problem

$$\begin{cases} \min\limits_{z,u} \sum\limits_{i=1}^{l} u_i \\ u_i = |A_i z - y_i| = \\ \qquad = max\{A_i z - y_i, y_i - A_i z\} \end{cases} \rightarrow$$

$$\rightarrow \begin{cases} \min\limits_{z,u} \sum\limits_{i=1}^{l} u_i \\ u_i \ge A_i z - y_i \quad i = 1,..,l \\ u_i \ge y_i - A_i z \quad i = 1,..,l \end{cases}$$

POL. REGR. MODEL

- We want to find the best approximation of experimental data with a polynomial p of degree $n-1$, with $n \le l$. Polynomial p has **coefficients** $z_0, .., z_{n-1}$:

$$p(x) = z_0 + z_1 x + z_2 x^2 + \ldots + z_{n-1}x^{n-1} =$$
$$= \sum_{i=0}^{n-1} z_i x^i$$

- Given the residual vector $r \in \mathbb{R}^l$, we want to find coefficients $z = (z_0, z_1, .., z_{n-1})$ of polynomial p s.t. $||r||$ is minimum, i.e. we want to solve the following optimization problem

$f(z)$ convex $\forall$ used norm $(||\cdot||_1, ||\cdot||_2, \ldots, ||\cdot||_\infty)$

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

j-th column $\rightarrow x_i^{j-1}$, $\forall i = 1, .., l$

i-th row $\rightarrow x_i$ exponentiations for $p(x_i)$

where

$$A = \begin{pmatrix} 1 & x_1 & x_1^2 & .. & x_1^{n-1} \\ 1 & x_2 & x_2^2 & .. & x_2^{n-1} \\ .. & .. & .. & .. & .. \\ 1 & x_l & x_l^2 & .. & x_l^{n-1} \end{pmatrix}, y = \begin{pmatrix} y_1 \\ y_2 \\ \ldots \\ y_l \end{pmatrix}$$

A is called **Vandermonde matrix**.

POL. REGR. MODEL with $||\cdot||_2$

- Euclidean norm $||\cdot||_2$ (**Least Squares** approximation) $\implies$ unconstrained quadratic programming problem :

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

- It can be proved that $rank(A) = n$, thus $A^T A$ is positive definite $\implies A^T A$ is invertible $\implies$ the unique optimal solution is the stationary point of the objective function $f(z)$, i.e. $\nabla_z f(z^*) = 0$, the solution of the system of linear equations :

$$A^T Az^* = A^T y \rightarrow$$
$$\rightarrow z^* = (A^T A)^{-1}A^T y$$

RESIDUAL

It's the vector $r \in \mathbb{R}^l$ s.t.

$$r_i = p(x_i) - y_i,$$
$$i = 1, .., l$$

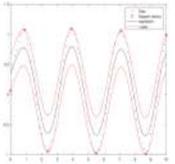
***predicted** value*

***actual** value*

In other words, the residual measures how much did our polynomial $p(x)$ get close to the experimental data.

REGRESSION with NON-LINEAR SVM

- We can generate a non-linear regression function f by using the kernel tricks by using a map $\phi : \mathbb{R}^n \rightarrow \mathcal{H}$, where $\mathcal{H}$ (**features space**) is a higher dimensional (potentially infinite) space and find the linear regression for the points $\{(\phi(x_i), y_i)\}$ in the feature space $\mathcal{H}$.



- **Primal** **problem** :

$$\begin{cases} min\,\frac{1}{2}||w||^2 + C\sum\limits_{i=1}^{l}(\xi_i^+ + \xi_i^-) \\ y_i \le w^T\phi(x_i) + b + \varepsilon + \xi_i^+ \qquad i = 1,..,l \\ y_i \ge w^T\phi(x_i) + b - \varepsilon - \xi_i^+ \qquad i = 1,..,l \end{cases}$$

CONs of primal :

- w is a vector in a high dimensional space (potentially infinite variables).

- **Dual** **problem** :

$\boldsymbol{k(x_i, x_j)}$

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

PROs of dual :

- number of variables is fixed and is $2\,l$

Therefore :

- choose a kernel k
- solve the dual $\implies$ find optimal (λ^+, λ^-)

- find b :

$$b = y_i - \varepsilon - \sum_{j=1}^{l}(\lambda_j^+ - \lambda_j^-)k(x_i, x_j)$$

for some i s.t. $0 < \lambda_i^+ < C$, or

$$b = y_i + \varepsilon - \sum_{j=1}^{l}(\lambda_j^+ - \lambda_j^-)k(x_i, x_j)$$

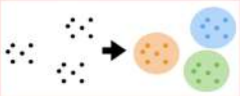
for some i s.t. $0 < \lambda_i^- < C$

- **Recession function**

$$f(\boldsymbol{x}) = \sum_{i=1}^{l}(\lambda_i^+ - \lambda_i^-)k(x_i, \boldsymbol{x}) + b$$

6. CLUSTERING

Clustering is an **unsupervised machine learning method** that, given a set S of patterns $p_1, .., p_l \in \mathbb{R}^n$ and an integer number k, it has the task to find a partition of S in k subsets $S_1, .., S_k$ (**clusters**) that are **homogeneous**(pattern inside a cluster must be as close as possible to each other) and **well separated**(differents clusters should be as much separated / distant as possible).



CLUSTERING OPTIMIZATION MODEL

1. Consider a distance $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ between vectors in $\mathbb{R}^n$
2. $\forall$ cluster S_j, introduce a centroid $x_j \in \mathbb{R}^n$. (unknown, i.e. a point that, potentially is not included in the data set.)
3. Define clusters so that each pattern $p_i, i = 1, .., l$, is associated to the closest centroid.
4. By using the obtained clusters of patterns, compute the new centroids and, if there's still room for improvement (maybe a pattern belongs to wrong cluster and another execution of this process makes that pattern go to the ideal cluster to which it should belong) go to step 3.

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

$$\begin{cases} min \sum_{i=1}^{l} \min_{j=1,..,k} d(p_i, x_j) \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases}$$

OPTIMIZATION MODEL with $|| \cdot ||_2^2$

- $d(x, y) = ||x - y||_2^2 \implies$ the optimization problem becomes

$$\begin{cases} min \sum_{i=1}^{l} \min_{j=1,..,k} ||p_i - x_j||_2^2 \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases}$$

- If $\boldsymbol{k = 1}$, then it's a **convex quadratic programming problem** w/o constraints

$$\begin{cases} min \sum_{i=1}^{l} ||p_i - x_j||_2^2 = \\ \qquad = \sum_{i=1}^{l} (x - p_i)^T (x - p_i) \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases} \qquad (1)$$

In this case, the global optimum is the stationary point

$$2\,l\,x - 2 \sum_{i=1}^{l} p_i = 0 \iff x = \frac{\sum_{i=1}^{l} p_i}{l}$$

which would be the **mean** (or **baricenter**) of all patterns $p_i, i = 1, .., l$.

- If $\boldsymbol{k > 1}$, then it's a **non-convex** and **non-smooth problem** :

$$\begin{cases} \min_{x} \sum_{i=1}^{l} \min_{j=1,..,k} ||p_i - x_j||_2^2 \\ x_j \in \mathbb{R}^n \qquad j = 1, .., l \end{cases} \qquad (2)$$

TH

- TH : problem (2) is equivalent to the following **non-convex** but **smooth** problem

$$\begin{cases} \min_{x,\alpha} \sum_{i=1}^{l} \sum_{j=1}^{k} \alpha_{ij} ||p_i - x_j||_2^2 \\ \sum_{j=1}^{k} \alpha_{ij} = 1, \quad i = 1, .., l \\ \alpha_{ij} \geq 0 \qquad i = 1, .., l \ , \ j = 1, .., k \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases} \qquad (3)$$

- PROOF : notice that

$$\min_{j=1,..,k} \{a_j\} = min \left\{ \sum_{j=1}^{k} \alpha_j a_j : \sum_{j=1}^{k} \alpha_j = 1, \alpha \geq 0 \right\}$$

K-MEANS

- The k-means algorithm is based on the following properties of problem (3) :
  - if x_j are fixed : (3) is decomposable into l very simple **linear** programming problems : $\forall i = 1, .., l$ the optimal solution is

$$\alpha_{ij}^* = \begin{cases} 1 & \text{if j is the 1st index s.t.} \\ & ||p_i - x_j||_2 = \min_{h=1,..,k} ||p_i - x_h||_2, \\ & \text{i.e. } x_j \text{ is the closest centroid to } p_i \\ 0 & otherwise \end{cases}$$

  - if $\alpha_{ij} \in \{0, 1\}$ are fixed : (3) is decomposable into k very simple **convex quadratic** programming problems similar to (1) : $\forall j = 1, .., k$, the optimal solution is

$$x_j^* = \frac{\sum_{i=1}^{l} \alpha_{ij} p_i}{\sum_{i=1}^{l} \alpha_{ij}}$$

which would be the weighted mean of the patterns.

- K-means algorithm consists in an **alternating minimization** of $f(x, \alpha) = \sum_{i=1}^{l} \sum_{j=1}^{k} \alpha_{ij} ||p_i - x_j||_2^2$ w.r.t. the two block of variables x and α

- **ALGORITHM** :
  1. **Inizialization**
     Set the loop index $t = 0$. Choose centroids $x_1^0, .., x_k^0 \in \mathbb{R}^n$ and assign patterns to clusters : $\forall i = 1, .., l$

$$\alpha_{ij}^0 = \begin{cases} 1 & \text{if j is the 1st index s.t.} \\ & ||p_i - x_j^0||_2 = \min_{h=1,..,k} ||p_i - x_h^0||_2 \\ 0 & otherwise \end{cases}$$

  2. **Update centroids**
     $\forall j = 1, .., k$ compute the mean

$$x_j^{t+1} = \frac{\sum_{i=1}^{l} \alpha_{ij}^t p_i}{\sum_{i=1}^{l} \alpha_{ij}^t}$$

  3. **Update clusters**
     $\forall i = 1, .., l$ compute

$$\alpha_{ij}^{t+1} = \begin{cases} 1 & \text{if j is the 1st index s.t.} \\ & ||p_i - x_j^{t+1}||_2 = \min_{h=1,..,k} ||p_i - x_h^{t+1}||_2 \\ 0 & otherwise \end{cases}$$

  4. **Stopping criterion**
     If $f(x^{t+1}, \alpha^{t+i}) = f(x^t, \alpha^t) \implies$ STOP, otherwise $t = t + 1$ and go to step 1.

TH

- TH : k-means algorithm **stops after a finite number of iterations** at a solution (x^*, α^*) of the KKT system of problem (3) s.t.

$$f(x^*, \alpha^*) \leq f(x^*, \alpha), \ \ \forall \alpha \geq 0 \ s.t. \ \sum_{j=1}^{k} \alpha_{ij} = 1, i = 1, .., l$$

$$f(x^*, \alpha^*) \leq f(x, \alpha^*), \ \ \forall x \in \mathbb{R}^{k\,n}$$

- NOTE : the k-means algorithm **doesn't give us the guarantee of finding a global optimum**.

OPTIMIZATION MODEL with $|| \cdot ||_1$

- $d(x, y) = ||x - y||_1 \implies$ the optimization problem becomes

$$\begin{cases} min \sum_{i=1}^{l} \min_{j=1,..,k} ||p_i - x_j||_1 \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases}$$

- If $\boldsymbol{k = 1}$, then it's a **convex problem** decomposable into n convex problems of one variable

$$\begin{cases} min \sum_{i=1}^{l} ||p_i - x_j||_1 = \\ \qquad = \sum_{i=1}^{l} \sum_{h=1}^{n} |x_h - (p_i)_h| = \\ \qquad = \sum_{h=1}^{n} \underbrace{\sum_{j=1}^{l} |x_h - (p_i)_h|}_{f_h(x_h)} \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases} \qquad (4)$$

Given l real numbers $a_1, .., a_l$, what's the optimal solution of the following problem?

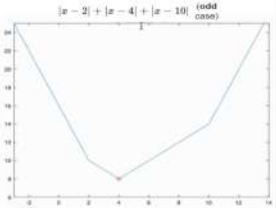
$$\begin{cases} min \sum_{i=1}^{l} |x - a_i| = f(x) \\ x \in \mathbb{R} \end{cases}$$

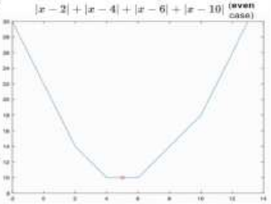
The objective function $f(x)$ is convex and piecewise linear :

$$f(x) = \begin{cases} -lx + \sum_{i=1}^{l} a_i & x < a_1 \\ (2 - l)x + \sum_{i=2}^{l} a_i - a_1 & x \in [a_1, a_2] \\ \dots & \dots \\ (2r - l)x + \sum_{i=r+1}^{l} a_i - \sum_{i=1}^{r} a_i & x \in [a_r, a_{r+1}] \\ \dots & \dots \\ (l - 2)x + a_l - \sum_{i=1}^{l-1} a_i & x \in [a_{l-1}, a_l] \\ lx - \sum_{i=1}^{l} a_i & x > a_l \end{cases}$$

The global optimum is

$$median(a_1, .., a_l) = \begin{cases} a_{(l+1)/2} & if \ \text{l is odd} \\ (a_{l/2} + a_{1+l/2})/2 & \text{if } l \text{ is even} \end{cases}$$





- If $\boldsymbol{k > 1}$, then it's a **non-convex** and **non-smooth problem** :

$$\begin{cases} \min_{x} \sum_{i=1}^{l} \min_{j=1,..,k} ||p_i - x_j||_1 \\ x_j \in \mathbb{R}^n \qquad j = 1, .., l \end{cases} \qquad (5)$$

TH

- TH : problem (5) is equivalent to the following problem (thus, replacing the $\min_{j=1,..,k} || \cdot ||_1$ operation) :

$$\begin{cases} \min_{x,\alpha} \sum_{i=1}^{l} \sum_{j=1}^{k} \alpha_{ij} ||p_i - x_j||_1 \\ \sum_{j=1}^{k} \alpha_{ij} = 1 \qquad i = 1, .., l \\ \alpha_{ij} \geq 0 \qquad i = 1, .., l \ , \ j = 1, .., k \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases} \qquad (6)$$

TH

- TH : problem (6) is, in turn, equivalent to the following **non-convex bilinear** problem :

$$u_{ijh} = |(p_i)_h - (x_j)_h| = = max\{(p_i)_h - (x_j)_h, (x_j)_h - (p_i)_h\}$$

$$\begin{cases} \min_{x,\alpha,u} \sum_{i=1}^{l} \sum_{j=1}^{k} \sum_{h=1}^{n} \alpha_{ij} u_{ijh} \\ u_{ijh} \geq (p_i)_h - (x_j)_h \quad i = 1, .., l \ , \ j = 1, .., k \ , \ h = 1, .., n \\ u_{ijh} \geq (x_j)_h - (p_i)_h \quad i = 1, .., l \ , \ j = 1, .., k \ , \ h = 1, .., n \\ \sum_{j=1}^{k} \alpha_{ij} = 1 \qquad i = 1, .., l \\ \alpha_{ij} \geq 0 \qquad i = 1, .., l \ , \ j = 1, .., k \\ x_j \in \mathbb{R}^n \qquad j = 1, .., k \end{cases} \qquad (7)$$

K-MEDIAN

- The k-means algorithm is based on the following properties of problem (6) :
  - if x_j are fixed : (6) is decomposable into l very simple **linear** programming problems : $\forall i = 1, .., l$ the optimal solution is

$$\alpha_{ij}^* = \begin{cases} 1 & \text{if j is the 1st index s.t.} \\ & ||p_i - x_j||_1 = \min_{h=1,..,k} ||p_i - x_h||_1, \\ & \text{i.e. } x_j \text{ is the closest centroid to } p_i \\ 0 & otherwise \end{cases}$$

  - if $\alpha_{ij} \in \{0, 1\}$ are fixed : (6) is decomposable into k very simple **convex quadratic** programming problems similar to (4) : $\forall j = 1, .., k$, the optimal solution is

$$x_j^* = median(p_i : \alpha_{ij} = 1)$$

which would be the weighted mean of the patterns.

- K-median algorithm consists in an **alternating minimization** of $f(x, \alpha) = \sum_{i=1}^{l} \sum_{j=1}^{k} \alpha_{ij} ||p_i - x_j||_1$ w.r.t. the two block of variables x and α

- **ALGORITHM** :
  1. **Inizialization**
     Set the loop index $t = 0$. Choose centroids $x_1^0, .., x_k^0 \in \mathbb{R}^n$ and assign patterns to clusters : $\forall i = 1, .., l$

$$\alpha_{ij}^0 = \begin{cases} 1 & \text{if j is the 1st index s.t.} \\ & ||p_i - x_j^0||_1 = \min_{h=1,..,k} ||p_i - x_h^0||_1 \\ 0 & otherwise \end{cases}$$

  2. **Update centroids**
     $\forall j = 1, .., k$ compute the mean

$$x_j^{t+1} = median(p_i : \alpha_{ij}^t = 1)$$

  3. **Update clusters**
     $\forall i = 1, .., l$ compute

$$\alpha_{ij}^{t+1} = \begin{cases} 1 & \text{if j is the 1st index s.t.} \\ & ||p_i - x_j^{t+1}||_1 = \min_{h=1,..,k} ||p_i - x_h^{t+1}||_1 \\ 0 & otherwise \end{cases}$$

  4. **Stopping criterion**
     If $f(x^{t+1}, \alpha^{t+i}) = f(x^t, \alpha^t) \implies$ STOP, otherwise $t = t + 1$ and go to step 1.

TH

- TH : k-median algorithm **stops after a finite number of iterations** at a solution (x^*, α^*) of the KKT system of problem (6) s.t.

$$f(x^*, \alpha^*) \leq f(x^*, \alpha), \ \ \forall \alpha \geq 0 \ s.t. \ \sum_{j=1}^{k} \alpha_{ij} = 1, i = 1, .., l$$

$$f(x^*, \alpha^*) \leq f(x, \alpha^*), \ \ \forall x \in \mathbb{R}^{k\,n}$$

- NOTE : the k-median algorithm **doesn't give us the guarantee of finding a global optimum**.

7. SOLUTION METHODS FOR UNCONSTRAINED PROBLEMS

Given a problem like the following

$$\begin{cases}\min_x f(x)\\ x \in \mathbb{R}^n\end{cases},$$

we want to use some techniques that'll help us find a solution to that problem.

GRADIENT METHOD

- Current point x^k
- Search direction $d^k = -\nabla f(x^k)$ (**steepest descent direction**). Why does d^k have to be equal to $\nabla f(x^k)$ to be the steepest descent direction? Let's see. We want to achieve that

$$\frac{\delta f}{\delta d}(x^k) = \langle \nabla f(x^k), d\rangle = \\ = ||\nabla f(x^k)||\ ||d||\ cos(\alpha) < 0$$

In other words, in order to find the steepest descent direction, we have to choose α in such a way that we minimize the derivative of f w.r.t. d. We can do that by minimizing that $cos(\alpha)$, thus we'll obtain

$$cos(\alpha) = -1 \implies \alpha = \pi$$

i.e. that means that d has to be opposite to $\nabla f(x^k)$, i.e.

$$d = -\nabla f(x^k)$$

- **Gradient method** :

```
1. choose $x^0 \in \mathbb{R}^n$
2. set $k = 0$
3. while $\nabla f(x^k) \neq 0$ do
    1. search direction : $d^k = -\nabla f(x^k)$
    2. step size : compute an optimal solution $t_k$ of the problem : $\min_{t>0} f(x^k + t\,d^k)$
    3. go to next point : $x^{k+1} = x^k + t_k\,d^k, k = k+1$
end.
```

Example. $f(x) = x_1^2 + 2x_2^2 - 3x_1 - 2x_2$, starting point $x^0 = (2,1)$.

$\nabla f(x^0) = (1,2)$, $d^0 = (-1,-2)$, $f(x^0 + td^0) = 9t^2 - 5t - 2$, $t_0 = 5/18$,

$$x^1 = (2,1) - \frac{5}{18}(1,2) = \left(\frac{31}{18}, \frac{4}{9}\right).$$

- **Step size** : if $f(x) = \frac{1}{2}x^T Q x + c^T x$, with Q being a positive definite matrix, then

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

where

$$g^k = \nabla f(x^k) = Q\,x^k + c.$$

Thus, the step size is equal to

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

- PROs :
  - **simple** method
- CONs :
  - convergence may be **slow** depending on what kind of hessian matrix Q we have at hand. In particular, what concerns us is the the condition number λ_n/λ_1 of Q

Is f quadratic?

YES

NO

PROPOSITION

- $(\mathbf{d}^k)^T \mathbf{d}^{k+1} = \mathbf{0}\ \forall\, k$, i.e. every direction d^k and the successively computed direction d^{k+1} are **orthogonal**.

PROOF :

$$f(x^k + t\,d^k) = \varphi(t) \rightarrow \\ \rightarrow \varphi'(t) = \nabla_t f(x^k + t\,d^k)^T d^k \rightarrow \\ \rightarrow \varphi'(t_k) = \nabla_t f(x^k + t_k\,d^k)^T d^k = 0 \rightarrow$$

$$\rightarrow \nabla_t f(x^{k+1})^T d^k = 0 \rightarrow \\ \rightarrow (d^{k+1})^T d^k = 0$$

- CONs :
  - two subsequent directions d^k, d^{k+1} are **orthogonal** to each other $\implies$ generated sequence has a zig-zag behaviour.

- If $\{x^k\}$ converges to x^*, then $\nabla f(x^*) = 0$, i.e. x^* is a stationary point of f, i.e. x^* is a global/local minimum candidate.

PROOF :

$$\nabla f(x^k)^T \nabla f(x^{k+1}) = 0 \rightarrow \\ \rightarrow \ldots \text{since } \lim_{k\to\infty}\{x^k\} = x^* \text{ we have...} \rightarrow \\ \rightarrow \nabla f(x^*)^T \nabla f(x^*) = 0 \implies \\ \implies ||\nabla f(x^*)||^2 = 0 \implies \nabla f(x^*) = 0$$

TH

- HP : f is **coercive**.
- TH : $\forall$ starting point x^0, the generated sequence $\{x^k\}$ is **bounded** (i.e. $\forall x^0$ we have that $\{x \in \{x^k\} : f(x) \leq f(x^0)\}$) and any of its cluster points is a **stationary point** of f.

NOTE : prof has written in the "bounded" part "$x \in \mathbb{R}^n$" instead of $x \in \{x^k\}$. Maybe there was a mistake.

COROLLARY

- HP : f is **coercive** and **convex**.
- TH : $\forall$ starting point x^0, the generated sequence $\{x^k\}$ is bounded (i.e. $\forall x^0$ we have that $\{x \in \{x^k\} : f(x) \leq f(x^0)\}$) and any of its cluster points is a **global minimum** of f.

COROLLARY

- HP : f is **strongly convex**.
- TH : $\forall$ starting point x^0, the generated sequence $\{x^k\}$ converges to the global minimum of f.

TH (Error Bound)

- HP :
  - $f(x) = \frac{1}{2}x^T Q x + c^T x$
  - Q **positive definite** matrix
  - x^* global min of $f(x)$
- TH : sequence $\{x^k\}$ satisfies the following inequality :

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

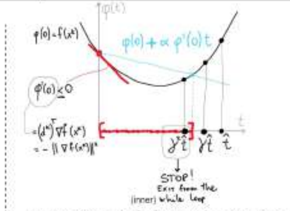
where $||\cdot||_Q$ is the matrix norm and with $\lambda_1 \leq, \ldots, \leq \lambda_n$ being the eigenvalues of Q.

- Note : if the **condition number** of $Q = \lambda_n/\lambda_1 \gg 1$, then the ratio $\left(\frac{\lambda_n}{\lambda_1} - 1\right)/\left(\frac{\lambda_n}{\lambda_1} + 1\right) \simeq 1$ and the convergence may be slow.

ARMIJO INEXACT LINE SEARCH

- 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 $\hat{t} > 0$.
2. Choose $x^0 \in \mathbb{R}^n$
3. Set $k = 0$
4. while $\nabla f(x^k) \neq 0$ do :
    1. $d^k = -\nabla f(x^k)$
    2. $t_k = \hat{t}$
    3. while
         $f(x^k + t_k d^k) > f(x^k) + \alpha t_k (d^k)^T \nabla f(x^k)$
       do
         1. $t_k = \gamma t_k$
       end
    4. $x^{k+1} = x^k + t_k d,\ \ k = k+1$
end
```



Example. 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

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

if $t_0 = 0.5$ then

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

if $t_0 = 0.25$ then

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

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

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

TH

- HP :
  - f is **coercive**
- TH : $\forall$ starting poing x^0 the generated sequence $\{x^k\}$ is **bounded** and any of its cluster points is a stationary point of f

CONJUGATE GRADIENT METHOD

- The search direction involves the gradient computed at the **current** iteration and the direction computed at the **previous** iteration.
- CASE f is quadratic, i.e.

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

where Q is **positive definite**. Set $g = \nabla f(x) = Qx + c$. At k^{th} iteration, the search direction is

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

where β_k is s.t. d^k and d^{k-1} are conjugate w.r.t. Q, i.e.

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

- Easy to compute β_k

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

- If we perform exact line search, then d^k is a descent direction
- The step size given by exact line search is

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

- **Conjugate gradient method for quadratic functions** :

```
1. Choose $x^0 \in \mathbb{R}^n$
2. Set $g^0 = Qx^0 + c$
3. k = 0
4. while $g^k \neq 0$ do
    1. if $k == 0$
         $\implies d^k = -g^k$,
       else
         $\implies \beta_k = \frac{(g^k)^T Q d^{k-1}}{(d^{k-1})^T Q d^{k-1}}$,
         $d^k = -g^k + \beta_k d^{k-1}$
    2. $t_k = -\frac{(g^k)^T d^k}{(d^k)^T Q d^k}$
       $x^{k+1} = x^k + t_k d^k$,
       $g^{k+1} = Qx^{k+1} + c$,
       $k = k+1$
```

- **Conjugate gradient method for general nonlinear functions** :

```
1. Choose $x^0 \in \mathbb{R}^n$
2. Set k=0
3. while $\nabla f(x^k) \neq 0$ do
    1. if $k == 0$
         $\implies d^k = -\nabla f(x^k)$
       else
         $\implies \beta_k = \frac{||\nabla f(x^k)||^2}{||\nabla f(x^{k-1})||^2}$,
         $d^k = -\nabla f(x^k) + \beta_k d^{k-1}$
    2. Compute step size $t_k$.
    3. $x^{k+1} = x^k + t_k d^k$,
       $k = k+1$
```

TH (Convergence)

- The Conjugate Gradient method finds the global minimum in numIterations $\leq n$. (why n? $x \in \mathbb{R}^n \implies$ we may find up to n orthogonal vectors)
- If Q has r distinct eigenvalues $\implies$ Conjugate Gradient method finds the global minimum in numIterations $\leq r$.

PROPOSITION

- Alternative formula for step size

$$t_k = \frac{||g^k||^2}{(d^k)^T Q\,d^k}$$

- Alternative formula for β_k is

$$\beta_k = \frac{||g^k||^2}{||g^{k-1}||^2}$$

- If we didn't 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 + Span$(d^0, d^1, \ldots, d^k)$

TH (general nonlinear functions)

- If f is **coercive**, then the conjugate gradient method, where t_k satisfies conditions (1) (see "*PROPOSITION (general non linear functions)*"), generates a sequence $\{x^k\}$ s.t.

$$\lim_{k\to\infty} inf||\nabla f(x^k)|| = 0$$

TH ERROR BOUND

If $0 \leq \lambda_1 \leq \ldots \leq \lambda_n$ are the eigenvalues of Q, then the following bounds hold :

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

PROPOSITION (general nonlinear functions)

- If t_k is computed by exact line search, then d^k is a descent direction.
- If t_k satisfies the following conditions

$$\begin{cases}f(x^k + t_k\,d^k) \leq f(x^k) + \alpha\,t_k\,\nabla f(x^k)^T d^k\\ |\nabla f(x^k + t_k\,d^k)^T d^k| \leq -\beta\,\nabla f(x^k)^T d^k\end{cases}, (1)$$

with $0 < \alpha < \beta < 1/2$ then d^k is a descent direction

NEWTON METHODS

- We want to find a stationary point $\nabla f(x) = 0$
- At kth iteration, 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 point 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

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

- **Newton method (basic version)** :

```
1. Choose $x^0 \in \mathbb{R}^n$
2. k = 0
3. while $\nabla f(x^k) \neq 0$
    1. Solve linear system
         $\nabla^2 f(x^k) d^k = -\nabla f(x^k)$
    2. $x^{k+1} = x^k + d^k$,
       $k = k+1$
```

- **Newton method with line search** : if f is **strongly convex**, we get global convergence because d^k is a descent direction

$$\nabla f(x^k)^T d^k = -\nabla f(x^k)^T \left(\nabla^2 f(x^k)\right)^{-1} \nabla f(x^k) < 0$$

Let's see how the method works :

```
1. Set $\alpha, \gamma \in (0,1)$
2. Set $\hat{t} > 0$
3. Choose $x^0 \in \mathbb{R}^n$
4. k = 0
5. while $\nabla f(x^k) \neq 0$ do
    1. [search direction] Solve the linear system
         $\nabla^2 f(x^k) d^k = -\nabla f(x^k)$
    2. $t_k = \hat{t}$
    3. while
         $f(x^k + t_k\,d^k) > f(x^k) + \alpha\,t_k\,(d_k)^T \nabla f(x^k)$
         1. $t_k = \gamma\,t_k$
```

- PROs :
  - **faster convergence** than the one of gradient method
- CONs :
  - **computationally heavy** : at each iteration we need to compute both $\nabla f(x^k)$ and the hessian matrix $\nabla^2 f(x^k)$
  - **local convergence** : convergence is guaranteed $\iff$ starting point x^0 is in the neighborhood of the solution x^*

TH (Convergence)

- HP : f **strongly convex**
- TH : $\forall x^0 \in \mathbb{R}^n$, 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.

TH (Convergence)

- HP :
  - x^* local minimum of f
  - $\nabla^2 f(x^k)$ is positive definite.
- TH : $\exists\delta > 0$, s.t. $\forall x^0 \in B(x^*, \delta)$, the sequence $\{x^k\}$ converges to x^* and
$||x^{k+1} - x^*|| \leq C||x^k - x^*||^2 \quad \forall k > \bar{k} \quad \left(\begin{matrix}\text{Quadratic}\\ \text{convergence}\end{matrix}\right)$
for some $C > 0$ and $\bar{k} > 0$

QUASI-NEWTON METHOD

- At each iteration, $\left(\nabla^2 f(x^k)\right)^{-1}$ is approximated by a **positive definite matrix** $\boldsymbol{H_k}$
- **Quasi-Newton method** :

```
1. Choose $x^0 \in \mathbb{R}^n$
2. Choose $H_0$ (e.g. identity matrix)
3. Set $k = 0$
4. while $\nabla f(x^k) \neq 0$
    1. $d^k = -H_k \nabla f(x^k)$
    2. Compute step size $t_k$
    3. Next point is
         $x^{k+1} = x^k + t_k\,d^k$
    4. Update hessian matrix $H_{k+1}$
    5. k = k+1
```

- PROs (w.r.t. Newton method) :
  - no whole-recomputation of hessian matrix

Updating H_k

TAYLOR APPROXIMATION

- We try to approximate the gradient $\nabla f(x^k)$:

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

- Set :
  - $p^k = x^{k+1} - x^k$
  - $g^k = \nabla f(x^{k+1}) - \nabla f(x^k)$
- We can thus obtain

$$\nabla^2 f(x^{k+1})\,p^k \simeq g^k \implies \\ \implies \left(\nabla^2 f(x^{k+1})\right)^{-1} g^k \simeq p^k \implies \\ \implies H_{k+1}\,g^k = p^k$$

DFP Method

We can update H_k as

$$H_{k+1} = H_k + \frac{p^k\,(p^k)^T}{(p^k)^T g^k} + \\ - \frac{H_k\,g^k\,(g^k)^T H^k}{(g^k)^T\,H_k\,g^k}$$

BFGS Method

- Since $\nabla^2 f(x^{k+1})\,p^k \simeq g^k$, we impose that

$$B_{k+1}p^k = g^k$$

- **Update** B_k as

$$B_{k+1} = B_k + \frac{g^k\,(g^k)^T}{(p^k)^T\,g^k} + \\ - \frac{B_k\,p_k\,(p_k)^T\,B_k}{(p^k)^T\,B_k\,p^k}, \ldots$$

... hence

$$H_{k+1} = H_k + \left(1 + \frac{(g^k)^T\,H_k\,g^k}{(p^k)^T\,g^k}\right)\frac{p^k\,(p^k)^T}{(p^k)^T\,g^k} + \\ - \frac{p^k\,(g_k)^T\,H_k + H_k\,g^k\,(p^k)^T}{(p^k)^T\,g^k}$$

DERIVATIVE-FREE METHODS

- There are situations where derivatives do not exist or are computationally expensive.
- Derivative-free methods sample the objective function at a finite number of points at each iteration, w/o any explicit/implicit derivative approximation.
- **Directional direct-search method** :

```
1. Choose $x^0 \in \mathbb{R}^n$
2. Choose step size $t_0 > 0$
3. Choose $\beta \in (0,1)$
4. Choose tolerance $\varepsilon > 0$
5. Choose a positive basis $D$
6. Set $k = 0$
7. while $t_k > \varepsilon$
    1. order the poll set
         $\{x^k + t^k\,d, d \in D\}$
    2. Evaluate $f$ at the poll points following the chosen order
    3. If $\exists$ poll point s.t.
         $f(x^k + t^k\,d) < f(x^k)$
       then we've got a successful iteration
         $x^{k+1} = x^k + t^k\,d,$
         $t_{k+1} = t_k,$
       else we've got to stay on the same point and decrease the step size
         $x^{k+1} = x^k$
         $t_{k+1} = \beta\,t_k$
```

- The last method is called **coordinate-search method** if $D = \{e_1, \ldots, e_n, -e_1, \ldots, -e_n\}$

- **Variant of directional direct-search method** :

```
1. Choose $x^0 \in \mathbb{R}^n$
2. Choose step size $t_0 > 0$
3. Choose $\beta \in (0,1)$
4. Choose tolerance $\varepsilon > 0$
5. Choose $\gamma \geq 1$
6. Choose a set of positive bases $\mathcal{D}$
7. Set $k = 0$
8. while $t_k > \varepsilon$
    1. Choose positive basis $D \in \mathcal{D}$
    2. order the poll set
         $\{x^k + t^k\,d, d \in D\}$
    3. Evaluate $f$ at the poll points following the chosen order
    4. If $\exists$ poll point s.t.
         $f(x^k + t^k\,d) < f(x^k)$
       then we've got a successful iteration and we update the point $x^k$ and also increase the step size
         $x^{k+1} = x^k + t^k\,d,$
         $t_{k+1} = \gamma\,t_k,$
       else we've got to stay on the same point and decrease the step size
         $x^{k+1} = x^k$
         $t_{k+1} = \beta\,t_k$
```

POSITIVE BASIS

It's a set of vectors $\{v^1, \ldots, v^p\} \subset \mathbb{R}^n$ s.t. :

- any $x \in \mathbb{R}^n$ is a conic combination of $v^1, \ldots, v^p$, i.e. $\exists\,\alpha_1, \ldots, \alpha_p \geq 0$ s.t. $x = \sum_{i=1}^p \alpha_i\,v^i$
- $\forall i = 1, \ldots, p$, v^i is not a conic combination of other vectors of the basis $\{v^1, \ldots, v^{i-1}, v^{i+1}, \ldots, v^p\}$

PROPOSITION

- HP : $\{v^1, \ldots, v^p\}$ is a **positive basis**
- TH : $\forall w \in \mathbb{R}^n \setminus(0)$, $\exists i \in \{1, \ldots, p\}$ s.t.

$$w^T\,v^i < 0$$

- PROOF (by contradiction) : $\{v^1, \ldots, v^p\}$ is a positive basis $\implies$ any vector ($w \neq 0$) and its opposite $-w$ are conic combinations of $\{v^1, \ldots, v^p\}$, i.e.

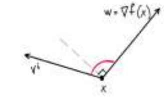
$$-w = \sum_{i=1}^p \alpha_i\,v^i, \alpha_i \geq 0$$

Let's suppose that $w^T\,v^i \geq 0, i = 1, \ldots, p$, thus

$$-w^T\,v^i \leq 0, i = 1, \ldots, p \rightarrow \\ \rightarrow -\alpha_i\,w^T\,v^i \leq 0, i = 1, \ldots, p \rightarrow \\ \rightarrow \sum_{i=1}^p(-\alpha_i\,w^T\,v^i) \leq 0 \rightarrow \\ \rightarrow -w^T\sum_{i=1}^p \alpha_i\,v^i \leq 0 \rightarrow \\ \rightarrow -w^T(-w) = ||w||^2 \leq 0,$$

but $w \neq 0 \implies$ CONTRADICTION!!

- How can we use this result?



We may use the particular v^i mentioned in the TH(esis) as a descent direction for lowering the value of the objective function w/o actually knowing the gradient $\nabla f(x)$.

TH (w.r.t. direct-search method)

- HP :
  - D is a positive basis
  - all vectors $\in D$ are $\in \mathbb{Z}^n$
  - f is **coercive** and **continuosly differentiable**
- TH : Generated sequence $\{x^k\}$ has a cluster point x^* s.t. $\nabla f(x^*) = 0$

- Remark 1 : the assumption that vectors of D are $\in \mathbb{Z}^n$ can be removed if we accept new iterates that satisfy a **"sufficient" decrease condition**

$$f(x^{k+1} \leq f(x^k) - t_k^2)$$

- Remark 2 : if a complete poll step is performed, i.e.

$$f(x^{k+1}) \leq f(x^k + t_k\,d), \forall d \in D,$$

then **any** cluster point of $\{x^k\}$ is a stationary point of f and $\lim_{k\to\infty}||\nabla f(x^k)|| = 0$

8. SOLUTION METHODS FOR CONSTRAINED PROBLEMS

- Here we've got constraints to deal with, but there are equivalent **unconstrained** problems that make our work easier by reconducting us in unconstrained domains and give us the opportunity to re-use, in some way, the algorithms that we've used in chapter "7. SOLUTION METHOD FOR UNCONSTRAINED PROBLEMS".

BARRIER METHOD

- Called also **interior point method**.
- Consider the problem (P)

$$\begin{cases} min\ f(x) \\ g_i(x) \leq 0 \qquad i = 1, .., m \end{cases} \qquad \text{(P)}$$

where :
  - f, g_i **convex** and **twice continuously differentiable**.
  - there is **no isolated point** in Ω
  - $\exists$ optimal solution (e.g. f coercive or Ω bounded)
  - Slater constraints (see "2 - CONVEX OPTIMIZATION PROBLEMS") qualification holds :

$$\exists \widehat{x} \text{ s.t.}$$
$$\widehat{x} \in dom(f), \quad g_i(\widehat{x}) < 0, \quad i = 1, .., m$$

hence strong duality holds.
Special cases : linear programming, convex quadratic programming

- **Unconstrained reformulation** : problem (P) is equivalent to the following unconstrained problem

$$\begin{cases} min\ f(x) + \sum_{i=1}^{m} I\_(g_i(x)) \\ x \in \mathbb{R}^n \end{cases}$$

where $I\_(\cdot)$ is an **indicator function** of $\mathbb{R}_-$, that is neither finite, nor differentiable.
- How can we overcome this problem of non-finiteness and non-differentiability of the indicator function? We approximate it by using **smooth** **convex** functions like the **logarithmic barrier**, $u \mapsto -\varepsilon\, log(-u), \varepsilon > 0$. Hence the problem becomes

$$\begin{cases} min f(x) - \varepsilon \sum_{i=1}^{m} log(-g_i(x)) \\ x \in int(\Omega) \end{cases}$$

- NOTE : $I\_(u)$ can also be approximated by the smooth convex function $u \mapsto -\frac{\varepsilon}{u}, u < 0$

- **Barrier method** :
  1. Set tolerance $\delta > 0, \varepsilon_1 > 0$. Choose $x^0 \in int(\Omega)$. Set $k = 1$
  2. Find optimal solution of problem
  $$\begin{cases} min\ f(x) - \varepsilon_k \sum_{i=1}^{m} log(-g_i(x)) \\ x \in int(\Omega) \end{cases}$$
  using x^{k-1} as starting point.
  3. If $m\, \varepsilon_k < \delta \implies$ STOP,
  else $\varepsilon_{k+1} = \tau\, \varepsilon_k, k = k + 1$ and go to step 2.

Note : choice of τ involves a trade-off : if
$$\tau \downarrow \implies \begin{cases} \text{nr. OUTer iterations}\downarrow \\ \text{nr. INner iterations}\uparrow \end{cases}$$

- **Choice of starting point** : consider auxiliary problem

$$\begin{cases} \min\limits_{x,s} s \\ g_i(x) \leq s \end{cases} \qquad \text{(AUX\_P)}$$

  1. take any $\widehat{x} \in \mathbb{R}^n$, find $\hat{s} > \max\limits_{i=1,..,m} g_i(\widehat{x})$, with $(\widehat{x}, \hat{s}) \in int(\text{feasib. reg. of (AUX\_P)}$
  2. Find optimal solution (x^*, s^*) of (AUX_P) using a barrier method starting from (x^*, s^*)
  3. If $s^* < 0 \implies x^* \in int(\Omega)$,
  else $int(\Omega) = \emptyset$

LOG BARRIER

- Logarithmic barrier

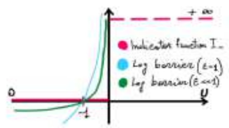
$$B(x) = -\sum_{i=1}^{m} log(-g_i(x))$$

- Properties of logarithmic barrier :
  - $dom(B) = int(\Omega)$
  - B convex
  - B is smooth with

$$\nabla B(x) = -\sum_{i=1}^{m} \frac{1}{g_i(x)} \nabla g_i(x)$$
$$\nabla^2 B(x) = \sum_{i=1}^{m} \frac{1}{g_i(x)^2} \nabla g_i(x) \nabla g_i(x)^T + + \sum_{i=1}^{m} \left(-\frac{1}{g_i(x)} \right) \nabla^2 g_i(x)$$

- Indicator function $I\_(u)$ may be approximated by the **smooth** **convex** function called logarithmic barrier

$$-\varepsilon\, log(-u), \varepsilon > 0$$



and the approximation improves as $\varepsilon \to 0$

- If x^*_ε is the optimal solution of (P_{LB}), then

$$\nabla f(x^*_\varepsilon) + \sum_{i=1}^{m} \left(-\frac{\varepsilon}{g_i(x^*_\varepsilon)} \right) \nabla g_i(x^*_\varepsilon) = 0$$

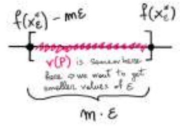
- By defining $\lambda^*_\varepsilon = \left(-\frac{\varepsilon}{g_1(x^*_\varepsilon)}, .., -\frac{\varepsilon}{g_m(x^*_\varepsilon)} \right) > 0$, we can say that the Lagrangian function

$$L(x, \lambda^*_\varepsilon) = f(x) + \sum_{i=1}^{m} (\lambda^*_\varepsilon)_i \cdot g_i(x)$$

is **convex** and $\nabla_x L(x^*_\varepsilon, \lambda^*_\varepsilon) = 0$, hence

$$f(x^*_\varepsilon) \geq v(P) \geq \varphi(\lambda^*_\varepsilon) = \min_x L(x, \lambda^*_\varepsilon) = = L(x^*_\varepsilon, \lambda^*_\varepsilon) = = f(x^*_\varepsilon) - \underbrace{m\, \varepsilon}_{\text{optimality gap}} \to$$

$$\to f(x^*_\varepsilon) - m\, \varepsilon \leq v(P) \leq f(x^*_\varepsilon)$$



- Interpretation via KKT conditions :

KKT of original problem

Approximation of the previous KKT system. The solution of this system is $(x^*_\varepsilon, \lambda^*_\varepsilon)$

$$\begin{cases} \nabla f(x) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x) = 0 \\ -\lambda_i g_i(x) = 0 \\ \lambda \geq 0 \\ g(x) \leq 0 \end{cases} \approx \begin{cases} \nabla f(x) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x) = 0 \\ -\lambda_i g_i(x) = \varepsilon \\ \lambda \geq 0 \\ g(x) \leq 0 \end{cases}$$

PROBLEMS w/ LINEAR EQUALITY CONSTRAINTS

- Consider a **constrained** problem

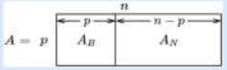
$$\begin{cases} min\ f(x) \\ A\, x = b \end{cases} \qquad (1)$$

where :
  - f is **strongly convex** and **twice continuously differentiable**.
  - $A \in \mathbb{R}^{p \times n}$, with $rank(A) = p$
- The problem (1) is equivalent to the following unconstrained problem

$$\begin{cases} min\ f(x_B, x_N) \\ x_N \in \mathbb{R}^{n-p} \end{cases}$$

...

...where :
  - $A = (A_B, A_N)$, with $A_B \in \mathbb{R}^{p \times p}$ matrix, and $A_N \in \mathbb{R}^{p \times (n-p)}$



  with A_B being a non-singular matrix (i.e. $det(A_B) \neq 0$)
  - $x^T = (x_B, x_N)$
  - Since $det(A_B) \neq 0$, we have that $A\, x = b$ is equivalent to

$$A_B\, x_B + A_N\, x_N = b \implies \implies x_B = A_B^{-1}(b - A_N\, x_N)$$

Thus, the alternative problem, becomes

$$\begin{cases} min\ f(A_B^{-1}(b - A_N\, x_N), x_N) \\ x_N \in \mathbb{R}^{n-p} \end{cases} \qquad (2)$$

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 $x_3 = -1/6$, $x_1 = 7/6$, $x_2 = 2/3$.

ACTIVE-SET METHOD

- Let's suppose we have inequality constraints in our problem

$$\begin{cases} min\ \frac{1}{2} x^T\, Q\, x + c^T\, x \\ A\, x \leq b \end{cases} \qquad (3)$$

where :
  - Q is a **positive definite** matrix
  - $\forall$ feasible point x, the vectors $\{A_i : A_i\, x = b_i\}$ are linearly independent.
- The **active-set method** solves at each iteration a quadratic programming problem with **equality constraints only**.
- **Active-set method** :
  1. Choose feasible point x^0;
  set $W_0 = \{i : A_i\, x^0 = b_i\}$ (**working set**);
  set $k = 0$
  2. Find optimal solution y^k of the problem
  $$\begin{cases} min\ \frac{1}{2} x^T\, Q\, x + c^T\, x \\ A_i\, x = b, \qquad \forall i \in W_k \end{cases}$$
  3. If $y^k \neq x^k$ then go to step 4.
  Go to step 5 otherwise.
  4. **If** y^k is feasible, then $t_k = 1$,
  else
  $$t_k = min \left\{ \frac{b_i - A_i\, x^k}{A_i\, (y^k - x^k)} : i \notin W_k, A_i(y^k - x^k) > 0 \right\},$$
  Update also :
     1. $x^k : x^{k+1} = x^k + t_k(y^k - x^k)$
     2. $W_k : W_{k+1} = W_k \cup \{i \notin W_k : A_i\, x^{k+1} = b_i\}$
     3. k = k+1
     Go to step 2.
  5. Compute the KKT (Karush-Kuhn-Tucker) system multipliers μ^k related to y^k.
  If $\mu^k \geq 0 \implies STOP$,
  else $x^{k+1} = x^k, \quad \mu_j^k = \min\limits_{i \in W_k} \mu_i^k, \quad W_{k+1} = W_k \setminus \{j\}$,
  k=k+1 and go to step 2.

PENALTY METHOD

- These methods are designed for general constrained optimization problems.
- If the objective function f is **non-quadratic** and the constraints are **non-linear**, penalty methods come into our aid.
- Let's consider a constrained optimization problem :

$$\begin{cases} min\ f(x) \\ g_i(x) \leq 0 \qquad i = 1, .., m \end{cases} \qquad \text{(P)}$$

We can transform the problem (P) into an unconstrained problem that adds a penalty

$$p(x) = \sum_{i=1}^{m} (max\{0, g_i(x)\})^2$$

in the objective function if the search solution is not included in the feasible space Ω.

- NOTE : $p(x)$ is defined as the $(\cdot)^2$ of a $\max\{\cdot, \cdot\}$ function in order to obtain a smooth function from another one that may not be smooth (i.e. $\max\{\cdot, \cdot\}$).
- Defining $p_\varepsilon(x)$ as

$$p_\varepsilon(x) = f(x) + \frac{1}{\varepsilon} p(x)$$

where

$$p_\varepsilon(x) \begin{cases} = f(x) & x \in \Omega \\ > f(x) & x \notin \Omega \end{cases}$$

we can thus define the new problem P_ε
$$\begin{cases} min\ p_\varepsilon(x) \\ x \in \mathbb{R}^n \end{cases} \qquad (P_\varepsilon)$$

- **Penalty method** :
  1. Set $\varepsilon_0 > 0, \tau \in (0, 1), k = 0$
  2. Find optimal solution x^k of (P_{ε_k})
  3. If $x^k \in \Omega \implies$ STOP.
  Else $\varepsilon_{k+1} = \tau\, \varepsilon_k$, $k = k + 1$ and go to step 2

PROPOSITIONs

PROPOSITION

- **HP** : f, g_i **convex**
- **TH** : p_ε **convex**

PROPOSITION

- **TH** : any (P_ε) is a relaxation of (P), i.e.

$$v(P_\varepsilon) \leq v(P), \quad \forall \varepsilon > 0$$

PROPOSITION

- **HP** : f, g_i **convex**
- **TH** : p_ε **convex**

PROPOSITION

- **HP** : x^*_ε solves (P_ε), $x^*_\varepsilon \in \Omega$
- **TH** : x^*_ε is optimal also for (P)

PROPOSITION

- **HP** : $\varepsilon_1, \varepsilon_2$ s.t.

$$0 < \varepsilon_1 < \varepsilon_2$$

- **TH** : $v(P_{\varepsilon_2}) \leq v(P_{\varepsilon_1})$

PROPOSITION

- **HP** : f, g_i **continuously differentiable**
- **TH** : p_ε is **continuously differentiable** and

$$\nabla p_\varepsilon(x) = \nabla f(x) + \frac{2}{\varepsilon} \sum_{i=1}^{m} max\{0, g_i(x)\} \nabla g_i(x)$$

EXACT PENALTY METHOD

- Instead of taking $p(x)$ as the sum of squares of the max functions between 0 and a perharps-violated constraints $g_i(x), i = 1, .., m$, we just take the *max* function instead, i.e.

$$\hat{p}(x) = \sum_{i=1}^{m} max\{0, g_i(x)\}$$

Then, the resulting penalized problem $(\widehat{P}_\varepsilon)$ is **unconstrained**, **convex** and **nonsmooth**.

- **Exact penalty method** :
  1. Set $\varepsilon_0 > 0, \tau \in (0, 1)$, $k = 0$
  2. Find an optimal sol. x^k of the penalized problem $(\widehat{P}_{\varepsilon_k})$
  3. If $x^k \in \Omega \implies$ STOP,
  else $\varepsilon_{k+1} = \tau\, \varepsilon_k$,
  $k = k + 1$ and go to step 2.

TH : the exact penalty method stops after a finite number of iterations at an optimal solution of (P)

- **PROs** : we don't need a sequence $\{\varepsilon_k \to 0\}$ to approximate an optimal solution of (P) (avoid numerica issues).
- **CONs** : $(\widehat{P}_\varepsilon)$ is nonsmooth

PROPOSITION

- **HP** :
  - $\exists$ opt. solution x^* of (P)
  - λ^* is a vector of KKT multipliers associated to x^*
- **TH** : the sets of optimal solutions of (P) and $(\widehat{P}_\varepsilon)$ coincide provided that $\varepsilon \in \left(0, \frac{1}{\|\lambda^*\|_\infty}\right)$

THEOREMs

THEOREM

- **HP** : f is coercive
- **TH** : the sequence $\{x^k\}$ is bounded and any of its cluster points is an optimal solution of (P)

THEOREM

- **HP** : $\{x^k\}$ converges to x^*
- **TH** : x^* optimal solution for (P)

THEOREM

- **HP** :
  - $\{x^k\}$ converges to x^*
  - gradients of **active** constraints at x^* are **linearly independent.**
- **TH** : x^* is an optimal solution of (P) and the sequence of vectors $\{\lambda^k\}$ defined as

$$\lambda_i^k = \frac{2}{\varepsilon_k} max\{0, g_i(x^k)\}, \quad i = 1, .., m$$

converges to a vector λ^* of KKT multipliers associated to x^*

9. MULTIOBJECTIVE OPTIMIZATION

Instead of a single objective function, we've got to deal with an **array of p objective functions**

$$\boldsymbol{f(x) = (f_1(x), f_2(x), .., f_p(x))}$$

e.g. Multi-flight-ticket purchase : what do we want to minimize first? Tot cost? Tot hours spent travelling + waiting at various aeroports? Tot distance travelled?

EXISTENCE RESULTS

Ω bounded

GENERALIZED WEIERSTRASS TH.

- HP :
  - $f_i(x)$ is **continuous** $\forall i = 1, .., p$
  - Ω is **closed** and **bounded**.
- TH : $\exists$ minimum of (P)

Ω unbounded

TH

- HP :
  - $f_i(x)$ is **continuous** $\forall i = 1, .., p$
  - Ω is **closed**.
  - $\exists v \in \mathbb{R}, j \in \{1, .., p\}$ s.t. the sublevel set

$$\{x \in \Omega : f_j(x) \leq v\}$$

is **non-empty** and **bounded**, i.e. the sublevel of just one objective function $f_j(x)$ has to be non-empty and bounded.

- TH : $\exists$ minimum of (P)

COROLLARY

- HP :
  - $f_i(x)$ is **continuous** $\forall i = 1, .., p$
  - Ω is **closed**.
  - $\exists j \in \{1, .., p\}$ s.t. $f_j(x)$ is **coercive**.
- TH : $\exists$ minimum of (P)

OPTIMALITY CONDITIONS

TH

- TH : x^* is a **minimum** of (P) $\iff$ the aux. optimization problem

$$\begin{cases} max \sum_{i=1}^{p} \varepsilon_i \\ f_i(x) + \varepsilon_i \leq f_i(x^*) \quad i = 1, .., p \\ x \in \Omega \\ \varepsilon \geq 0 \end{cases} \quad \text{(AUX\_P1)}$$

has optimal value equal to 0.

TH

- TH : x^* is a **weak minimum** of (P) $\iff$ the aux. optimization problem

$$\begin{cases} max\ v \\ v \leq \varepsilon_i \quad i = 1, .., p \\ f_i(x) + \varepsilon_i \leq f_i(x^*) \\ x \in \Omega \\ \varepsilon > 0 \end{cases} \quad \text{(AUX\_P2)}$$

has optimal value equal to 0.

UNCONSTRAINED PROBLEMS

1st ORDER OPTIMALITY CONDITIONS (UNCONST. PROB.s)

- We're given an unconstrained multiobjective problem like the following

$$\begin{cases} min\ f(x) = (f_1(x), f_2(x), .., f_p(x)) \\ x \in \mathbb{R}^n \end{cases} \quad \text{(P\_unconstr)}$$

where f_i is continuously differentiable $\forall i = 1, .., p$

- TH (Necessary condition) : if x^* is a **weak minimum** of $(P\_unconstr) \implies \exists \xi^* \in \mathbb{R}^p$ s.t.

$$\begin{cases} \sum_{i=1}^{p} \xi_i^* \nabla f_i(x^*) = 0 \\ \xi^* \geq 0 \\ \sum_{i=1}^{p} \xi_i^* = 1 \end{cases} \quad \text{(S)}$$

- TH (Sufficient condition) : if problem $(P\_uncostr)$ is **convex**, i.e. $f_i(x)$ convex $\forall i = 1, .., p$, and x^*, ξ^* is a solution of the system $(S) \implies x^*$ is a **weak minimum** of (P)

CONSTRAINED PROBLEMS

1st ORDER OPTIMALITY CONDITIONS (CONSTR. PROB.s)

- We're given a constrained multiobjective problem like the following

$$\begin{cases} min\ f(x) = KKT(f_1(x), f_2(x), .., f_p(x)) \\ g_j(x) \leq 0 \quad j = 1, .., m \\ h_k(x) = 0 \quad k = 1, .., q \end{cases} \quad \text{(P\_constr)}$$

where f_i, g_j, h_k are continuously differentiable with $i = 1, .., p\ ,\ j = 1, .., m\ ,\ k = 1, .., q$

- TH (Necessary condition) : if x^* is a **weak minimum** of $(P\_constr) \implies \exists \xi^* \in \mathbb{R}^p, \lambda^* \in \mathbb{R}^m, \mu^* \in \mathbb{R}^q$ s.t. $(x^*, \xi^*, \lambda^*, \mu^*)$ solves the KKT system

$$\begin{cases} \sum_{i=1}^{p} \xi_i^* \nabla f_i(x^*) + \sum_{j=1}^{m} \lambda_j^* \nabla g_j(x^*) + \sum_{k=1}^{q} \mu_k^* \nabla h_k(x^*) = 0 \\ \xi^* \geq 0 \\ \sum_{i=1}^{p} \xi_i^* = 1 \\ \lambda^* \geq 0 \\ \lambda_j^* g_j(x^*) = 0, \quad j = 1, .., m \end{cases}$$

- TH (Sufficient condition) : if problem (P_costr) is **convex**, i.e. $f_i(x), g_j(x), h_k(x)$ convex $i = 1, .., p\ ,\ j = 1, .., m\ ,\ k = 1, .., q$, and $(x^*, \xi^*, \lambda^*, \mu^*)$ is a solution of the system $\implies x^*$ is a **weak minimum** of (P)

SOLUTION METHODS

SCALARIZATION METHOD

- Let's define a vector of **weights** associated to the objectives :

$$\alpha = (\alpha_1, .., \alpha_p) \geq 0,\ s.t.\ \sum_{i=1}^{p} \alpha_i = 1$$

- That vector of weights is used to **scalarize** the objective function by **giving each objective a certain weight**, depending on the importance of the objective

$$\begin{cases} min \sum_{i=1}^{p} \alpha_i f_i(x) \\ x \in \Omega \end{cases} \quad (P_\alpha)$$

- Let S_α be the set of optimal solutions of (P_α)
- NOTE : solving (P_α) $\forall$ possible choice α doesn't allow finding all the minima and the weak minima

TH

- TH1 : (P) **linear** $\implies$
  - $\{\boldsymbol{weak\ minima}\ of\ (P)\} = \bigcup_{\alpha \geq 0} S_\alpha$
  - $\{\boldsymbol{minima}\ of\ (P)\} = \bigcup_{\alpha > 0} S_\alpha$
- TH2 : (P) **convex** $\implies$ $\{\boldsymbol{weak\ minima}\ of\ (P)\} = \bigcup_{\alpha \geq 0} S_\alpha$
- TH3 : (P) **convex**, f_i **strongly convex** $i = 1, .., p \implies$ $\{\boldsymbol{weak\ minima}\ of\ (P)\} = \bigcup_{\alpha \geq 0} S_\alpha$

TH

- TH1 : $\bigcup_{\alpha \geq 0} S_\alpha \subseteq \boldsymbol{weak\ minima}$ of (P)
- TH2 : $\bigcup_{\alpha > 0} S_\alpha \subseteq \boldsymbol{minima}$ of (P)

GOAL METHOD

- Let's define in the objective space $\mathbb{R}^p$ the **ideal point z** as

$$z_i = \min_{x \in \Omega} f_i(x), i = 1, .., p$$

- Since very often the problem (P) has no ideal minimum (i.e. z \not\in f(\Omega)), we want to find the point of $f(\Omega)$ which is as close as possible to z :

$$\begin{cases} min\ ||f(x) - z||_s \\ x \in \Omega, \quad s \in [1, +\infty] \end{cases} \quad \text{(G)}$$

TH

- **TH1** : if $s \in [1, +\infty[\implies$ any optimal solution of G is a **minimum** of (P).
- **TH2** : if $s = +\infty \implies$ any optimal solution of G is a **weak minimum** of (P)

GOAL METHOD ON LINEAR PROGR. PROBLEMS

- Assume that (P) is a linear multiobjective optimization problem, i.e.

$$\begin{cases} min\ C\,x \\ A\,x \leq b \end{cases} \quad (P_{linear})$$

where $C \in \mathbb{R}^{p \times n}$

- $\boldsymbol{s = 2} \implies (G)$ is equivalent to a quadratic programming problem

$$\begin{cases} min\ \frac{1}{2}||C\,x - z||_2^2 = \\ = \frac{1}{2} x^T C^T C\,x - x^T C^T z + \frac{1}{2} z^T z \\ A\,x \leq b \end{cases} \quad (G_2)$$

- $\boldsymbol{s = 1} \implies (G)$ is equivalent to the linear programming problem

$$\begin{cases} \min_{x,y} \sum_{i=1}^{p} y_i \\ y_i \geq C_i\,x - z_i \quad i = 1, .., p \\ y_i \geq z_i - C_i\,x \quad i = 1, .., p \\ A\,x \leq b \end{cases} \quad (G_1)$$

- $\boldsymbol{s = +\infty} \implies (G)$ is equivalent to the linear programming problem

$$\begin{cases} \min_{x,y} y \\ y \geq C_i\,x - z_i \quad i = 1, .., p \\ y \geq z_i + C_i\,x \quad i = 1, .., p \\ A\,x \leq b \end{cases} \quad (G_\infty)$$

Example. Consider

$$\begin{cases} \min\ (x_1 - x_2\ ,\ x_1 + x_2) \\ -2\,x_1 + x_2 \leq 0 \\ -x_1 - x_2 \leq 0 \\ 5\,x_1 - x_2 \leq 6 \end{cases}$$

The set $f(\Omega)$ is shown in the figure below.
The ideal point is $z = (-2, 0)$ (black point).
The optimal solution of (G_2) is $x^* = (1/5, 2/5)$ and $f(x^*) = (-1/5, 3/5)$.
The optimal solution of (G_1) is $\bar{x} = (0, 0)$ and $f(\bar{x}) = (0, 0)$.
The optimal solution of (G_∞) is $\hat{x} = (1/2, 1)$ and $f(\hat{x}) = (-1/2, 3/2)$.

PARETO ORDER

- There are often **conflicting objectives** (e.g. cost vs distance in the multi-ticket purchase example) $\implies$ definition of optimality is not obvious. We need to define an **order** in $\mathbb{R}^p$.
- **Pareto order** : given $x, y \in \mathbb{R}^p$, we say that

$$x \geq y \iff x_i \geq y_i \ \forall i = 1, .., p$$

This relation is a partial order in $\mathbb{R}^p$ and it is :

  - **reflexive** : $x \geq x$
  - **asymmetric** : if $x \geq y$ and $y \geq x \implies x = y$
  - **transitive** : if $x \geq y$ and $y \geq z \implies x \geq z$

but it is not a total order : if $x = (1, 4)$ and $y = (3, 2)$, $\implies x \not\geq y$ and $y \not\geq x$

PARETO MINIMUM

Given a subset $A \subseteq \mathbb{R}^p$ we call :

- Pareto **ideal minimum** of A a point $x \in A$ s.t. $y \geq x, \forall y \in A$
- Pareto **minimum** of A a point $x \in A$ s.t. $\nexists y \in A, y \neq x$ s.t. $x \geq y$.
- Pareto **weak minimum** of A a point $x \in A$ s.t. $\nexists y \in A, y \neq x$ s.t. $x > y$

PROPOSITION

- Let's call $IMin(A)$ the set of Pareto Ideal minima, $Min(A)$ the set of Pareto minima and $WMin(A)$ the set of Pareto weak minima. These sets are s.t.

$$IMin(A) \subseteq Min(A) \subseteq WMin(A)$$

- If $IMin(A) \neq \emptyset$ (i.e. $IMin(A)$ contains the only ideal minimum point $\widehat{x}$) $\implies IMin(A) = Min(A) = \{\widehat{x}\}$

PARETO MINIMUM OF MULTIOBJ. OPTIMIZATION PROBLEM

- Given the multiobjective minimization problem

$$\begin{cases} min\ f(x) = \Big(f_1(x), .., f_p(x)\Big) \\ x \in \Omega \end{cases} \quad \text{(P)}$$

we call :

  - $x^* \in \Omega$ a Pareto **ideal minimum** of (P) if $f(x^*)$ is a Pareto ideal minimum of $f(\Omega)$, i.e. $f(x) \geq f(x^*), \forall x \in \Omega$
  - $x^* \in \Omega$ a Pareto **minimum** of (P) if $f(x^*)$ is a Pareto minimum of $f(\Omega)$, i.e. $\nexists x \in \Omega$ s.t.

$$f_i(x^*) \geq f_i(x),\ \ \forall i = 1, .., p$$
$$f_j(x^*) > f_j(x),\ \ \text{for some j} \in \{1, .., p\}$$

  - $x^* \in \Omega$ a Pareto **weak minimum** of (P) if $f(x^*)$ is a Pareto weak minimum of $f(\Omega)$, i.e. $\nexists x \in \Omega$ s.t.

$$f_i(x^*) > f_i(x),\ \ \forall i = 1, .., p$$

10. GAME THEORY (GT)

- Game theory deals with the analysis of **conflictual situations** among different decision makers (**players**), each of them having different interests.
- The decision (**strategy**) of each player can produce different results depending on the strategies chosen by other players.
- Game theory studies the possibility to forecast the strategies that will be chosen by each player which is assumed to be "rational".

STRATEGIES

STRICTLY DOMINATED STRATEGY

- Given a two-person non-coop game, a strategy $x \in X$ is **strictly dominated** by $\hat{x} \in X$ if

$$f_1(x,y) > f_1(\hat{x},y), \quad \forall y \in Y$$

- Similarly, a strategy $y \in Y$ is **strictly dominated** by $\hat{y} \in Y$ if

$$f_2(x,y) < f_2(x,\hat{y}), \quad \forall x \in X$$

- Strictly dominated strategies can be deleted from the game (because they'll never be used the considered player).

MIXED STRATEGY

- Not all two-person non-coop games have strategies that may strictly dominate other ones. Neither all of these games have Nash equilibria. This is the case for e.g. of the "Odds and evens" two-player non-coop game :

		Player 2	
		1 (odd)	2 (even)
Player 1	1 (odd)	1	−1
	2 (even)	−1	1

- **Definition** of **mixed strategy** : if C is a $m \times n$ matrix game, then a mixed strategy for P_1 is an m-vector of probabilities and we consider

$X = \{x \in \mathbb{R}^m : x \geq 0, \sum_{i=1}^{m} x_i = 1\}$ as the set of mixed strategies of P_1.

$Y = \{y \in \mathbb{R}^n : y \geq 0, \sum_{j=1}^{n} y_j = 1\}$ is the set of mixed strategies of P_2.

- Expected costs are
  - $f_1(x,y) = x^T\, C\, y$, for P_1
  - $f_2(x,y) = -x^T\, C\, y$, for P_2
- The vertices of X, i.e. $e_i = (0,\dots,0,1,0,\dots,0)$, are called **pure strategies** of P_1 because P_1 uses just one strategy.

MIXED STRATEGIES NASH EQUILIBRIA

If C is a $m \times n$ matrix game, then $\hat{x}, \hat{y} \in X \times Y$ is a **mixed strategies nash equilibrum** if

$$\max_{y \in Y} \hat{x}^T\, C\, y = \hat{x}^T\, C\, \hat{y} = \min_{x \in X} x^T\, C \hat{y},$$

i.e. $(\hat{x},\hat{y})$ is a **saddle point** (*punto di sella*) of the function $x^T\, C\, y$

TH

$(\hat{x},\hat{y})$ is a mixed strategies Nash equilibrium $\iff$

$$\begin{cases} \hat{x} \text{ is an opt. sol. of } \min\limits_{x \in X} \max\limits_{y \in Y} x^T\, C\, y \\ \hat{y} \text{ is an opt. sol. of } \max\limits_{y \in Y} \min\limits_{x \in X} x^T\, C\, y \end{cases}$$

Note : we can reformulate these min/max problem into linear programming problems.

TH

- **TH1** : the problem $\min\limits_{x \in X} \max\limits_{y \in Y} x^T\, C\, y$ is equivalent to the linear programming problem

$$\begin{cases} min\ v \\ v \geq \sum_{j=1}^{m} c_{ij}\, x_i \quad j = 1,\dots,n \\ x \geq 0 \\ \sum_{i=1}^{m} x_i = 1 \end{cases} \qquad (Prob_1)$$

$C^T\, x$

- **TH2** :

$$\begin{cases} max\ w \\ w \leq \sum_{j=1}^{n} c_{ij}\, y_j \quad i = 1,\dots,m \\ y \geq 0 \\ \sum_{i=1}^{m} y_i = 1 \end{cases} \qquad (Prob_2)$$

$C\, y$

- **TH3** : $(Prob_2)$ is the dual of $(Prob_1)$
- **COROLLARY** : any matrix game has **at least a mixed strategies Nash equilibrium**.

example of "Odds and evens" problem

		Player 2	
		1 (odd)	2 (even)
Player 1	1 (odd)	1	−1
	2 (even)	−1	1

$$(P_1) \begin{cases} \min\ v \\ v \geq x_1 - x_2 \\ v \geq -x_1 + x_2 \\ x \geq 0 \\ x_1 + x_2 = 1 \end{cases} \text{ is equivalent to } \begin{cases} \min\ v \\ v \geq 2x_1 - 1 \\ v \geq 1 - 2x_1 \\ 0 \leq x_1 \leq 1 \end{cases} \Rightarrow \bar{x} = (1/2, 1/2)$$

$$(P_2) \begin{cases} \max\ w \\ w \leq y_1 - y_2 \\ w \leq -y_1 + y_2 \\ y \geq 0 \\ y_1 + y_2 = 1 \end{cases} \text{ is equivalent to } \begin{cases} \max\ w \\ w \leq 2y_1 - 1 \\ w \leq 1 - 2y_1 \\ 0 \leq y_1 \leq 1 \end{cases} \Rightarrow \bar{y} = (1/2, 1/2)$$

NASH EQUILIBRIUM

- Let's consider a two-player (players P_1, P_2) non-coop game :

$$P_1 : \begin{cases} min\ f_1(x,y) \\ x \in X \end{cases}, \quad P_2 : \begin{cases} min\ f_2(x,y) \\ y \in Y \end{cases}$$

controls

controls

- **Definition** : in a two-person non-coop game, a **pair of strategies** $(\hat{x},\hat{y})$ is a Nash equilibrium if no player can decrease his own cost by **unilateral deviation** ("what is the best possible solution for P_1 if P_2 doesn't change his strategy?"), i.e.

$$f_1(\hat{x},\hat{y}) = \min_{x \in X} f_1(x,\hat{y}),$$

$$f_2(\hat{x},\hat{y}) = \min_{y \in Y} f_1(\hat{x},y)$$

- Equivalent **definition** : $(\hat{x},\hat{y})$ is a Nash equilibrium $\iff$:
  - $\hat{x}$ is the best response of P_1 to strategy $\hat{y}$ of P_2
  - $\hat{y}$ is the best response of P_2 to strategy $\hat{x}$ of P_1

NON-COOPERATIVE GT

- A Non-Cooperative game in normal form is given by :
  - set of N players
  - each player i has a set Ω_i of strategies and a cost function $f_i : \Omega_1 \times \Omega_2 \times \ldots \times \Omega_N \to \mathbb{R}$
- The aim of each player i consists in solving the optimization problem

$$\begin{cases} min\ f_i(x_1, x_2, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_N) \\ x_i \in \Omega_i \end{cases}$$

managed by other ($\neq i$) players

managed by i^{th} player

TYPES OF GAMES

MATRIX GAMES

- Two-person non-coop game where :
  - X, Y are finite sets : $X = \{1,\dots,m\}, Y = \{1,\dots,n\}$
  - $f_2 = -f_1$ (**zero-sum** game).

It can be represented by a $m \times n$ matrix C, where c_{ij} is the cost that P_1 pays to P_2 if P_1 chooses strategy i and P_2 chooses strategy j.
Example :

		Player 2		
		1	2	3
Player 1	1	1	−1	0
	2	3	−2	−1
	3	2	3	−2

For P_2, strategy 3 is dominated by strategy 1, because in strategy 3 we have all non-positive values, i.e. P_2 has to pay a cost or, at best, nothing to P_1 in strategy 3, while strategy 1 guarantees P_2 a secure profit for any strategy of P_1, thus P_2 will never use strategy 3 $\Longrightarrow$ strategy 3 can be deleted from the game. The game is thus equivalent to

		Player 2	
		1	2
Player 1	1	1	−1
	2	3	−2
	3	2	3

Now, for P_1 strategy 3 is worse (they're all strictly positive values $\Longrightarrow$ P_1 always pays a cost to P_2 for any strategy of P_2) than strategy 1. The reduced problem becomes

		Player 2	
		1	2
Player 1	1	1	−1
	2	3	−2

For P_2, strategy 2 is worse than strategy 1 $\Longrightarrow$ remove strategy 2 for P_2. The reduced game is

		Player 2
		1
Player 1	1	1
	2	3

For P_1, strategy 2 is worse than strategy 1 $\Longrightarrow$ we can remove strategy 2 for P_1. We are left with just one choice which is strategy 1 for P_1 and strategy 1 for P_2 $\Longrightarrow$ (1,1) is a Nash equilibrium.

BIMATRIX GAMES

- Two-person non-coop game where :
  - sets of pure strategies are finite, thus the sets of mixed strategies are

$$X = \{x \in \mathbb{R}^m : x \geq 0, \sum_{i=1}^{m} x_i = 1\},$$

$$Y = \{y \in \mathbb{R}^n : y \geq 0, \sum_{j=1}^{n} y_j = 1\}$$

  - $f_2 \neq -f_1$ (**non-zero sum** game); the cost functions are :
    - $f_1(x,y) = x^T\, C_1\, y$, with $C_1 \in \mathbb{R}^{m \times n}$
    - $f_2(x,y) = x^T\, C_2\, y$, with $C_2 \in \mathbb{R}^{m \times n}$
- Example : "prisoner's dilemma" game. P_1 chooses rows, while P_2 chooses columns.

$$C_1 = \begin{pmatrix} 5 & 1 \\ 10 & 2 \end{pmatrix} \qquad C_2 = \begin{pmatrix} 5 & 10 \\ 1 & 2 \end{pmatrix}$$

Are there strictly dominated strategies ? Yes. Let's see it / them :

- SOLUTION, version 1 : P_1 has to evaluate if he's got some strictly unconvenient row (i.e. row with costs > some other row). We can see as strategy (or row) 1 is strictly better than strategy 2 $\Longrightarrow$ delete strategy 2 for P_1 and delete 2^{nd} row of C_2. Since we've got just two columns left, now it's time for P_2 to decide. In C_2, strategy (or column) 1 is better than strategy 2 $\Longrightarrow$ delete strategy 2 for P_2 and 2^{nd} column of C_1. We're left with the unique left strategy which is a Nash equilibrium.
- SOLUTION, version 2 : P_2 has to evaluate if he's got some strictly unconvenient column (i.e. row with costs > some other column).We can see as strategy (or column) 1 is strictly better than strategy 2 $\Longrightarrow$ delete strategy 2 for P_2 and delete 2^{nd} column of C_1. Since we've got just two rows left, now it's time for P_1 to decide. In C_1, strategy (or row) 1 is better than strategy 2 $\Longrightarrow$ delete strategy 2 for P_1 and 2^{nd} row of C_2. We're left with the unique left strategy (1,1) which is a Nash equilibrium.

TH

Any bimatrix game has at least a mixed strategies Nash equilibrium.

BEST RESPONSE

- We define as **best response mappings** $\boldsymbol{B_1(y)} : Y \to X$ and $\boldsymbol{B_2(x)} : X \to Y$ as

$$B_1(y) = \{\text{opt. sol.s of } \min_{x \in X} x^T\, C_1\, y\}$$

$$B_2(x) = \{\text{opt. sol.s of } \min_{y \in Y} x^T\, C_2\, y\}$$

- $(\hat{x},\hat{y})$ is a Nash equilibrium $\iff$ $\hat{x} \in B_1(\hat{y})$ and $\hat{y} \in B_2(\hat{x})$
- Example :

$$C_1 = \begin{pmatrix} -5 & 0 \\ 0 & -1 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -1 & 0 \\ 0 & -5 \end{pmatrix}$$

Given $y \in Y$, we have to solve the problem

$$\begin{cases} min\ x^T\, C_1\, y = \\ \quad = -5\, x_1\, y_1 - x_2\, y_2 \\ x \in X \end{cases}$$

is equivalent to

$$\begin{cases} min\ (1 - 6\, y_1)\, x_1 + y_1 - 1 \\ 0 \leq x_1 \leq 1 \end{cases}$$

Hence, the optimal solution set is

$$B_1(y_1) = \begin{cases} 0 & y_1 \in [0, 1/6] \\ [0,1] & y_1 = 1/6 \\ 1 & y_1 \in [1/6, 1] \end{cases}$$

Similarly, given $x \in X$, we have to solve the problem

$$\begin{cases} min\ x^T\, C_2\, y = \\ \quad = -x_1\, y_1 - 5\, x_2\, y_2 \\ y \in Y \end{cases}$$

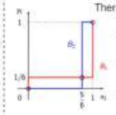
That problem is equivalent to

$$\begin{cases} min\ (5 - 6\, x_1)\, y_1 + 5\, x_1 - 5 \\ 0 \leq y_1 \leq 1 \end{cases}$$

hence the optimal set of solutions is

$$B_2(x_1) = \begin{cases} 0 & x_1 \in [0, 5/6] \\ [0,1] & x_1 = 5/6 \\ 1 & x_1 \in [5/6, 1] \end{cases}$$

Nash equilibria are given by the intersections of the graphs of the best response mappings B_1, B_2



There are 3 Nash equilibria :

- $\hat{x} = (0,1),\ \hat{y} = (0,1)$ (*pure strategies*)
- $\hat{x} = (\frac{5}{6}, \frac{1}{6}),\ \hat{y} = (\frac{1}{6}, \frac{5}{6})$ (*mixed strategies*)
- $\hat{x} = (1,0),\ \hat{y} = (1,0)$ (*pure strategies*)

CONVEX GAMES

- Two-person (can be extended also to N players as well) non-coop game, with players P_1, P_2, where :

$$P_1 : \begin{cases} min_x\ f_1(x, \boldsymbol{y}) \\ g^1_i(x) \leq 0 \quad i = 1,\dots,p \end{cases}$$

$$P_2 : \begin{cases} min_y\ f_2(\boldsymbol{x}, y) \\ g^2_j(y) \leq 0 \quad j = 1,\dots,q \end{cases}$$

with :

- f_1, f_2 being the cost functions of, respectively, P_1, P_2
- $f_1, g^1_i\ (\forall i = 1,\dots,p), f_2, g^2_j\ (\forall j = 1,\dots,q)$ are all continuously differentiable.
- The game is said **convex** $\iff$ the optimization problem of each player is convex.

TH

- **HP** :
  - feasible regions

$$X = \{x \in \mathbb{R}^m : g^1_i(x) \leq 0, i = 1,\dots,p\}$$

$$Y = \{y \in \mathbb{R}^n : g^2_j(y) \leq 0, j = 1,\dots,q\}$$

are **closed**, **convex** and **bounded**

  - cost function $f_1(\cdot,y)$ w.r.t. x is **quasiconvex** (i.e. $\exists$ sublevel set of that function $f_1(\cdot,y)$ that is convex) $\forall y \in Y$
  - cost function $f_2(x,\cdot)$ w.r.t. y is **quasiconvex** (i.e. $\exists$ sublevel set of that function $f_2(x,\cdot)$ that is convex) $\forall x \in X$

$\forall \alpha \in \mathbb{R}, \forall y \in \mathbb{R}^n$ the set $\left\{x \in \mathbb{R}^m : f_1(x,y) \leq \alpha\right\}$ *is convex (remember that y is a parameter here!)*

- **TH** : $\exists$ Nash equilibrium.
- NOTE : quasiconvexity of f_1, f_2 is crucial(!!). For example, the game defined as $X = Y = [0,1]$, $\boldsymbol{f_1(x,y)} = -x^2 + 2x\,y$, $\boldsymbol{f_2(x,y)} = y\,(1 - 2\,x)$ has no Nash equilibrium.

KKT CONDITIONS

- **TH1** : if $(\hat{x},\hat{y})$ is a Nash equilibrium and the ACQ (Abadie Constraint Qualification) holds both in $\hat{x}$ and $\hat{y}$ $\Longrightarrow$ $\exists \lambda^1 \in \mathbb{R}^p, \lambda^2 \in \mathbb{R}^q$ s.t.

$$\begin{cases} \nabla_x f_1(\hat{x},\hat{y}) + \sum_{i=1}^{p} \lambda^1_i\, \nabla g^1_i(\hat{x}) = 0 \\ \lambda^1 \geq 0 \\ g^1(\hat{x}) \leq 0 \\ \lambda^1_i\, g^1_i(\hat{x}) = 0 \quad i = 1,\dots,p \\ \nabla_x f_2(\hat{x},\hat{y}) + \sum_{j=1}^{q} \lambda^2_j\, \nabla g^2_j(\hat{y}) = 0 \\ \lambda^2 \geq 0 \\ g^2(\hat{y}) \leq 0 \\ \lambda^2_j\, g^2_j(\hat{y}) = 0 \quad j = 1,\dots,q \end{cases}$$

KKT system of P_1

KKT system of P_2

- **TH2** : if $(\hat{x},\hat{y},\lambda^1,\lambda^2)$ solves the above system and the game is **convex** $\Longrightarrow$ $(\hat{x},\hat{y})$ is a Nash equilibrium.

CHARACTERIZATION OF NASH EQUILIBRIA

KKT CONDITIONS FOR NASH EQUILIBRIA

- **TH** : $(\hat{x},\hat{y})$ is a Nash equilibrium $\iff$ $\exists \mu_1, \mu_2 \in \mathbb{R}$ s.t.

$$\begin{cases} C_1\, \hat{y} + \mu_1\, e \geq 0 \\ \hat{x} \geq 0 \\ \sum_{i=1}^{m} \hat{x}_i = 1 \\ \hat{x}_i\, (C_1\, \hat{y} + \mu_1\, e)_i = 0 \quad i = 1,\dots,m \\ C_2^T\, \hat{x} + \mu_2\, e \geq 0 \\ \hat{y} \geq 0 \\ \sum_{j=1}^{n} \hat{y}_j = 1 \\ \hat{y}_j\, (C_2^T\, \hat{x} + \mu_2\, e)_j = 0 \quad j = 1,\dots,n \end{cases}$$

$\hat{x}$ chosen by P_1

$\hat{y}$ chosen by P_2

where $e = (1,\dots,1)^T$

- To get the to the above system, do the following : start from the systems,

$$\begin{cases} \min\limits_{x} x^T C_1 y \\ x_i \geq 0 \quad i = 1,\dots,m \\ \sum_{i=1}^{m} x_i = 1 \end{cases} \qquad \begin{cases} \min\limits_{y} x^T C_2 y \\ y_j \geq 0 \quad j = 1,\dots,n \\ \sum_{j=1}^{n} y_j = 1 \end{cases}$$

then obtain the KKT of each of them, obtain vector $\lambda^1 = (\lambda^1_1,\dots,\lambda^1_m)$ for P_1 and $\lambda^2 = (\lambda^2_1,\dots,\lambda^2_n)$ for P_2 and then replace λ^1 and λ^2 in the systems, then join the systems into one.

TH

Assume that $C_1 < 0$ and $C_2 < 0$ (this is not a restrictive assumption, since you can alway take the matrix (C_1 or C_2, whatever!) and subtract to it a matrix having all equal values s.t. each component of the resulting matrix is < 0, and you can still obtain the Nash equilibria of the initial matrix) :

- if $\hat{x}, \hat{y}$ is a Nash equilibrium $\Longrightarrow$ $\exists u > 0, v > 0$ s.t.

$$\tilde{x} = \frac{\hat{x}}{u}, \quad \tilde{y} = \frac{\hat{y}}{v}$$

solve the following system (S)

$$\begin{cases} C_1\, \tilde{y} + e \geq 0 \\ \tilde{x} \geq 0 \\ \tilde{x}_i\, (C_1\, \tilde{y} + e)_i = 0 \quad i = 1,\dots,m \\ C_2^T\, \tilde{x} + e \geq 0 \\ \tilde{y} \geq 0 \\ \tilde{y}_j\, (C_2^T\, \tilde{x} + e)_j = 0 \quad j = 1,\dots,n \end{cases} \qquad \text{(S)}$$

If $(\tilde{x},\tilde{y})$ solves system (S), with $\tilde{x} \neq 0$ and $\tilde{y} \neq 0$, then

$$\left(\frac{\tilde{x}}{\sum_{i=1}^{m} \tilde{x}_i}, \frac{\tilde{y}}{\sum_{j=1}^{n} \tilde{y}_j} \right)$$

is a Nash equilibrium.

TH

- Define the polyhedra :

$$P = \left\{ (x_1,\dots,x_m) : \begin{array}{ll} x_i \geq 0 & \forall i = 1,\dots,m \\ (C_2^T x + e)_j \geq 0 & \forall j = m+1,\dots,m+n \end{array} \right\}$$

$$Q = \left\{ (y_{m+1},\dots,y_{m+n}) : \begin{array}{ll} (C_1 y + e)_i \geq 0 & \forall i = 1,\dots,m \\ y_j \geq 0 & \forall j = m+1,\dots,m+n \end{array} \right\}$$

- **TH** : $(\tilde{x},\tilde{y})$ solves system (S) $\iff$ $\tilde{x} \in P, \tilde{y} \in Q$, and $\forall k = 1,\dots,m+n$, either the k^{th} constraint of P is active in $\tilde{x}$, or the k^{th} constraint of Q is active in $\tilde{y}$.
- **TH** : if the vertices of P and Q are non-degenerate (i.e. m constraints active on x, and n constraints active on y) and $(\tilde{x},\tilde{y})$ solves system (S) $\Longrightarrow$ $\tilde{x}$ is a vertex of P and $\tilde{y}$ is a vertex of Q.
- Therefore, if $C_1 < 0, C_2 < 0$ and vertices of P, Q are non-degenerate $\Longrightarrow$ we can find all Nash equilibria analyzing all the pairs (x,y) of vertices of P and Q, checking if for any $k = 1,\dots,m+n$ either the k^{th} constraint of P is active in x, or the k^{th} constraint of Q is active in y.

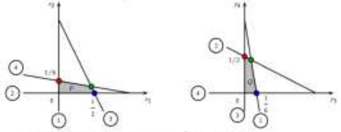
Example. (Battle of the buddies)

$$C_1 = \begin{pmatrix} -5 & 0 \\ 0 & -1 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -1 & 0 \\ 0 & -5 \end{pmatrix}$$

Since the elements of C_1 and C_2 are not all negative, we can reformulate the game setting $(C_1)_{ij} = (C_1)_{ij} - 1$ and $(C_2)_{ij} = (C_2)_{ij} - 1$:

$$C_1 = \begin{pmatrix} -6 & -1 \\ -1 & -2 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -2 & -1 \\ -1 & -6 \end{pmatrix}$$

$P = \{(x_1,x_2) : x_1 \geq 0,\ x_2 \geq 0,\ -2x_1 - x_2 + 1 \geq 0,\ -x_1 - 6x_2 + 1 \geq 0\}$
$Q = \{(y_3,y_4) : -6y_3 - y_4 + 1 \geq 0,\ -y_3 - 2y_4 + 1 \geq 0,\ y_3 \geq 0,\ y_4 \geq 0\}$
Vertices of P and Q are non-degenerate.



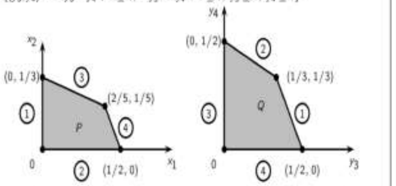
Solutions of system (S)	Nash equilibria
x = (0, 1/6) (active const. 1, 4) y = (0, 1/2) (active const. 2, 3)	x = (0,1) y = (0,1)
x = (5/11, 1/11) (active const. 3, 4) y = (1/11, 5/11) (active const. 1, 2)	x = (5/6,1/6) y = (1/6,5/6)
x = (1/2,0) (active const. 2, 3) y = (1/6,0) (active const. 1, 4)	x = (1,0) y = (1,0)

LEMKE-HOWSON ALGORITHM

- When $C_1 < 0, C_2 < 0$ and vertices of P, Q are non-degenerate, a Nash equilibrium (beware : not ALL Nash equilibria, but just one) can be found by using this algorithm :
  1. Set $x = 0, y = 0$. Define $I_x = \{1,\dots,m\}, I_y = \{m+1,\dots,m+n\}$. Choose an exiting index $h \in 1,\dots,m$.
  2. In polyhedron P, move away from x along the edge given by constraints $I_x \setminus \{h\}$, towards the adjacent vertex x'
  3. Find the entering index k corresponding to the new active constraint at x'. Set $x = x'$ and $I_x = (I_x \setminus \{h\}) \cup \{k\}$
  4. If $k \notin I_y$ $\Longrightarrow$ STOP : (x,y) solves system (S), i.e. we can find a Nash equilibrium, else set $h = k$ and in polyhedron Q move away from y along the edge given by constraints $I_y \setminus \{h\}$, towards the adjacent vertex y'
  5. Find the entering index k corresponding to the new active constraint at y'. Set $y = y'$ and $I_y = (I_y \setminus \{h\}) \cup k$
  6. If $k \notin I_x$ $\Longrightarrow$ STOP : (x,y) solves system (S), i.e. we can find a Nash equilibrium, else set $h = k$ and go to step 2.

Example. Consider the following bimatrix game: $C_1 = \begin{pmatrix} -2 & -1 \\ -1 & -2 \end{pmatrix}$ $C_2 = \begin{pmatrix} -1 & -2 \\ -3 & -1 \end{pmatrix}$

$P = \{(x_1,x_2) : x_1 \geq 0,\ x_2 \geq 0,\ -x_1 - 3x_2 + 1 \geq 0,\ -2x_1 - x_2 + 1 \geq 0\}$
$Q = \{(y_3,y_4) : -2y_3 - y_4 + 1 \geq 0,\ -y_3 - 2y_4 + 1 \geq 0,\ y_3 \geq 0,\ y_4 \geq 0\}$



Iter	h	k	x	I_x	y	I_y
1			(0,0)	{1,2}	(0,0)	{3,4}
2	1	4	(1/2,0)	{2,4}	(0,0)	{3,4}
3	4	2	(1/2,0)	{2,4}	(0,1/2)	{2,3}
4	2	3	(2/5,1/5)	{3,4}	(0,1/2)	{2,3}
5	3	1	(2/5,1/5)	{3,4}	(1/3,1/3)	{1,2}
	Nash	equil.	(2/3,1/3)		(1/2,1/2)	

MERIT FUNCTIONS

- Merit functions $\psi(x,y)$ allow reformulating the Nash equilibrium problem into an equivalent optimization problem (whose global optimum solution is a Nash equilibrium), where we want to minimize a function that takes into account two different choices of P_1 and two different choices of P_2.
- We can define $\psi(x,y)$ as one of the following convex functions:
  - **gap function**
  - **regularized gap function**
  - **D-gap function**

GAP FUNCTION

- Let's consider the Nikaido-Isoda function

$$f(x,y,u,v) = f_1(u,y) - f_1(x,y) + f_2(x,v) - f_2(x,y), \quad x, u \in \mathbb{R}^m, \quad y, v \in \mathbb{R}^n$$

difference of cost between choosing u vs choosing x

difference of cost between choosing v vs choosing y

- We can thus define the **gap function** as

$$\psi(x,y) = \max_{\substack{u \in X, \\ v \in Y}} \left(-f(x,y,\boldsymbol{u},\boldsymbol{y}) \right)$$

- Then
  - problem defining $\psi(x,y)$ is convex
  - $\psi(x,y) \geq 0, \forall (x,y) \in X \times Y$
  - $(\hat{x},\hat{y})$ is a Nash equilibrium $\iff$ $(\hat{x},\hat{y}) \in X \times Y$ and $\psi(\hat{x},\hat{y}) = 0$
- Hence, finding Nash equilibria is equivalent to solving the **constrained** optimization problem

$$\begin{cases} min\ \psi(x,y) \\ (x,y) \in X \times Y \end{cases}$$

REGULARIZED GAP FUNCTION

- In general $\psi(x,y)$ is not always differentiable, but we can regularize it. Given a parameter $\alpha > 0$, the **regularized gap function** is defined as

$$\psi_\alpha(x,y) = \max_{\substack{u \in X, \\ v \in Y}} \left(-f(x,y,\boldsymbol{u},\boldsymbol{v}) - \frac{\alpha}{2} ||(x,y) - (\boldsymbol{u},\boldsymbol{v})||^2 \right)$$

- Then :
  - problem defining $\psi_\alpha(x,y)$ is **convex** and has unique optimal solution
  - ψ_α is **continuously differentiable**
  - $\psi_\alpha(x,y) \geq 0, \forall (x,y) \in X \times Y$
  - $\hat{x}, \hat{y}$ is a Nash equilibrium $\iff$ $(\hat{x},\hat{y}) \in X \times Y$ and $\psi_\alpha(\hat{x},\hat{y}) = 0$
  - Hence, finding Nash equilibria is equivalent to solving the **smooth constrained** optimization problem

$$\begin{cases} min\ \psi_\alpha(x,y) \\ (x,y) \in X \times Y \end{cases}$$

D-GAP FUNCTION

- We can reformulate the problem of finding Nash equilibria as an **unconstrained** optimization problem.
- Given two params $\beta > \alpha > 0$, the **D-gap function** is defined as

$$\psi_{\alpha,\beta}(x,y) = \psi_\alpha(x,y) - \psi_\beta(x,y)$$

- Then :
  - $\psi_{\alpha,\beta}(x,y)$ is **continuously differentiable**.
  - $\psi_{\alpha,\beta}(x,y) \geq 0, \forall (x,y) \in \mathbb{R}^m \times \mathbb{R}^n$
  - $(\hat{x},\hat{y})$ is a Nash equilibrium $\iff$ $\psi_{\alpha,\beta}(\hat{x},\hat{y}) = 0$
- Hence, finding Nash equilibria is equivalent to solving the **smooth unconstrained** optimization problem

$$\begin{cases} min\ \psi_{\alpha,\beta}(x,y) \\ (x,y) \in \mathbb{R}^m \times \mathbb{R}^n \end{cases}$$