Continuous optimization
ENT305A

Elise Grosjean

Ensta-Paris
Institut Polytechnique de Paris
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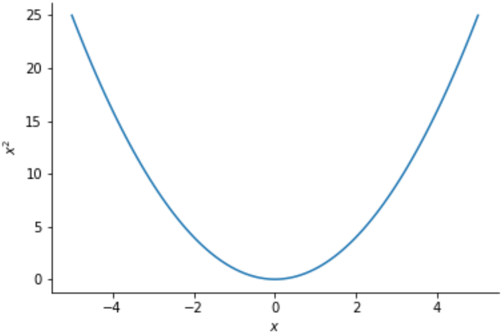
What is an optimization problem?

$$f : x \to x^2, x \in [-5, 5]$$

$\mathcal{D} = K = \mathbb{R}$



What is an optimization problem?

Notation.
Let $\bar{B}(\bar{x}, \varepsilon)$ denote the closed ball of center $\bar{x}$ and radius ε.

Definition.
A feasible point $\bar{x}$ is a local solution to (P) if and only if there exists $\varepsilon > 0$ such that $\bar{x}$ is a **global** solution to the following **localized** problem:

$$\inf_{x \in \mathbb{R}^n} f(x), \quad x \in K \cap \bar{B}(\bar{x}, \varepsilon).$$

What is an optimization problem?

Constraints.
Most of the time, the feasible set K is described by

$$K = \left\{ x \in \mathbb{R}^n \,\middle|\, \begin{array}{ll} h_i(x) = 0, & \forall i \in \mathcal{E} \\ g_j(x) \leq 0, & \forall j \in \mathcal{I} \end{array} \right\},$$

where $h\colon \mathbb{R}^n \to \mathbb{R}^{m_1}$, $g : \mathbb{R}^n \to \mathbb{R}^{m_2}$.

We call the expressions

- $h_i(x) = 0$: **equality constraint**
- $g_j(x) \leq 0$: **inequality constraint**.

Existence of a solution

Theorem 1 (existence of extreme value (Weierstrass))

Assume the following:

- *?*
- *?*

Then the optimization problem (P) has (at least) one solution.

Existence of a solution

Theorem 2 (existence of extreme value (Weierstrass))

Assume the following:

- K *is* **non-empty** *and* **compact** *(i.e. closed and bounded)*
- f *is* **continuous** *on* K*.*

Then the optimization problem (P) *has (at least) one solution.*

Remarks. If $K = \{x \in \mathbb{R}^n \mid h_i(x) = 0, \forall i \in \mathcal{E}, g_j(x) \leq 0, \forall j \in \mathcal{I}\}$, where h_i, g_j are continuous, then K is closed. In practical exercises, it is not necessary to justify the continuity of h_i or g_j.

Optimality conditions

Let us fix a continuously differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ for the whole section. Let us consider

$$\inf_{x \in \mathbb{R}^n} f(x) \tag{P}$$

The function f is said to be **stationary** at $x \in \mathbb{R}^n$ if $\nabla f(x) = 0$.

Theorem 3 (Necessary optimality condition)

Let $\bar{x} \in \mathbb{R}^n$ be a **local solution** *of (P). Then, f is* **stationary** *at $\bar{x}$.*

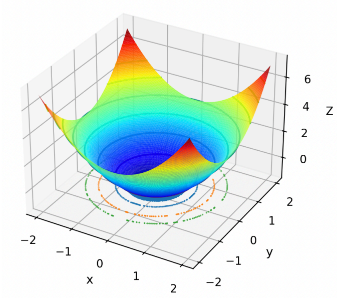
Remark. Stationarity is only a necessary condition!

And to sum up the courses ...

	Necessary conditions	Sufficient conditions
Abstract formulation (exist.)		if K compact, $f \in C^0(K)$ then at least one solution
		if K closed, $f \in C^0(K)$, coercive then at least one solution

	Necessary conditions	Sufficient conditions
No constraints $K = \mathbb{R}^d$ (opt.)	if $\overline{x}$ local sol., $f \in C^2(K)$ then, $D^2 f(\overline{x})$ is positive semi-def.	if $f \in C^2(K)$, $\nabla f(\overline{x}) = 0$, $D^2 f(\overline{x})$ positive def. then $\overline{x}$ local sol.
Affine constraints		
Non-linear constraints		then KKT=global sol.

Gradient methods



Our goal: solving **numerically** the problem

$$\inf_{x\in\mathbb{R}^n} f(x). \qquad (P)$$

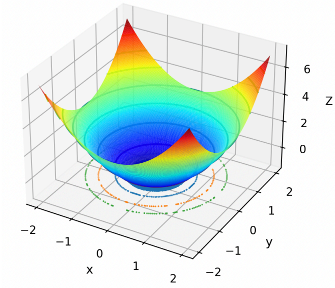
General idea: to compute a sequence $(x_k)_{k\in\mathbb{N}}$ such that

$$f(x_{k+1}) \leq f(x_k), \quad \forall k \in \mathbb{N},$$

the inequality being strict if $\nabla f(x_k) \neq 0$. $\rightarrow$ **Iterative** method.

How to compute x_{k+1}?

Gradient methods



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the inequality being strict if $\nabla f(x_k) \neq 0$. $\rightarrow$ **Iterative** method.
How to compute x_{k+1}?

Gradient methods

Main idea of gradient methods.

Let $x_k \in \mathbb{R}^n$. Let d_k be a descent direction at x_k. Let $\alpha > 0$. Then

$$f(x_k + \alpha d_k) = f(x_k) + \alpha \underbrace{\langle \nabla f(x_k), d_k \rangle}_{<0} + o(\alpha).$$

Therefore, if α is small enough,

$$f(x_k + \alpha d_k) < f(x_k).$$

We can set

$$x_{k+1} = x_k + \alpha d_k.$$

Gradient methods

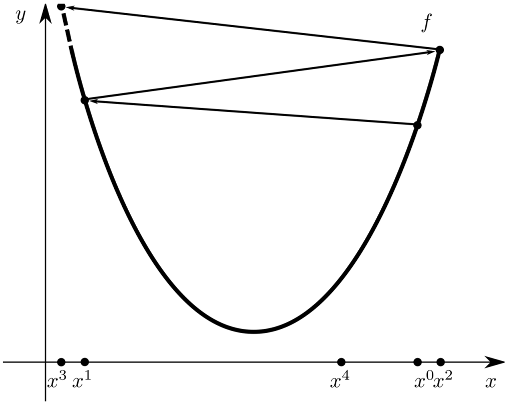
Gradient descent algorithm.

1. Input: $x_0 \in \mathbb{R}^n$, $\varepsilon > 0$.
2. Set $k = 0$.
3. While $\|\nabla f(x_k)\| \geq \varepsilon$, do
   (a) Find a descent direction d_k.
   (b) Find $\alpha_k > 0$ such that $f(x_k + \alpha_k d_k) < f(x_k)$.
   (c) Set $x_{k+1} = x_k + \alpha_k d_k$.
   (d) Set $k = k + 1$.
4. Output: x_k.

Remark. Step (b) is crucial; it is called **line search**.
The real α_k is called **stepsize**.
Exercice: Code the gradient descent algorithm

Gradient methods

On the choice of α_k.



Gradient methods

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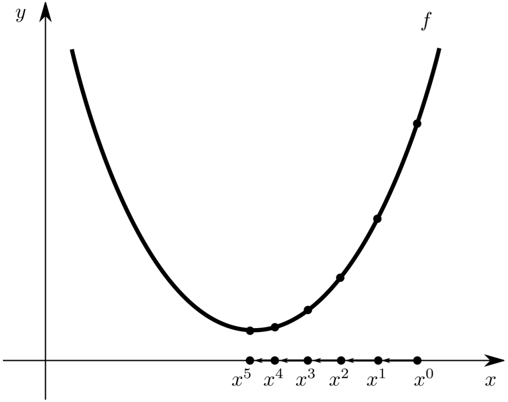


Gradient methods

On the choice of α_k.

Let us fix $x_k \in \mathbb{R}^n$. Let us define

$$\phi_k : \alpha \in \mathbb{R} \mapsto f(x_k + \alpha d_k).$$

The condition $f(x_k + \alpha_k d_k) < f(x_k)$ is equivalent to

$$\phi_k(\alpha_k) < \phi_k(0).$$

A natural idea: define α_k as a solution to

$$\inf_{\alpha \geq 0} \phi_k(\alpha).$$

Minimizing ϕ_k would take too much time! A **compromise** must be found between simplicity of computation and quality of α.

Gradient methods

Observation. Recall that $\phi_k(\alpha) = f(x_k + \alpha d_k)$. We have

$$\phi_k'(\alpha) = \langle \nabla f(x_k + \alpha d_k), d_k \rangle.$$

In particular, since d_k is a descent direction,

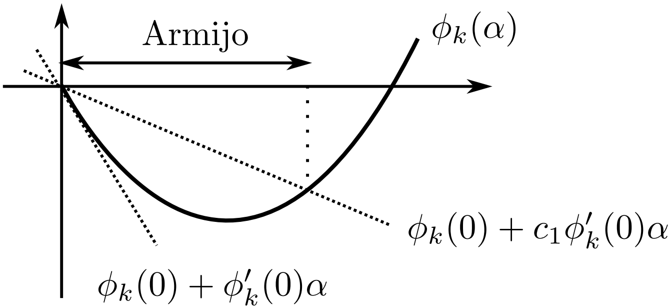
$$\phi_k'(0) = \langle \nabla f(x_k), d_k \rangle < 0.$$

Definition 4

Let us fix $0 < c_1 < 1$. We say that α satisfies **Armijo's rule** if

$$\phi_k(\alpha) \leq \phi_k(0) + c_1 \phi_k'(0)\alpha.$$

Gradient methods



Gradient methods

Backstepping algorithm for Armijo's rule

1. Input: $c_1 \in (0,1)$, $\beta > 0$, and $\gamma \in (0,1)$.
2. Set $\alpha = \beta$.
3. While α does not satisfy Armijo's rule,
   - Set $\alpha = \gamma\alpha$.
4. Output α.

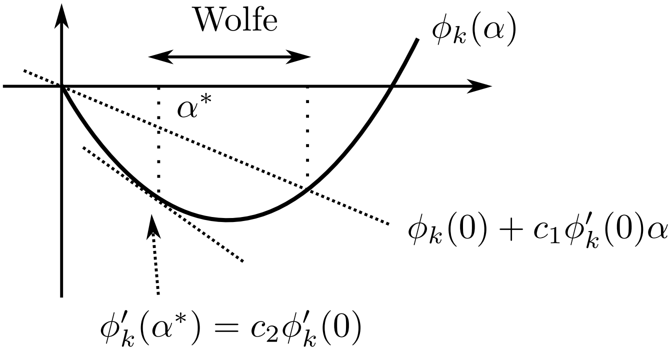
Gradient methods

Definition 5

Let $0 < c_1 < c_2 < 1$. We say that $\alpha > 0$ satisfies **Wolfe's rule** if

$$\phi_k(\alpha) < \phi_k(0) + c_1 \phi_k'(0)\alpha \quad \text{and} \quad \phi_k'(\alpha) \geq c_2 \phi'(0).$$

Gradient methods



Gradient methods

Bisection method for Wolfe's rule

1. Input: $c_1 \in (0,1)$, $c_2 \in (c_1, 1)$, $\beta > 0$, $\alpha_{min}, \alpha_{max}$.
2. Set $\alpha = \beta$.

While Wolfe's rule not satified:

1. if α does not satisfy Armijo's rule :
   - Set $\alpha_{max} = \alpha$
   - $\alpha = 0.5(\alpha_{min} + \alpha_{max})$
2. if α satisfies Armijo's rule and $\phi_k'(\alpha) < c2\phi_k'(0)$, do
   - Set $\alpha_{min} = \alpha$
   - $\alpha = 0.5(\alpha_{min} + \alpha_{max})$
3. Output: α.

Gradient methods

General comments on theoretical results from literature.

- In practice: $(x_k)_{k\in\mathbb{N}}$ "usually" **converges to a local solution**. Thus a good **initialization** (that is the choice of x_0) is crucial.
- In general, **slow** convergence.

1. Reminders
   - Optimization problem
   - Existence of a solution
   - Gradient methods
   - Newton's method

2. Optimality conditions for constrained problems
   - Linear constraints
   - Non-linear constraints
   - Sensitivity analysis

Newton's method

Main idea.

Originally, Newton's method aims at solving non-linear equations of the form

$$F(x) = 0,$$

where $F\colon \mathbb{R}^n \to \mathbb{R}^n$ is a given continuously differentiable function. It is an iterative method, generating a sequence $(x_k)_{k\in\mathbb{N}}$. Given x_k, we have

$$F(x) \approx F(x_k) + DF(x_k)(x - x_k).$$

Thus we look x_{k+1} as the solution to the linear equation

$$F(x_k) + DF(x_k)(x - x_k) = 0$$

that is, $x_{k+1} = x_k - DF(x_k)^{-1}F(x_k)$.

Newton's method

Remarks.

- If there exists $\bar{x}$ such that $F(\bar{x}) = 0$ and $DF(\bar{x})$ is regular, then for x_0 close enough to $\bar{x}$, the sequence $(x_k)_{k\in\mathbb{N}}$ is well-posed and converges "**quickly**" to $\bar{x}$.
- On the other hand, if x_0 is far away from $\bar{x}$, there is **no guaranty** of convergence.

Back to problem (P). Assume that f is continuously twice differentiable. Apply Newton's method with $F(x) = \nabla f(x)$ so as to solve $\nabla f(x) = 0$. Update formula:

$$x_{k+1} = x_k - D^2 f(x_k)^{-1} \nabla f(x_k).$$

The difficulties mentioned above are still relevant.

Newton's method

Optimization with Newton's method.

- Newton's formula can be written in the form:

$$x_{k+1} = x_k + \alpha_k d_k,$$

where

$$\alpha_k = 1 \quad \text{and} \quad d_k = -D^2 f(x_k)^{-1} \nabla f(x_k).$$

- If $D^2 f(x_k)$ is positive definite (and $\nabla f(x_k) \neq 0$), then $D^2 f(x_k)^{-1}$ is also positive definite, and therefore d_k is descent direction:

$$\langle \nabla f(x_k), d_k \rangle = -\langle \nabla f(x_k), D^2 f(x_k)^{-1} \nabla f(x_k) \rangle < 0.$$

Newton's method

Globalised Newton's method.

1. Input: $x_0 \in \mathbb{R}^n$, $\varepsilon > 0$, a linesearch rule (Armijo, Wolfe,...).
2. Set $k = 0$.
3. While $\|\nabla f(x_k)\| \geq \varepsilon$, do
   (a) If $-D^2 f(x_k)^{-1} \nabla f(x_k)$ is computable and is a descent direction, set $d_k = -D^2 f(x_k)^{-1} \nabla f(x_k)$, otherwise set $d_k = -\nabla f(x_k)$.
   (b) If $\alpha = 1$ satisfies the linesearch rule, then set $\alpha_k = 1$. Otherwise, find α_k with an appropriate method.
   (c) Set $x_{k+1} = x_k + \alpha_k d_k$.
   (d) Set $k = k + 1$.
4. Output: x_k.

Newton's method

Comments.

- The numerical computation of $D^2 f(x_k)$ may be **very time consuming** and may generate storage issues because of n^2 figures in general).
- **Quasi-Newton** methods construct a sequence of positive definite matrices H_k such that $H_k \approx D^2 f(x_k)^{-1}$. The matrix H_k can be stored efficiently (with $O(n)$ figures). Then $d_k = -H_k \nabla f(x_k)$ is a descent direction. Good speed of convergence is achieved. $\rightarrow$ **The ideal compromise!**

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2. Optimality conditions for constrained problems
   - Linear constraints
   - Non-linear constraints
   - Sensitivity analysis

Linear equality constraints

- We investigate in this section the problem

$$\inf_{x \in \mathbb{R}^n} f(x), \quad \text{s.t.} \begin{cases} h_i(x) = 0, & \forall i \in \mathcal{E} \\ g_j(x) \leq 0, & \forall j \in \mathcal{I}. \end{cases} \qquad (P)$$

- Let $x \in \mathbb{R}^n$ be feasible. Let $j \in \mathcal{I}$. We say that
  - the inequality constraint j is **active** if $g_j(x) = 0$
  - the inequality constraint j is **inactive** if $g_j(x) < 0$.

Linear constraints

- Let $f\colon \mathbb{R}^n \to \mathbb{R}$ and let $h\colon \mathbb{R}^n \to \mathbb{R}^{m_1}$ and $g\colon \mathbb{R}^n \to \mathbb{R}^{m_2}$ be two continuously differentiable functions.
- Let the **Lagrangian** $L\colon \mathbb{R}^n \times \mathbb{R}^{m_1} \times \mathbb{R}^{m_2} \to \mathbb{R}$ be defined by

$$\begin{aligned} L(x,\mu,\lambda) &= f(x) + \langle \mu, h(x)\rangle + \langle \lambda, g(x)\rangle \\ &= f(x) + \sum_{i=1}^{m_1} \mu_i h_i(x) + \sum_{j=1}^{m_2} \lambda_j g_j(x). \end{aligned}$$

The variables μ, λ are referred to as **dual variables**.

Linear equality constraints

Theorem 6

Assume that h and g are affine, that it to say, there exists $A \in \mathbb{R}^{m_2 \times n}$ *and* $b \in \mathbb{R}_2^m$ *such that*

$$g(x) = Ax + b.$$

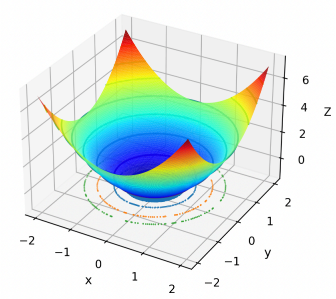
Let $\bar{x}$ *be a* **local solution** *to* (P).

Then there exists $(\mu, \lambda) \in \mathbb{R}^{m1} \times \mathbb{R}^{m_2}$ *such that the following three conditions, referred to as Karush-Kuhn-Tucker (KKT) conditions, are satisfied:*

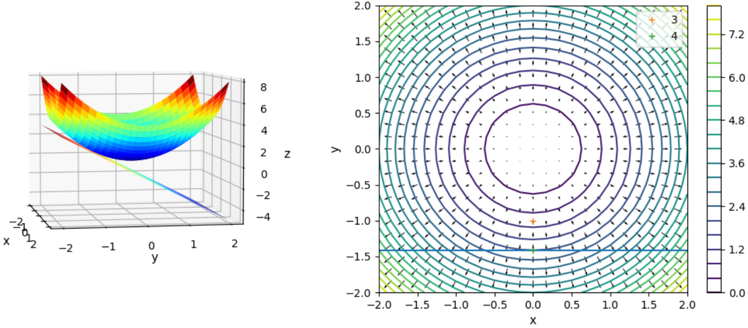
1. **Stationarity** *condition:* $\nabla_x L(\bar{x}, \mu, \lambda) = 0$.
2. **Sign** *condition: for all* $j \in \mathcal{I}$, $\lambda_j \geq 0$.
3. **Complementarity** *condition: for all* $j \in \mathcal{I}$, $g_j(\bar{x}) < 0 \Longrightarrow \lambda_j = 0$.

Linear constraints

Illustration.



KKT stationarity



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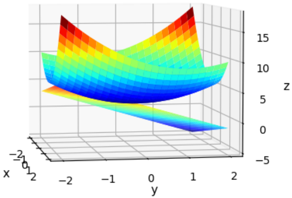
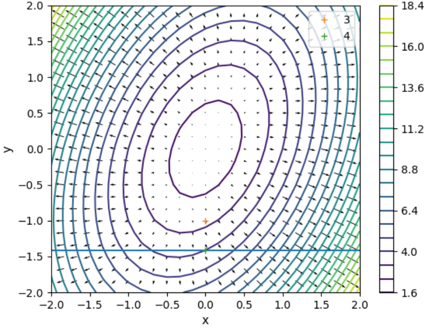
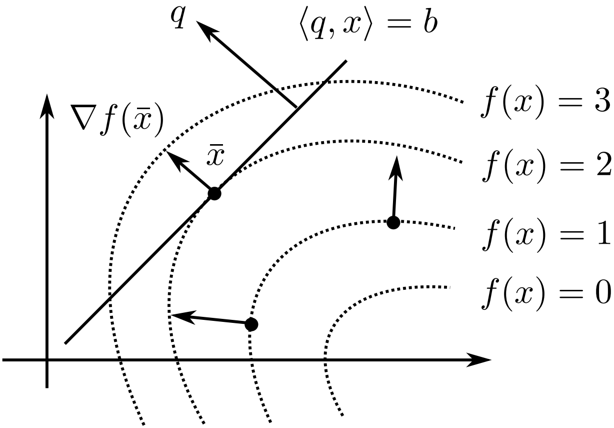


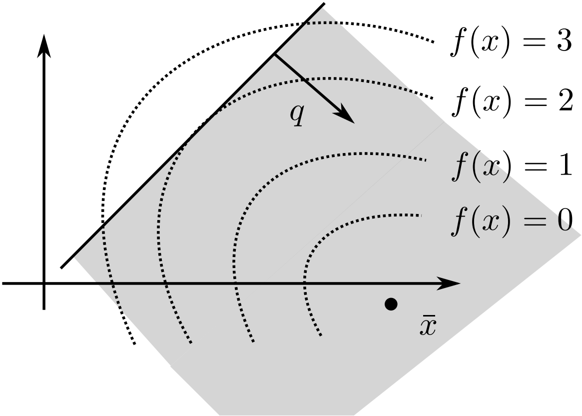


Linear constraints



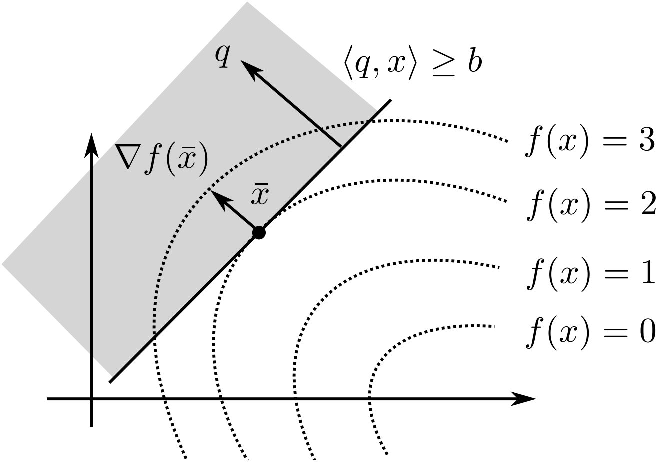
Linear constraints

Example 2(a). Case of **one (inactive) inequality equality constraint**:



Linear constraints

Example 2(b). Case of **one (active) inequality equality constraint**:



1. Reminders
   - Optimization problem
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Non-linear constraints

Definition 7

Let $\bar{x}$ be a feasible point. Let the set of **active inequality constraints** $\mathcal{I}_0(\bar{x})$ be defined by

$$\mathcal{I}_0(\bar{x}) = \{j \in \mathcal{I} \,|\, g_j(\bar{x}) = 0\}.$$

We say that the **Linear Independence Qualification Condition (LICQ)** holds at $\bar{x}$, if the following set of vectors is linearly indepedent:

$$\{\nabla h_i(\bar{x})\}_{i \in \mathcal{E}} \cup \{\nabla g_j(\bar{x})\}_{j \in \mathcal{I}_0(\bar{x})}$$

Non-linear constraints

Non-linear constraints

Theorem 8

Let $\bar{x}$ be a **local solution** *to (P). Assume that the LICQ holds at $\bar{x}$. Then there exists a unique (μ, λ) such that the* **KKT conditions** *are satisfied.*

Remarks.

- At a numerical level, a solution that does not satisfy the LICQ is hard to compute.

Non-linear constraints

Example 4.

Consider the problem

$$\inf_{x \in \mathbb{R}} x, \quad \text{subject to: } x^2 \leq 0.$$

Unique feasible point: $\bar{x} = 0$, thus the solution.

Lagrangian:

$$L(x, \lambda) = x + \lambda x^2.$$

At zero:

$$\nabla_x L(0, \lambda) = 1 + 2\lambda \bar{x} = 1 \neq 0.$$

The LICQ is not satisfied, since $\nabla g_1(0) = 0$.

Non-linear constraints

Theorem 9

Assume that

- *f is* **convex**
- *for all $i \in \mathcal{E}$, the map $x \mapsto h_i(x)$ is* **affine**
- *for all $j \in \mathcal{I}$, the map $x \mapsto g_j(x)$ is* **convex***.*

Then any feasible point $\bar{x}$ satisfying the **KKT conditions** *is a* **global solution** *to the problem.*

Remark. The result holds whether the LICQ holds or not at $\bar{x}$.

Exercise

Exercise. Consider the function $f\colon (x,y) \in \mathbb{R}^2 \mapsto \exp(x+y^2) + y + x^2$.

1. Prove that f is coercive. *Indication: Use* $\exp(z) \geq 1+z$
2. Compute $\nabla f(x,y)$ and $\nabla^2 f(x,y)$.
3. We recall that a symmetric matrix of size 2 of the form $\begin{pmatrix} a & b \\ b & c \end{pmatrix}$ is positive semidefinite if and only if $a+c \geq 0$ and $ac - b^2 \geq 0$. Using this fact, prove that f is convex.
4. We consider the following problem:
$$\inf_{(x,y)\in\mathbb{R}^2} f(x,y), \quad \text{subject to: } \begin{cases} -x-y \leq 0 \\ -x-2 \leq 0. \end{cases} \tag{$\mathcal{P}$}$$
Verify that $(0,0)$ is feasible and satisfies the KKT conditions.
5. Is the point $(0,0)$ a global solution to problem $(\mathcal{P})$?

Non-linear constraints

Exercise.

Consider:

$$\inf_{x\in\mathbb{R}^2} f(x) := -x_1 - x_2, \quad \text{s.t.} \begin{cases} g_1(x) = & x_1^2 + 2x_2^2 - 3 & \leq 0 \\ g_2(x) = & x_1 - 1 & \leq 0. \end{cases}$$

- Show that $\bar{x} = (1, 1)$ is feasible
- Verify that the LICQ and the KKT conditions hold at $\bar{x} = (1, 1)$.
- Prove that $\bar{x} = (1, 1)$ is a global solution.

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2 Optimality conditions for constrained problems
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- Sensitivity analysis

Sensitivity analysis

- Consider the family of optimization problems

$$\inf_{x \in \mathbb{R}^n} f(x), \quad \text{s.t.} \begin{cases} h_i(x) = y_i, & \forall i \in \mathcal{E}, \\ g_j(x) \leq y_j, & \forall j \in \mathcal{I}, \end{cases} \qquad (P(y))$$

  parametrized by the vector $y \in \mathbb{R}^m$.

- Let the **value function** V be defined by

$$V(y) = \mathrm{val}(P(y)).$$

- A variation δy_i in the i-th constraint generates a variation of the optimal cost of $\lambda_i \delta y_i$.

Sensitivity analysis

Exercise.

A company decides to rent an engine over d days. The engine can be used to produce two different objects. The two objects are not produced simultaneously. Let x_1 and x_2 denote the times dedicated to the production of each object. The resulting benefits (in k€) are given by:

$$\frac{x_1}{1+x_1} \quad \text{and} \quad \frac{x_2}{4+x_2}.$$

Sensitivity analysis

1. Formulate the problem as a minimization problem.
2. Justify the existence of a solution.
3. Write the KKT conditions. What is the unit of the dual variable?
4. Verify that $\bar{x} = (4, 6)$ satisfies the KKT conditions for $d = 10$ days. Is it a global solution to the problem?
5. The renting cost of the engine is 70€/day. Is it of interest for the company to rent the engine for a longer time?

Sensitivity analysis

1. Problem:

$$\inf_{x\in\mathbb{R}^2} -\frac{x_1}{1+x_1} - \frac{x_2}{4+x_2}, \quad \text{s.t.} \begin{cases} x_1 + x_2 = & d \\ -x_1 \leq & 0 \\ -x_2 \leq & 0 \end{cases}$$

2. The feasible set is obviously compact and non-empty and the cost function is continuous. Therefore, there exists a solution.

Sensitivity analysis

3. Let $\bar{x}$ be a solution. Let $\mu \in \mathbb{R}^2$ and $\lambda \in \mathbb{R}^2$ be the associated Lagrange multipliers. Lagrangian:

$$L(x, \mu, \lambda) = -\frac{x_1}{1+x_1} - \frac{x_2}{4+x_2} + \mu(x_1 + x_2 - d) - \lambda_1 x_1 - \lambda_2 x_2.$$

KKT conditions:

- Stationarity:

$$-\frac{1}{(1+\bar{x}_1)^2} + \mu - \lambda_1 = 0, \qquad -\frac{4}{(4+\bar{x}_2)^2} + \mu - \lambda_2 = 0.$$

- Sign condition: $\lambda_1 \geq 0$, $\lambda_2 \geq 0$.
- Complementarity: $\bar{x}_1 > 0 \Rightarrow \lambda_1 = 0$, $\bar{x}_2 > 0 \Rightarrow \lambda_2 = 0$.

- Units: $[\mu] = [\lambda_1] = [\lambda_2] =$k€/day.

Sensitivity analysis

4. Let μ, λ be such that the KKT conditions hold true. By complementarity condition, we necessarily have $\lambda_1 = \lambda_2 = 0$. The stationarity condition holds true with

$$\mu = \frac{1}{(1+\bar{x}_1)^2} = \frac{4}{(4+\bar{x}_2)^2} = \frac{1}{25} = 0.04.$$

The sign condition trivially holds true since the inequality constraints are inactive. Lagrangian:

$$L(x,\mu,\lambda) = -\frac{x_1}{1+x_1} - \frac{x_2}{4+x_2} + 0.04(x_1+x_2-d).$$

If $x_1 + x_2 > d$, the cost associated to constraints is increased, otherwise decreased (company rents the engine for the $d - x_1 - x_2$ remaining days).

The point $\bar{x}$ is feasible and satisfies the KKT conditions. We have affine constraints and a convex cost function, therefore, the KKT conditions are sufficient. The point $\bar{x}$ is a global solution.

Sensitivity analysis

5. d is fixed.

   Increasing the renting time of y days will generate a variation of cost of μy (approximately), that is, an augmentation of the benefit of 40€/day (less the renting price). It corresponds to the benefit that the company can have from another firm for renting the engine. Thus, the cost will corresponds to:

$$c(\bar{x}, \mu, \lambda) = -\frac{4}{1+4} - \frac{6}{4+6} - 0.04y + 0.07y = -1.4 + 0.03y.$$

   It would be of interest for the company to reduce the renting time.

And to sum up the courses ...

	Necessary conditions	Sufficient conditions
Abstract formulation (exist.)		if K compact, $f \in C^0(K)$ then at least one solution
		if K closed, $f \in C^0(K)$, coercive then at least one solution

	Necessary conditions	Sufficient conditions
No constraints $K = \mathbb{R}^d$ (opt.)	if $\overline{x}$ local sol., $f \in C^2(K)$ then, $D^2 f(\overline{x})$ is positive semi-def.	if $f \in C^2(K)$, $\nabla f(\overline{x}) = 0$, $D^2 f(\overline{x})$ positive def. then $\overline{x}$ local sol.
Affine constraints	$\overline{x}$ local sol. then KKT	f convex, then KKT=global sol.
Non-linear constraints	$\overline{x}$ local sol., LICQ then KKT	f convex, h affine, g convex, then KKT=global sol.

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