Continuous optimization ENT305A

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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).

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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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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

Definition 1

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

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

where:

- \mathbf{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: $\mathcal{D} = \mathcal{K} = \mathbb{R}^n$.

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

Abbreviation: "subject to" → "s.t.".



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

$$f(x) \ge f(\bar{x})$$
, 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 val(P).

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

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

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:

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

Definition 3

General introduction

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 $x \in K$,

$$||x - \bar{x}|| \le \varepsilon \Longrightarrow f(x) \ge f(\bar{x}).$$

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.

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:

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

Constraints.

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

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

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

We call the expressions

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

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

- 1 Economical problems
- 2 Physical problems
- 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",...).

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.

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

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

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

where the constraints may model a priori knowledge on x.

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 $(x_k, y_k)_{k=1}$ 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.

Approach by least-square.

- Fix an explicit function $F: X \times R \rightarrow Y$, 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

$$F(x,r)=r_1+r_2x.$$

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Lemma 4

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 $K = \{x \in \mathbb{R}^n | g_i(x) \ge 0, \forall i \in \mathcal{I}, g_i(x) = 0, \forall i \in \mathcal{E} \}$, where g is continuous, then K is closed. In practical exercises, it is not necessary to justify the continuity of g.

Definition 5

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.

Exercise. Consider

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

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

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

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

Therefore

$$f(x,y) \ge 2x^2 - 1 - 2xy + 2y^2$$

= $(x^2 + y^2) - 1 + (x - y)^2$
 $\ge ||(x,y)||^2 - 1 \xrightarrow{||(x,y)|| \to \infty} \infty,$

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

Lemma 6

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.

Remark. This is a generalization of the previous lemma, since if K is bounded, f is necessarily coercive.

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

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

- lackbreak 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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Definition 7

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

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

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

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.

■ The function F is said to be continuously differentiable if the Jacobian $DF: x \in \mathbb{R}^n \to \mathbb{R}^{m \times n}$ 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 $F: \mathbb{R}^n \to \mathbb{R}^m$ and let $G: \mathbb{R}^p \to \mathbb{R}^n$ be continuously differentiable functions. Let $H = F \circ G$ (that is, H(x) = F(G(x)). Then

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

Definition 8

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:

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

Definition 9

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

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

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

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 $b \in \mathbb{R}^n$.

Solution. We have

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

Therefore,

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

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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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 10 (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 11

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 $D^2f(\bar{x})$ is positive semi-definite, that is to say,

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

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

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

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

Definition 12

The function f is said to be convex if

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

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

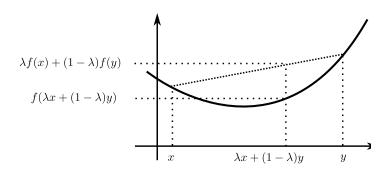
Theorem 13

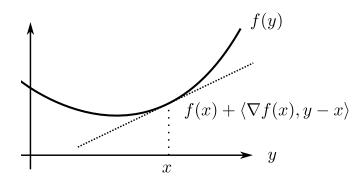
■ The function f is convex if and only if

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

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

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





Theorem 14

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

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

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.

Solution.

- We have $\nabla f(x) = Ax$ and $\nabla^2 f(x) = A$. Since A is positive definite, thus positive semi-definite, the function f is convex.
- For a convex function, a point is a solution if and only if it is a stationary point. Thus it suffices to prove the existence and uniqueness of a stationary point.
- We have

$$x$$
 is stationary $\iff \nabla f(x) = 0$
 $\iff Ax + b = 0$
 $\iff x = -A^{-1}b$.

Therefore there is a unique stationary point, which concludes the proof.

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

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How to compute x_{k+1} ?

Definition 15

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.

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

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 descent algorithm.

- 1 Input: $x_0 \in \mathbb{R}^n$, $\varepsilon > 0$.
- 2 Set k = 0.
- 3 While $\|\nabla f(x_k)\| > \varepsilon$, 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**.

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 .

Optimality conditions

General introduction

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

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

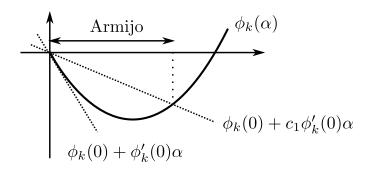
In particular, since d_k is a descent direction,

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

Definition 16

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

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



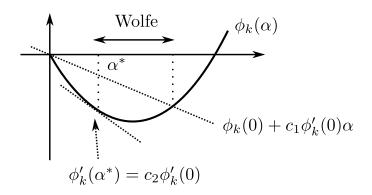
Backstepping algorithm for Armijo's rule

- **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,
 - \blacksquare Set $\alpha = \gamma \alpha$.
- 4 Output α .

Definition 17

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

$$\phi_k(\alpha) < \phi_k(0) + c_1 \phi_k'(0) \alpha$$
 and $\phi_k'(\alpha) \ge c_2 \phi'(0)$.



Bisection method for Wolfe's rule

- **1** Input: $c_1 \in (0,1), c_2 \in (c_1,1), \beta > 0, \eta > 1.$
- Set $\alpha = \beta$.
- 3 While α satisfies Armijo's rule, do
 - Set $\alpha = \eta \alpha$.
- 4 Set $\alpha_{\min} = 0$, α_{\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 .

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

General introduction

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

$$F(x)=0$$

where $F: \mathbb{R}^n \to \mathbb{R}^n$ 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

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

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:

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

General introduction

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 $\|\nabla f(x_k)\| > \varepsilon$, 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 $H_k \approx D^2 f(x_k)^{-1}$. 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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- Gradient methods
- Newton's method

3 Optimality conditions for constrained problems

- Linear constraints
- Non-linear constraints
- Sensitivity analysis

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

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

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

Linear equality constraints

We investigate in this section the problem

$$\inf_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}), \quad \text{s.t.} \quad \begin{cases} g_i(\mathbf{x}) = 0, & \forall i \in \mathcal{E} \\ g_i(\mathbf{x}) \ge 0, & \forall i \in \mathcal{I}. \end{cases}$$
 (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 18

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: $\nabla_{\mathbf{x}} L(\bar{\mathbf{x}}, \lambda) = 0$.
- 2 Sign condition: for all $i \in \mathcal{I}$, $\lambda_i > 0$.
- **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 $m \ge n$.

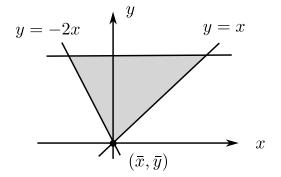
Exercise.

Consider the problem

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

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

Solution.



- 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:

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

■ This linear system has a unique solution

$$\lambda_1 = 1/3 \ge 0$$
 $\lambda_2 = 2/3 \ge 0$.

The sign condition is satisfied.

Example 1. Case of one equality constraint:

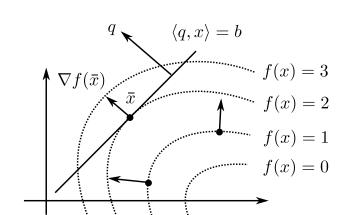
$$m=1, \quad \mathcal{E}=\{1\}, \quad \mathcal{I}=\emptyset.$$

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

Proof of KKT conditions.

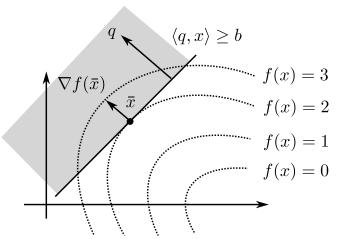
- Geometrically, we understand that $\nabla f(x)$ and q are **colinear**.
- Let $\lambda \in \mathbb{R}$ be such that $\nabla f(x) = \lambda q$.
- We have:

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

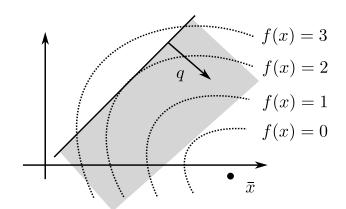


Linear constraints

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



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



Optimality conditions

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

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

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

We deduce that

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

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

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



General introduction

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

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Definition 19

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

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

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

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

Theorem 20

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.

Example 4.

Consider the problem

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

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

Lagrangian:

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

At zero:

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

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

Theorem 21

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

- \blacksquare Prove that f is coercive.
- 2 Calcule $\nabla f(x, y)$ 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 $a+c \ge 0$ and $ac-b^2 \ge 0$. Using this fact, prove that f is convex.
- 4 We consider the following problem:

$$\inf_{(x,y)\in\mathbb{R}^2} f(x,y), \quad \text{subject to: } \begin{cases} x+y \geq 0 \\ x+2 \geq 0. \end{cases}$$
 (\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: $\exp(z) \ge 1 + z$, which yields:

$$f(x,y) \ge x + y^2 + y + x^2$$

$$= \frac{1}{2}(x^2 + y^2) + \frac{1}{2}(x^2 + 2x + 1) + \frac{1}{2}(y^2 + 2y + 1) - 1$$

$$= \frac{1}{2}\|(x,y)\|^2 + (x+1)^2 + (y+1)^2 - 1 \xrightarrow[\|(x,y)\| \to \infty]{} \infty.$$

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^2f . It holds:

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

and

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

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

Exercise

4. Feasibility of (0,0): we have $0+0 \ge 0$ 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: $\frac{\partial L}{\partial v}(0,0,1,0) = \frac{\partial L}{\partial v}(0,0,1,0) = 0$.
- 2 Sign condition: $\lambda_1 > 0$, $\lambda_2 > 0$.
- 3 Complementarity: the second constraint is inactive and the corresponding Lagrange multiplier is null.

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.

Exercise.

Consider:

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

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

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} .

General introduction

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 $\lambda_1 = 1/4 \ge 0$ and $\lambda_2 = 1/2 \ge 0$.

- The sign condition is satisfied.
- The complementarity condition is satisfied (all inequality constraints are active).

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Consider the family of optimization problems

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

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

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

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

Theorem 22

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**).

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 $k \in$) are given by:

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

General introduction

- 1 Formulate the problem as a minimization problem.
- 2 Justify the existence of a solution.
- 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?
- The renting cost of the engine is 70€/day. Is it of interest for the company to rent the engine for a longer time?

1. Problem:

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

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

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

$$L(x,\lambda) = -\frac{x_1}{1+x_1} - \frac{x_2}{4+x_2} - \lambda_1(x_1+x_2-d) - \lambda_2x_1 - \lambda_3x_2.$$

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: $\lambda_2 > 0$, $\lambda_3 > 0$.
- Complementarity: $\bar{x}_1 > 0 \Rightarrow \lambda_2 = 0$, $\bar{x}_2 > 0 \Rightarrow \lambda_3 = 0$.
- Units: $[\lambda_1] = [\lambda_2] = [\lambda_3] = k \in /day$.

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.

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 $40 \in /\text{day}$ (less the renting price). It would be of interest for the company to reduce the renting time.