Continuous optimization
PGE305

Laurent Pfeiffer
Inria and CentraleSupélec, Université Paris-Saclay

Ensta-Paris
Institut Polytechnique de Paris
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Organisation

Organization:

- Class 1: lecture
- Class 2: lecture (1h 30) + programming exercises (2h)
- Class 3: lecture (1h 30) + programming exercises (2h)
- Class 4: programming exercises
- Class 5: programming exercise (1h 30) + exam (2h).

Contact me:

laurent.pfeiffer@inria.fr

Main objectives

Skills to be developped:

- **Modelling** of practical situations involving decision variables, constraints to be satisfied, a cost to minimize, as an *optimization problem*.
- **Numerical resolution** of such problems with the help of AMPL (A Mathematical Programming Language).
- Basic knowledge in optimization **theory and numerics**.

Pre-requisite:

- Programming: none
- Maths: little.

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1 General introduction
- What is an optimization problem?
- Classes of problems
- Existence of a solution
- Derivatives

2 Methods for unconstrained optimization
- Optimality conditions
- Gradient methods
- Newton's method

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

What is an optimization problem?

Definition 1

An **optimization problem** is a mathematical expression of the form:

$$\inf_{x\in\mathcal{D}} f(x), \quad \text{subject to: } x \in K, \tag{P}$$

where:

- $\mathcal{D}$ is a set, called **domain** of f
- $f : \mathcal{D} \to \mathbb{R}$ is called **cost function** (or **objective** function)
- $K \subseteq \mathcal{D}$ is called **feasible set**.

In this class: $\mathcal{D} = \mathbb{R}^n$. **Unconstrained** optimization: $\mathcal{D} = K = \mathbb{R}^n$.

Straightforward adaptation of all results of the class to **maximization** problems, replacing f by $-f$.

Abbreviation: "subject to" $\rightsquigarrow$ "s.t.".

What is an optimization problem?

Definition 2

- A point x is called **feasible** if $x \in K$.
- A feasible point $\bar{x}$ is called **(global) solution** (to problem P) if

$$f(x) \geq f(\bar{x}), \quad \text{for all } x \in K.$$

- If $\bar{x}$ is a global solution, then the real number $f(\bar{x})$ is called **value** of the problem, it is denoted $\mathrm{val}(P)$.

Example. The point $x = \pi$ is the solution of the problem

$$\inf_{x \in \mathbb{R}} \cos(x), \quad x \in [0, 2\pi].$$

What is an optimization problem?

Remarks.

- An optimization problem may **not** have a solution. *Examples*:

$$\inf_{x \in \mathbb{R}} e^x, \tag{P_1}$$

$$\inf_{x \in \mathbb{R}} x^3. \tag{P_2}$$

- The concept of **value** of an optimization can also be defined whether the problem has a solution or not, as an element of $\mathbb{R} \cup \{-\infty, \infty\}$. In particular:

$$\mathrm{val}(P_1) = 0, \quad \mathrm{val}(P_2) = -\infty.$$

What is an optimization problem?

Definition 3

Let $\bar{x} \in K$. We call $\bar{x}$ a **local solution** to (P) if there exists $\varepsilon > 0$ such that the following holds true: for all $x \in K$,

$$\|x - \bar{x}\| \leq \varepsilon \Longrightarrow f(x) \geq f(\bar{x}).$$

Example: $\inf_{x \in \mathbb{R}} -x^2$, s.t. $x \in [-1, 2]$. Local solutions: -1 and 2.

Remarks.

- A global solution is also a local solution.
- The notion of local optimality does not depend on the norm, if K is a subset of a finite dimensional vector space.

What is an optimization problem?

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

Equivalent 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

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

where $g : \mathbb{R}^n \to \mathbb{R}^m$ and $(\mathcal{I}, \mathcal{E})$ is a partition of $\{1, \ldots, m\}$.

We call the expressions

- $g_i(x) \geq 0$: **inequality constraint**
- $g_i(x) = 0$: **equality constraint**.

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Classes of optimization problems

From the point of view of **applications**, one can distinguish four classes of optimization problems.

1. Economical problems
2. Physical problems
3. Inverse problems
4. Learning problems.

1. Economical problems.

Any practical situation involving

- a **cost** to be minimized, some revenue or performance index to be maximized
- **operational decisions** (production level in thermal power plants, amount of water flowing out from a hydropower plant, begin and end of the maintenance of nuclear power plant, etc.)
- constraints **bounding** the decisions (which are often non-negative!)
- **physical constraints** ("total production=demand", "variation of stock= input - output",...).

Classes of optimization problems

2. Physical problems.

Some equilibrium problems in **physics** can be formulated as optimization problems, involving an energy to be minimized.

- Mechanical structures
- Electricity networks
- Gas networks

Some similar problems arise in **economics** and game theory:

- Cournot models with competing firms
- Traffic models on road networks.

Classes of optimization problems

3. Inverse problems

Context. A variable x must be identified, with the help of another variable y, related to x via a relation $y = F(x)$.

Examples:

- the epicenter x of an earthquake, given seismic measurements y.
- localization x of a crack in a mechanical structure, given displacements measurements y provided by captors
- temperature in the core of nuclear plant, given external temperature measurements

Classes of optimization problems

The equation $y = F(x)$ (with unknown x)...

- may not have a solution (because of inaccurate measurements)
- may have several solutions (too few measurements).

Optimization is the solution! Consider

$$\inf_{x \in \mathcal{D}} \|y - F(x)\|^2, \quad \text{subject to: } x \in K,$$

where the constraints may model a priori knowledge on x.

Classes of optimization problems

4. Learning problems

Context. A heuristical relation must be found between two (or more) variables $x \in X$ and $y \in Y$, with the help of measurements $(x_k, y_k)_{k=1,\dots,K}$.

Examples.

- the size of a population in function of time
- the efficiency of solar pannel in function of its age, temperature, enlightment, etc
- the identity of a person on a picture.

Classes of optimization problems

Approach by least-square.

- Fix an explicit function $F\colon X \times R \to Y$, for some parameter set R.
- "Tune the parameter r", that is, solve the least-squares problem
$$\inf_{r \in R} \sum_{k=1}^{K} \|y_k - F(x_k, r)\|^2.$$
- Heuristical relation $y \approx F(x, \bar{r})$ for the optimal $\bar{r}$.

Example: linear regression. For $X = \mathbb{R}$ and $Y = \mathbb{R}$, take $R = \mathbb{R}^2$ and
$$F(x, r) = r_1 + r_2 x.$$

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Existence of a solution

Definition 4

We say that f is **coercive** on the set K if the following holds: for any sequence $(x_k)_{k\in\mathbb{N}}$ in K,

$$\|x_k\| \to \infty \Longrightarrow f(x_k) \to +\infty.$$

Remark. The definition is independent of the norm.

Existence of a solution

Exercise. Consider

$$f : (x, y) \in \mathbb{R}^2 \mapsto x^4 - 2xy + 2y^2.$$

Prove that f is coercive on $\mathbb{R}^2$.

Existence of a solution

Solution. We have $x^4 \geq 2x^2 - 1$, since

$$0 \leq (x^2 - 1)^2 = x^4 - 2x^2 + 1.$$

Therefore

$$\begin{aligned} f(x, y) &\geq 2x^2 - 1 - 2xy + 2y^2 \\ &= (x^2 + y^2) - 1 + (x - y)^2 \\ &\geq \|(x, y)\|^2 - 1 \underset{\|(x,y)\|\to\infty}{\longrightarrow} \infty, \end{aligned}$$

where $\| \cdot \|$ denotes the Euclidean norm. Thus f is coercive.

Existence of a solution

Lemma 5

Assume the following:

- K *is* non-empty *and* closed
- f *is* continuous *on* K
- f *is* coercive *on* K.

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

Remarks.

- If $K = \{x \in \mathbb{R}^n \,|\, g_i(x) \geq 0,\ \forall i \in \mathcal{I}, g_i(x) = 0,\ \forall i \in \mathcal{E}\}$, where g is continuous, then K is closed.
- If K is bounded, then f is coercive because there is no sequence $(x_k)_{k \in \mathbb{N}}$ in K such that $\|x_k\| \to \infty$.

Existence of a solution

Elements of proof. Fix $x_0 \in K$ and define:

$$K' = \{x \in K \mid f(x) \leq f(x_0)\}.$$

- K' is **closed**, since f is continuous and K is closed
- K' is **bounded**, since f is coercive (proof by contradiction)
- The problem $\inf f(x)$, s.t. $x \in K'$ is known to have a **global solution** $\bar{x}$ since f is continuous and K' compact.
- Show that $\bar{x}$ is a global solution to the original problem.

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Derivatives

Definition 6

A function $F : \mathbb{R}^n \to \mathbb{R}^m$ is called **differentiable** at $\bar{x}$ if for all $i = 1, \dots m$, for all $j = 1, \dots, n$, the function

$$x \in \mathbb{R} \mapsto F_i(\bar{x}_1, \dots, \bar{x}_{j-1}, x, \bar{x}_{j+1}, \dots) \in \mathbb{R}$$

is differentiable. Its derivative at $\bar{x}_j$ is called **partial derivative** of F, it is denoted $\frac{\partial F_i}{\partial x_j}(\bar{x})$.

The matrix

$$DF(\bar{x}) = \left(\frac{\partial F_i}{\partial x_j}(\bar{x}) \right)_{\substack{i=1,\dots,m \\ j=1,\dots,n}} \in \mathbb{R}^{m \times n}$$

is called **Jacobian** matrix.

Derivatives

- The function F is said to be continuously differentiable if the Jacobian $DF \colon x \in \mathbb{R}^n \to \mathbb{R}^{m \times n}$ is continuous.
- If F is continuously differentiable, then we have the **first order Taylor expansion**

$$F(x + \delta x) = F(x) + DF(x)\delta x + o(\|\delta x\|).$$

- **Chain rule**. Let $F \colon \mathbb{R}^n \to \mathbb{R}^m$ and let $G \colon \mathbb{R}^p \to \mathbb{R}^n$ be continuously differentiable functions. Let $H = F \circ G$ (that is, $H(x) = F(G(x))$). Then

$$DH(x) = DF(G(x))DG(x), \quad \text{for all } x \in \mathbb{R}^p.$$

Derivatives

Definition 7

Let $f : \mathbb{R}^n \to \mathbb{R}$ be differentiable at $x \in \mathbb{R}^n$. We call **gradient** of f (at x) the column vector:

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(x) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x) \end{pmatrix} = Df(x)^\top .$$

Derivatives

Definition 8

The function $F: \mathbb{R}^n \to \mathbb{R}^m$ is said to be **twice differentiable** if it is differentiable and DF is differentiable.

We denote: $\frac{\partial^2 F_i}{\partial x_j \partial x_k}(x) = \frac{\partial}{\partial x_j}\left(\frac{\partial F}{\partial x_k}\right)(x)$.

If $m = 1$, the matrix

$$D^2 F(x) = \left(\frac{\partial^2 F}{\partial x_j \partial x_k}(x)\right)_{\substack{j=1,\ldots,n \\ k=1,\ldots,n}}$$

is called **Hessian** matrix. It is symmetric.

Derivatives

Exercise.
Calculate the gradient and the Hessian of the function

$$f : x \in \mathbb{R}^n \mapsto \frac{1}{2}\langle x, Ax\rangle + \langle b, x\rangle,$$

where $A \in \mathbb{R}^{n\times n}$ and $b \in \mathbb{R}^n$.

Derivatives

Solution. We have

$$f(x) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}x_i x_j + \sum_{i=1}^{n} b_i x_i.$$

Therefore,

$$\begin{aligned}\frac{\partial f}{\partial x_k}(x) &= \frac{1}{2}\sum_{j=1}^{n} A_{kj}x_j + \frac{1}{2}\sum_{i=1}^{n} A_{ik}x_i + b_k\\ &= \frac{1}{2}(Ax)_k + \frac{1}{2}(A^\top x)_k + b_k.\end{aligned}$$

Therefore,

$$\nabla f(x) = \frac{1}{2}(A + \bar{A}^\top)x + b.$$

Hessian: $D^2 f(x) = \frac{1}{2}(A + A^\top)$.

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Optimality conditions

Let us fix a continuously differentiable function $f\colon \mathbb{R}^n \to \mathbb{R}$ 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 9 (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!

Optimality conditions

Theorem 10

Assume that f is twice continuously differentiable. Let $\bar{x}$ be a stationary *point.*

- Necessary *condition.*
  If $\bar{x}$ is a local solution *of (P), then $D^2 f(\bar{x})$ is* positive semi-definite, *that is to say,*

$$\langle h, D^2 f(\bar{x}) h \rangle \geq 0, \quad \textit{for all } h \in \mathbb{R}^n.$$

- Sufficient *condition.*
  If $D^2 f(\bar{x})$ is positive definite, *that is to say if*

$$\langle h, D^2 f(\bar{x}) h \rangle > 0, \quad \textit{for all } h \in \mathbb{R}^n \backslash \{0\} \ ,$$

then $\bar{x}$ is a local solution *of (P).*

Optimality conditions

Definition 11

The function f is said to be convex if

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda) f(y),$$

for all x and $y \in \mathbb{R}^n$ and for all $\lambda \in [0,1]$.

Theorem 12

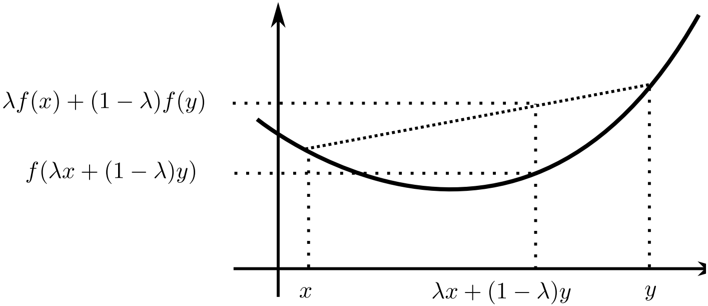
- *The function f is convex if and only if*

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle,$$

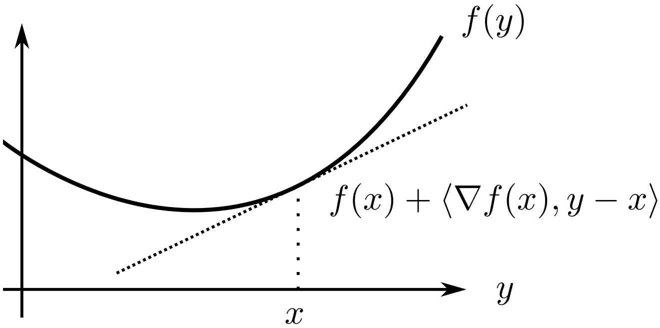
for all x and $y \in \mathbb{R}^n$.

- *If f is twice differentiable, then f is convex if and only if $D^2 f(x)$ is symmetric* positive semi-definite *for all $x \in \mathbb{R}^n$.*

Optimality conditions



Optimality conditions



Optimality conditions

Theorem 13

Assume that f is convex. *Let $\bar{x}$ be a* stationary *point of f. Then it is a* global solution *of (P).*

Proof. For all $x \in \mathbb{R}^n$, we have

$$f(x) \geq f(\bar{x}) + \langle \nabla f(\bar{x}), x - \bar{x} \rangle = f(\bar{x}).$$

Optimality conditions

Exercise.
Let $A \in \mathbb{R}^{n\times n}$ be symmetric positive definite and let $b \in \mathbb{R}^n$. Let

$$f : x \in \mathbb{R}^n \mapsto \frac{1}{2}\langle x, Ax\rangle + \langle b, x\rangle.$$

Prove that

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

has a unique solution. *Hint:* A is regular.

Optimality conditions

Solution.

- We have

$$\nabla f(x) = Ax + b.$$

  Since A is regular, there exists a unique solution $\bar{x}$ to the equation $Ax + b = 0$ (that is, $\bar{x} = -A^{-1}b$).

- We also have $D^2 f(x) = A$. Therefore, f is convex and $\bar{x}$ is a global solution.

- Any solution is stationary. Since $\bar{x}$ is the unique stationary point, it is also the unique solution.

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Gradient methods

Our goal: solving **numerically** the problem

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

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 $\nabla f(x_k) \neq 0$. $\to$ **Iterative** method.

How to compute x_{k+1}?

Gradient methods

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

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How to compute x_{k+1}?

Gradient methods

Definition 14

Let $x \in \mathbb{R}^n$ and let $d \in \mathbb{R}^n$. The vector d is called **descent direction** if

$$\langle \nabla f(x), d \rangle < 0.$$

Remark. If $\nabla f(x) \neq 0$, then $d = -\nabla f(x)$ is a descent direction. Indeed,

$$\langle \nabla f(x), d \rangle = -\langle \nabla f(x), \nabla f(x) \rangle = -\|\nabla f(x)\|^2 < 0.$$

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**.

Gradient methods

On the choice of α_k.

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

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

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,

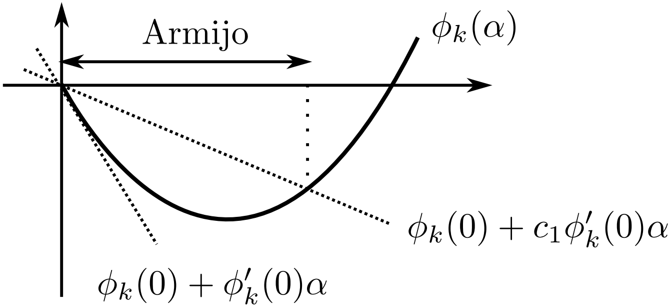
$$\phi_k'(0) = \langle \nabla f(x_k), d_k \rangle < 0.$$

Definition 15

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.

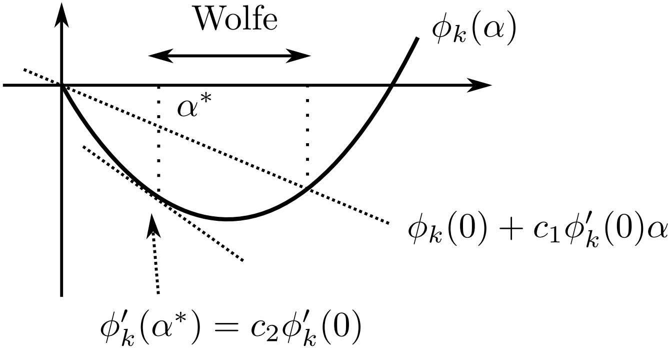
Gradient methods

Definition 16

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: $c_1 \in (0,1)$, $c_2 \in (c_1, 1)$, $\beta > 0$, $\eta > 1$.
2. Set $\alpha = \beta$.
3. While α satisfies Armijo's rule, do
   - Set $\alpha = \eta\alpha$.
4. Set $\alpha_{\min} = 0$, $\alpha_{\max}$, $\alpha = \frac{1}{2}(\alpha_{\min} + \alpha_{\max})$.
5. While α does not satisfy Wolfe's rule, do
   - If α does not satisfy Armijo's rule, then set $\alpha_{\max} = \alpha$. Else set $\alpha_{\min} = \alpha$.
   - Set $\alpha = \frac{1}{2}(\alpha_{\min} + \alpha_{\max})$.
6. Output: α.

Gradient methods

General comments on theoretical results from literature.

- The algorithms for the computation of stepsizes satisfying Armijo and Wolfe's rules converge in **finitely many iterations** (under non-restrictive assumptions).
- Without convexity assumption on f, very little can be said about the convergence of the sequence $(x_k)_{k\in\mathbb{N}}$. Typical results ensure that any accumulation point is stationary.
- 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.

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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 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

Globalization of 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.

- Under non-restrictive assumptions, the globalized method converges, whatever the initial condition. Convergence is fast.
- The numerical computation of $D^2f(x_k)$ may be **very time consuming** and may generate storage issues n^2 figures in general).
- **Quasi-Newton** methods construct a sequence of positive definite matrices H_k such that $H_k \approx D^2f(x_k)^{-1}$. 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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Linear constraints

- Let $f\colon \mathbb{R}^n \to \mathbb{R}$ ang let $g\colon \mathbb{R}^n \to \mathbb{R}^m$ be two continuously differentiable functions.
- Let $(\mathcal{E},\mathcal{I})$ be a partition of $\{1,\dots,m\}$ (that is, $\mathcal{E}\cap\mathcal{I}=\emptyset$, $\mathcal{E}\cup\mathcal{I}=\{1,\dots,m\}$).
- Let the **Lagrangian** $L\colon \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ be defined by

$$L(x,\lambda) = f(x) - \langle \lambda, g(x)\rangle = f(x) - \sum_{i=1}^{n} \lambda_i g_i(x).$$

The variable λ is referred to as **dual variable**.

Linear equality constraints

- We investigate in this section the problem

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

- Let $x \in \mathbb{R}^n$ be feasible. Let $i \in \mathcal{I}$. We say that
  - the inequality constraint i is **active** if $g_i(x) = 0$
  - the inequality constraint i is **inactive** if $g_i(x) > 0$.
- *Remark*. All results of the section are true if $\mathcal{E} = \emptyset$ or $\mathcal{I} = \emptyset$.

Linear equality constraints

Theorem 17

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

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

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

Then there exists $\lambda \in \mathbb{R}^m$ such that the following three conditions, refered to as Karush-Kuhn-Tucker (KKT) conditions, are satisfied:

1. Stationarity *condition:* $\nabla_x L(\bar{x}, \lambda) = 0$.
2. Sign *condition: for all $i \in \mathcal{I}$,* $\lambda_i \geq 0$.
3. Complementarity *condition: for all $i \in \mathcal{I}$,* $g_i(\bar{x}) > 0 \Longrightarrow \lambda_i = 0$.

Linear equality constraints

Remarks.

- A dual variable λ satisfying the KKT conditions is called **Lagrange multiplier** (associated with $\bar{x}$).
- Further assumptions are required to have uniqueness of λ.
- If $\mathcal{I} = \emptyset$, then the sign condition and the complementarity conditions are trivially satisfied.
- The theorem allows to have $m \geq n$.

Linear constraints

Exercise.

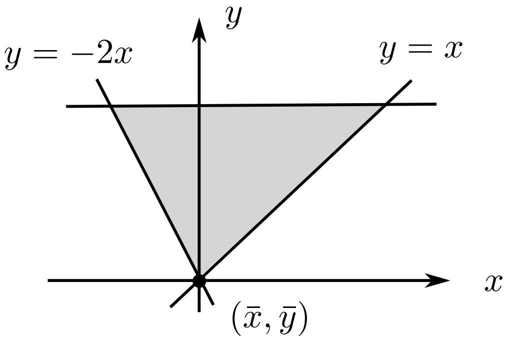
Consider the problem

$$\inf_{(x,y)\in\mathbb{R}^2} f(x,y) := y, \quad \text{s.t.} \begin{cases} g_1(x,y) := & 2x + y & \geq 0, \\ g_2(x,y) := & -x + y & \geq 0, \\ g_3(x,y) := & -y + 3 & \geq 0. \end{cases}$$

- Draw the feasible set and find (geometrically) the solution.
- Verify that the KKT conditions are satisfied.

Linear constraints

Solution.



Linear constraints

- Solution to the problem: $(\bar{x}, \bar{y}) = 0$.
- Let $\lambda \in \mathbb{R}^3$ be the associated Lagrange multiplier. Necessarily $\lambda_3 = 0$, since $g_3(\bar{x}, \bar{y}) > 0$, by complementarity.
- Lagrangian:

$$L(x, y, \lambda) = y - \lambda_1(2x + y) - \lambda_2(-x + y).$$

- The stationarity condition yields:

$$\begin{aligned} 0 &= \frac{\partial L}{\partial x}(0,0) = -2\lambda_1 + \lambda_2 \\ 0 &= \frac{\partial L}{\partial y}(0,0) = 1 - \lambda_1 - \lambda_2. \end{aligned}$$

Linear constraints

- This linear system has a unique solution

$$\lambda_1 = 1/3 \geq 0 \quad \lambda_2 = 2/3 \geq 0.$$

The sign condition is satisfied.

Linear constraints

Example 1. Case of **one equality constraint**:

$$m = 1, \quad \mathcal{E} = \{1\}, \quad \mathcal{I} = \emptyset.$$

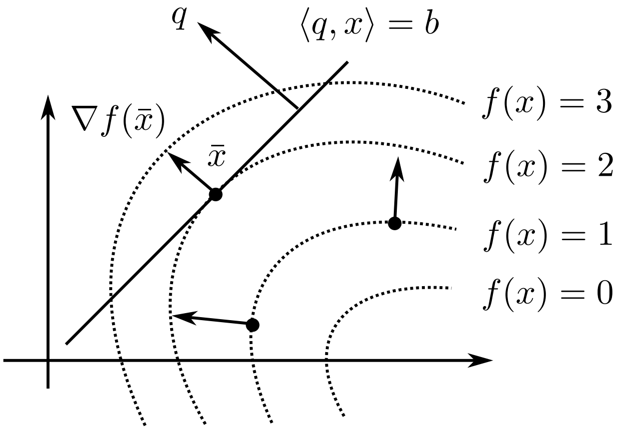
The matrix A is a row vector, let $q = A^\top$.

Proof of KKT conditions.

- Geometrically, we understand that $\nabla f(x)$ and q are **colinear**.
- Let $\lambda \in \mathbb{R}$ be such that $\nabla f(x) = \lambda q$.
- We have:

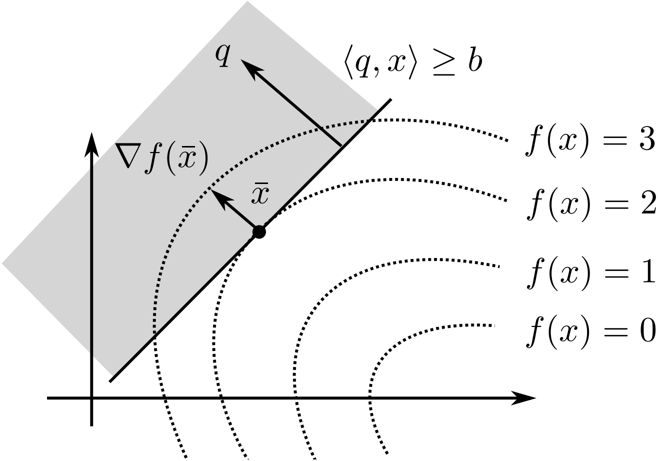
$$\nabla L(x, \lambda) = \nabla f(x) - \lambda \nabla g(x) = \nabla f(x) - \lambda q = 0.$$

Linear constraints



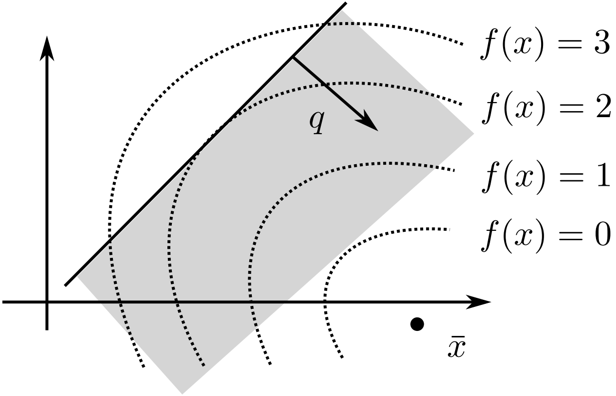
Linear constraints

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



Linear constraints

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



Linear constraints

Example 3. Case of m equality constraints ($\mathcal{I} = \emptyset$).

Proof.

- Let $\varepsilon > 0$ be given by the definition of a local solution.
  Let $h \in \mathrm{Ker}(A)$ (that is $Ah = 0$).
  For all $\theta \in \mathbb{R}$, let $x_\theta = \bar{x} + \theta h$.
- For all $\theta \in \mathbb{R}$, x_θ is **feasible:**

$$g(x_\theta) = Ax_\theta + b = A\bar{x} + b + \theta Ah = 0.$$

- For all $\theta \in [0, \varepsilon/\|h\|]$, we have $\|x_\theta - \bar{x}\| \leq \varepsilon$ and thus

$$f(x_\theta) \geq f(\bar{x}).$$

Linear constraints

- We deduce that

$$0 \leq \lim_{\theta \downarrow 0} \frac{f(\bar{x} + \theta h) - f(\bar{x})}{\theta} = \langle \nabla f(\bar{x}), h \rangle.$$

- Since $h \in \mathrm{Ker}(A)$, we also have $-h \in \mathrm{Ker}(A)$. Therefore,

$$0 \leq \langle \nabla f(\bar{x}), -h \rangle$$

  and therefore $\langle \nabla f(\bar{x}), h \rangle = 0$.

- We deduce that

$$\nabla f(x) \in (\mathrm{Ker}(A))^{\perp} = \mathrm{Im}(A^{\top}),$$

  that is, there exists $\lambda \in \mathbb{R}^m$ such that $\nabla f(x) = A^{\top} \lambda$.

- We have $\nabla_x L(x, \lambda) = \nabla f(x) - A^{\top} \lambda = 0$.

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Non-linear constraints

Definition 18

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

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

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

$$\{\nabla g_i(\bar{x})\}_{i \in \mathcal{E} \cup \mathcal{I}_0(\bar{x})}.$$

Non-linear constraints

Theorem 19

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

Remarks.

- Many available **variants** of this theorem in the literature, with different qualification conditions.
- At a numerical level, a solution that does not satisfy the LICQ is hard to compute.

Non-linear constraints

Example 4.

Consider the problem

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

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 20

Assume that

- f *is* convex
- *for all* $i \in \mathcal{E}$, *the map* $x \mapsto g_i(x)$ *is* affine
- *for all* $i \in \mathcal{I}$, *the map* $x \mapsto -g_i(x)$ *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 $f : (x, y) \in \mathbb{R}^2 \mapsto \exp(x + y^2) + y + x^2$.

1. Prove that f is coercive.
2. Calculate $\nabla f(x, y)$ 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:

$$\inf_{(x,y)\in\mathbb{R}^2} f(x, y), \quad \text{subject to: } \begin{cases} x + y \geq 0 \\ x + 2 \geq 0. \end{cases} \tag{$\mathcal{P}$}$$

   Verify that $(0, 0)$ is feasible and satisfies the KKT conditions.
5. Is the point $(0, 0)$ a global solution to problem $(\mathcal{P})$?

Exercise

Solution.

1. We use the inequality: $\exp(z) \geq 1 + z$, which yields:

$$
\begin{aligned}
f(x,y) &\geq x + y^2 + y + x^2 \\
&= \frac{1}{2}(x^2 + y^2) + \frac{1}{2}(x^2 + 2x + 1) + \frac{1}{2}(y^2 + 2y + 1) - 1 \\
&= \frac{1}{2}\|(x,y)\|^2 + (x+1)^2 + (y+1)^2 - 1 \underset{\|(x,y)\| \to \infty}{\longrightarrow} \infty.
\end{aligned}
$$

Exercise

2. It holds:

$$\frac{\partial f}{\partial x} = \exp(x + y^2) + 2x, \qquad \frac{\partial f}{\partial y} = 2y\exp(x + y^2) + 1.$$

Therefore, $\nabla f(x, y) = \begin{pmatrix} \exp(x + y^2) + 2x \\ 2y\exp(x + y^2) + 1 \end{pmatrix}$.

We also have

$$\frac{\partial^2 f}{\partial x^2} = \exp(x + y^2) + 2, \qquad \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} 2y\exp(x + y^2),$$

$$\frac{\partial^2 f}{\partial y^2} = 2\exp(x + y^2) + 4y^2\exp(x + y^2).$$

Thus, $D^2 f(x, y) = \begin{pmatrix} \exp(x + y^2) + 2 & 2y\exp(x + y^2) \\ 2y\exp(x + y^2) & (2 + 4y^2)\exp(x + y^2) \end{pmatrix}$.

Exercise

3. Proof of positive definiteness of $D^2 f$. It holds:

$$a + c = (3 + 4y^2)\exp(x + y^2) + 2 \geq 0$$

and

$$ac - b^2 = 2\exp(2x + 2y^2) + 4(1 + 2y^2)\exp(x + y^2) \geq 0.$$

It follows that $D^2 f(x, y)$ is positive semidefinite, for all (x, y). Therefore f is a convex function.

Exercise

4. Feasibility of $(0,0)$: we have $0+0 \geq 0$ and $0+2>0$.
KKT conditions. Lagrangian:

$$L(x,y,\lambda_1,\lambda_2) = \exp(x+y^2)+y+x^2-\lambda_1(x+y)-\lambda_2(x+2).$$

Therefore,

$$\frac{\partial L}{\partial x}(0,0,\lambda_1,\lambda_2) = 1-\lambda_1-\lambda_2, \qquad \frac{\partial L}{\partial y}(0,0) = 1-\lambda_1.$$

Taking $\lambda_1 = 1$ and $\lambda_2 = 0$, we have:

1. Stationarity: $\frac{\partial L}{\partial x}(0,0,1,0) = \frac{\partial L}{\partial y}(0,0,1,0) = 0$.
2. Sign condition: $\lambda_1 \geq 0$, $\lambda_2 \geq 0$.
3. Complementarity: the second constraint is inactive and the corresponding Lagrange multiplier is null.

Exercise

5. We have the following:
   - The cost function is convex.
   - The functions $-(x+y)$ and $-(x+2)$ are convex.
   - The point $(0,0)$ is feasible and satisfies the KKT conditions.

   Therefore $(0,0)$ is a global solution.

Non-linear constraints

Exercise.

Consider:

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

- Draw the feasible set and prove the existence of a solution.
- Verify that the LICQ at the KKT conditions hold at $\bar{x} = (1, 1)$.

Non-linear constraints

Verification of the LICQ.

$$\nabla g_1(\bar{x}) = \begin{pmatrix} -2\bar{x}_1 \\ -4\bar{x}_2 \end{pmatrix} = \begin{pmatrix} -2 \\ -4 \end{pmatrix} \quad \text{and} \quad \nabla g_2(\bar{x}) = \begin{pmatrix} -1 \\ 0 \end{pmatrix}.$$

We have: $\mathcal{E} = \emptyset$, $\mathcal{I}_0(\bar{x}) = \{1, 2\}$. The vectors $\nabla g_1(\bar{x})$ and $\nabla g_2(\bar{x})$ are linearly independant, since

$$\det \begin{pmatrix} -2 & -4 \\ -1 & 0 \end{pmatrix} = -4 \neq 0.$$

Thus the LICQ is satisfied at $\bar{x}$.

Non-linear constraints

KKT conditions.

- Lagrangian:
  $L(x, \lambda) = (-x_1 - x_2) - \lambda_1(-x_1^2 - 2x_2^2 + 3) - \lambda_2(-x_1 + 1).$
- Stationarity condition:

$$\begin{pmatrix} -1 \\ -1 \end{pmatrix} + \begin{pmatrix} 2\bar{x}_1 \\ 4\bar{x}_2 \end{pmatrix} \lambda_1 + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \lambda_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

  It is satisfied at $\bar{x}$ with $\lambda_1 = 1/4 \geq 0$ and $\lambda_2 = 1/2 \geq 0$.
- The sign condition is satisfied.
- The complementarity condition is satisfied (all inequality constraints are active).

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Sensitivity analysis

- Consider the family of optimization problems

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

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

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

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

Sensitivity analysis

Theorem 21

Assume that for some $\bar{y}$, the problem $(P(\bar{y}))$ has a solution $\bar{x}$ satisfying the KKT conditions. Let λ denote the corresponding Lagrange multiplier.
Then, under some technical assumptions, V is differentiable *at $\bar{y}$ and*

$$\nabla V(\bar{y}) = \lambda.$$

Interpretation. A variation δy_i in the i-th constraint generates a variation of the optimal cost of $\lambda_i \delta y_i$ (in **first approximation**).

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:

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

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 $\lambda \in \mathbb{R}^3$ be the associated Lagrange multiplier. Lagrangian:

$$L(x, \lambda) = -\frac{x_1}{1 + x_1} - \frac{x_2}{4 + x_2} - \lambda_1(x_1 + x_2 - d) - \lambda_2 x_1 - \lambda_3 x_2.$$

KKT conditions:

- Stationarity:

$$-\frac{1}{(1 + \bar{x}_1)^2} - \lambda_1 - \lambda_2 = 0, \qquad -\frac{4}{(4 + \bar{x}_2)^2} - \lambda_1 - \lambda_3 = 0.$$

- Sign condition: $\lambda_2 \geq 0$, $\lambda_3 \geq 0$.
- Complementarity: $\bar{x}_1 > 0 \Rightarrow \lambda_2 = 0$, $\bar{x}_2 > 0 \Rightarrow \lambda_3 = 0$.

- Units: $[\lambda_1] = [\lambda_2] = [\lambda_3] =$k€/day.

Sensitivity analysis

4. Let λ be such that the KKT conditions hold true. By complementarity condition, we necessarily have $\lambda_2 = \lambda_3 = 0$. The stationarity condition holds true with

$$\lambda_1 = -\frac{1}{(1+\bar{x}_1)^2} = -\frac{4}{(4+\bar{x}_2)^2} = -\frac{1}{25} = -0.04.$$

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

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. Increasing the renting time of y days will generate a variation of cost of $\lambda_1 y$ (approximately), that is, an augmentation of the benefit of 40€/day (less the renting price). It would be of interest for the company to reduce the renting time.