Numerical optimization

Mines Nancy – Fall 2024

session 1 – general introduction

Lecturer: Julien Flamant (CNRS, CRAN)

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Course material:

`arche.univ-lorraine.fr/course/view.php?id=74098`

`github.com/jflamant/mines-nancy-fall24-optimization`

Outline of the course

36h of classes, including lectures, exercices and lab work (Python)

Course material in english, lecture given in french or english

Main results will be on lecture slides, but detailed computations, proofs and exercises solution will not, in general. Take notes!

Prerequisites: elementary differential calculus and linear algebra

Evaluation

- intermediate exams (40%)
- final exam (60%): January 7th, 2025

Lecturers Julien Flamant (CNRS) and Christophe Zhang (INRIA)
Contact info `julien.flamant@univ-lorraine.fr`

What to expect from this course

in short: an introduction to numerical optimization

Objectives

- learn the basic language of optimization;
- characterize objective functions and critical points;
- solve least squares problems;
- learn about classical first and second-order descent algorithms;
- first principles and algorithms in constrained optimization.

hands-on approach with Python notebooks

Some useful references

Books

- D. Bertsekas (1999). *Nonlinear programming*. Second edition. Belmont, MA: Athena Scientific
- J. Nocedal and S. J. Wright (1999). *Numerical optimization*. Springer
- S. P. Boyd and L. Vandenberghe (2004). *Convex optimization*. Cambridge university press
- A. Beck (2017). *First-order methods in optimization*. SIAM

Online material (include lecture slides and notebooks)

- MIT OpenCourseWare | Optimization (Boyd and Bertsekas courses)
- Numerical tours | Optimization

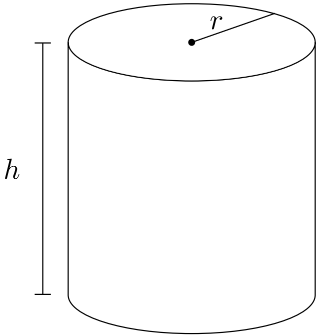
Outline

1. A first example
2. More examples
3. Optimization: vocabulary and nomenclature
4. Some standard optimization problems
5. Recap

A first example

A can produce wants to optimize his consumption of raw material.

The only constraint is that their volume $V = 1\text{L}$ is fixed.



How to formulate this shape optimization problem?

quantity of raw material $\equiv$ area of cylinder $\times$ constant thickness

$\rightarrow$ how to minimize the area A of a cylinder with given volume V?

Formulation of the optimization problem

Expression of the area A (objective function or criterion)

$$A(r,h) = A_{\text{cylinder}}(r,h) + A_{\text{lids}}(r,h) = 2\pi rh + 2\pi r^2$$

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The dimensions r and h are the variables of the optimization problem

r and h must be non-negative $\rightarrow$ constraint $\quad r \geq 0, h \geq 0$

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The condition of constant volume is also a constraint.

$$V(r,h) = \pi r^2 h = V_0$$

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$$r \text{ and } h \text{ must be non-negative} \rightarrow \text{constraint} \quad r \geq 0, h \geq 0$$

The condition of constant volume is also a constraint.

$$V(r,h) = \pi r^2 h = V_0$$

The constrained optimization problem is finally written as

$$\text{Find } (\hat{r},\hat{h}) \text{ such that } A(\hat{r},\hat{h}) \text{ is minimal and } \begin{cases} r \geq 0 \text{ and } h \geq 0 \\ \pi r^2 h = V_0 \end{cases}$$

Simplification of the problem

We notice that h and r are related by the constraint $V_0 = \pi r^2 h$.
$\rightarrow$ The area $A(r, h)$ can be rewritten as a function of r only.

$$h(r) = \frac{V_0}{\pi r^2} \quad (h \geq 0 \quad \text{OK!})$$

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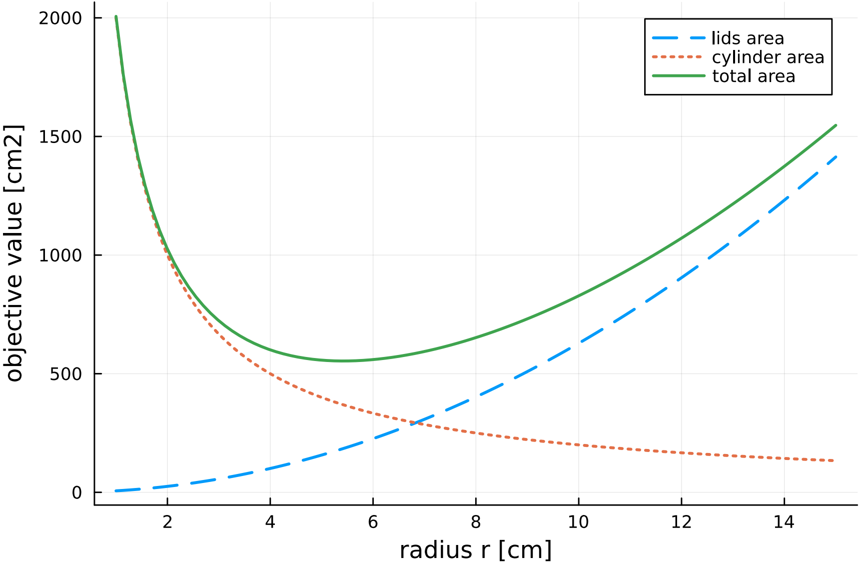
$$h(r) = \frac{V_0}{\pi r^2} \quad (h \geq 0 \quad \text{OK!})$$

By substituting this into the expression for $A(r, h)$, we then obtain

$$\begin{aligned} A(r, h) &= 2\pi r h + 2\pi r^2 \\ &= 2\pi r \frac{V_0}{\pi r^2} + 2\pi r^2 \\ &= \frac{2V_0}{r} + 2\pi r^2 \\ &:= \tilde{A}(r) \end{aligned}$$

The volume constraint is directly taken into account in the new objective function $\tilde{A}(r)$. We consider the constraint $r \geq 0$ when searching for the minimum of $\tilde{A}(r)$ over $\mathbb{R}^+$.

Objective function of the problem ($V_0 = 1$L)



Explicit solution

The derivative of the objective function vanishes at its minimum.

$$\frac{\mathrm{d}\tilde{A}(r)}{\mathrm{d}r} = 4\pi r - \frac{2V_0}{r^2}$$

We solve

$$\left.\frac{\mathrm{d}\tilde{A}(r)}{\mathrm{d}r}\right|_{r=\hat{r}} = 0 \Leftrightarrow 4\pi\hat{r} = \frac{2V_0}{\hat{r}^2}$$

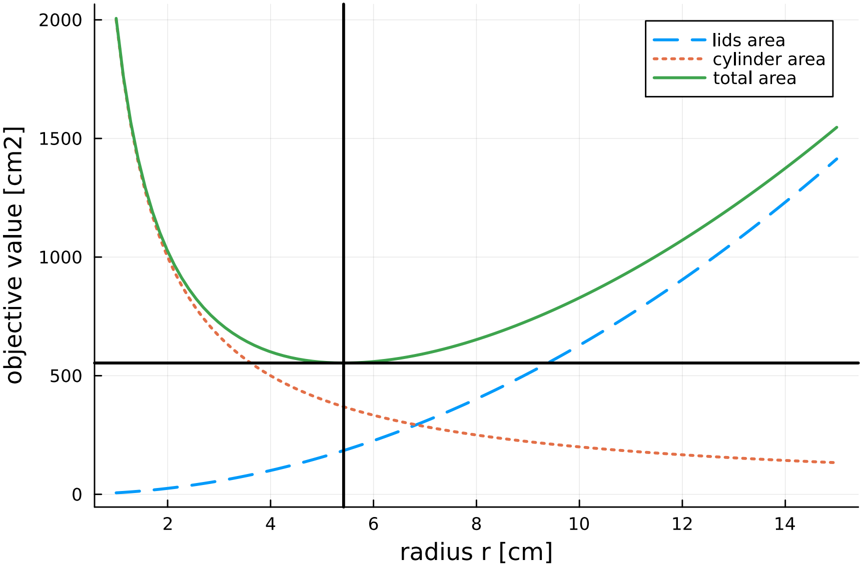
$$\Leftrightarrow \hat{r} = \left[\frac{V_0}{2\pi}\right]^{1/3}$$

In summary, the solutions to the optimization problem are

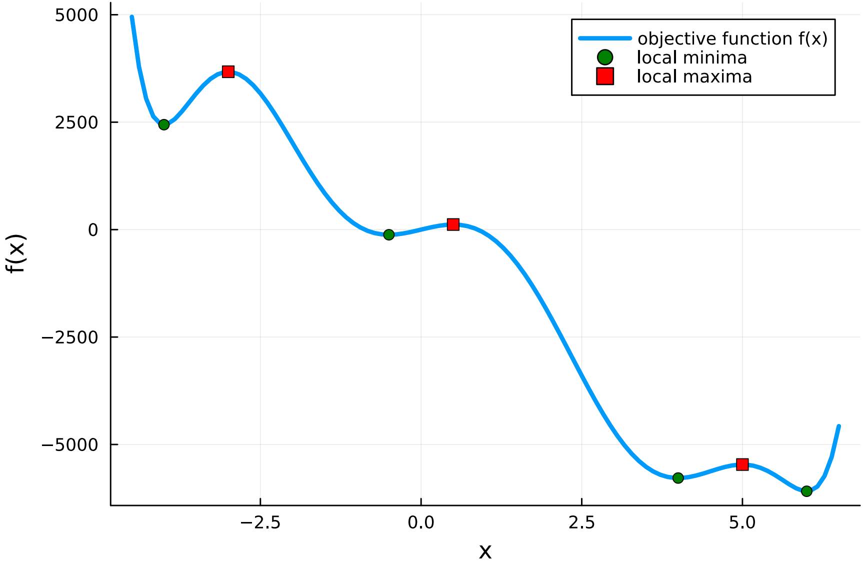
$$\hat{r} = \left[\frac{V_0}{2\pi}\right]^{1/3} \qquad \hat{h} = \frac{V_0}{\pi\hat{r}^2} = 2\hat{r}$$

In this simple case, the solution is explicit and does not require a resolution algorithm $\rightarrow$ this is not the case in general.

Objective function of the problem ($V_0 = 1L$) and solution



It's not always that simple... example in 1D



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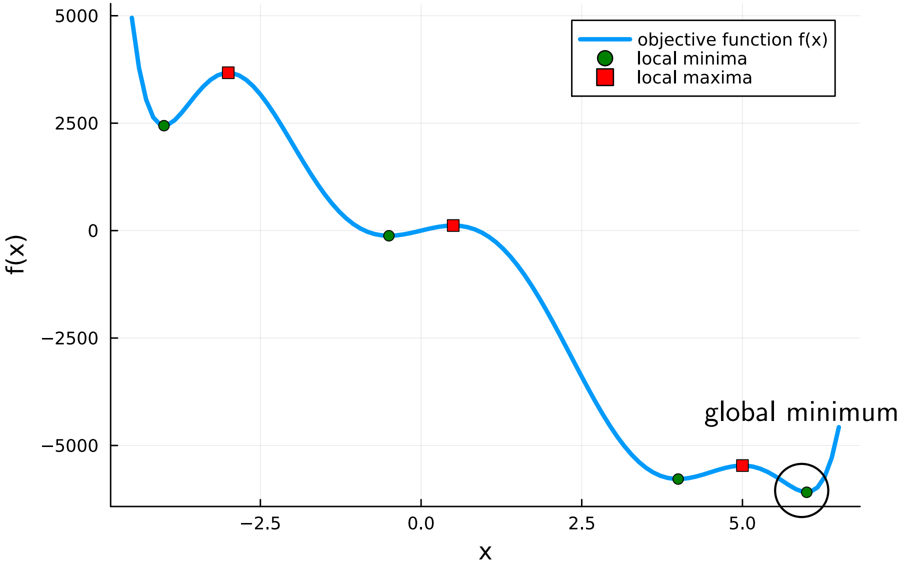

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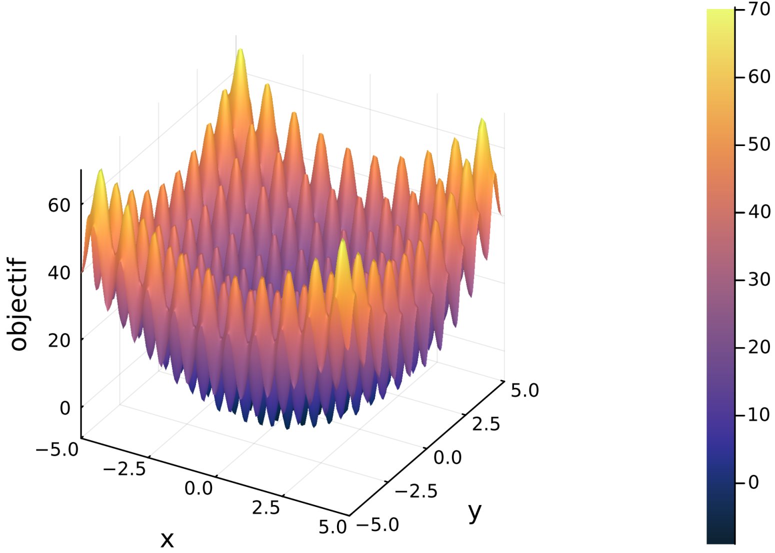

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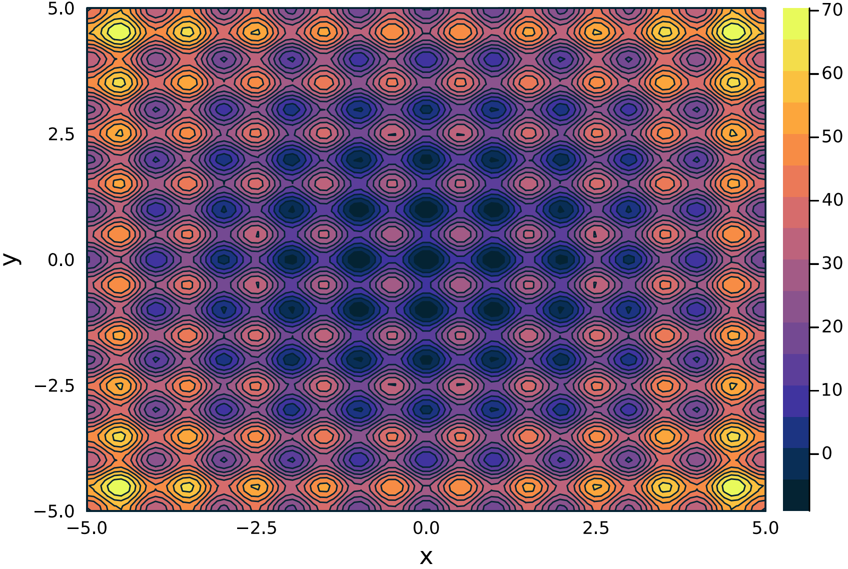
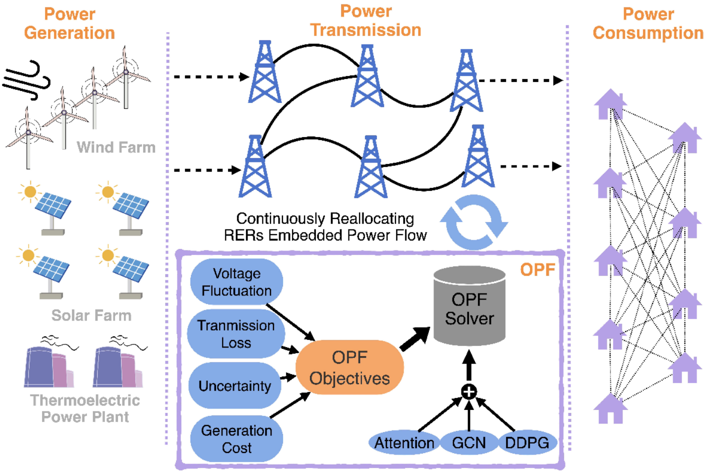


Outline

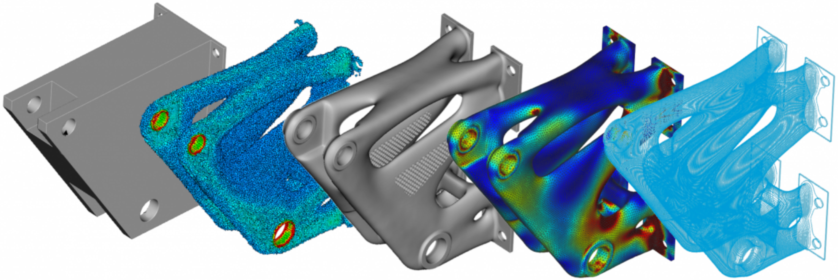
Energy chain optimization



often a multi-objective problem: maximize system efficiency + minimize costs, etc.

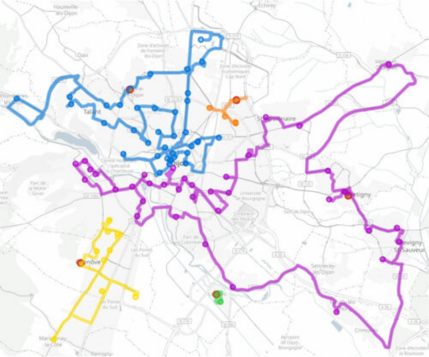
variables of different types: discrete + continuous

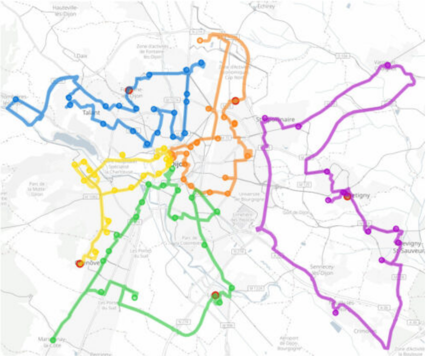
Shape optimization



objective: strongly non-linear, based on physics/mechanics
variables: several billion positions of 3D mesh points

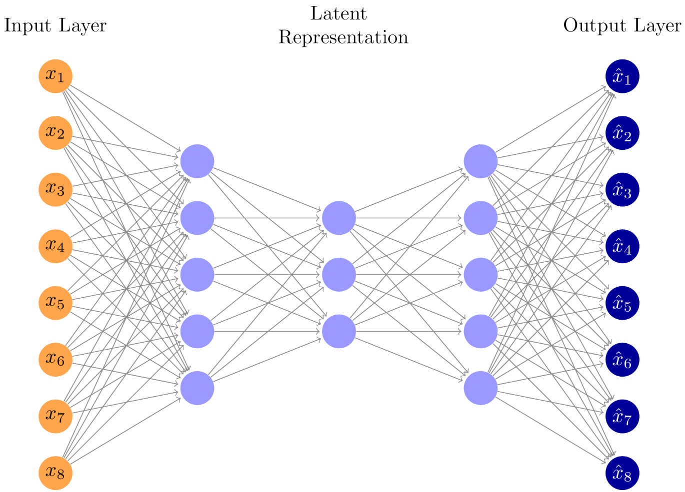
Route or path optimization





objective: minimize the distance/time of each path/journey/yield/etc., often multi-objective
generally discrete variables

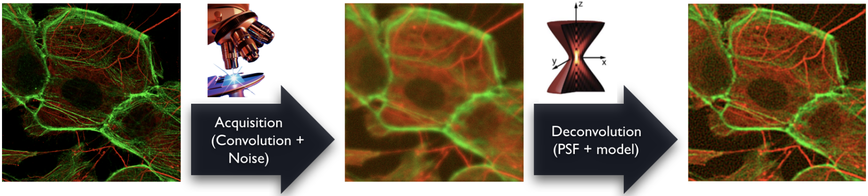
Learning and neural networks



objective: minimize the error between input and output

$\sim 10^6$ to 10^9 optimization variables

Image processing: deconvolution and denoising



Inverse problem: reconstruct an image X from the measurements
$$Y = \text{PSF} * X + \text{noise}$$

Objective: minimize the error between the measurements and the direct model

image X with several megapixels $\to$ as many optimization variables

Outline

General form of an optimization problem

$$\min_{\mathbf{x} \in \mathbb{X}^N} f(\mathbf{x}) \text{ subject to } \mathbf{x} \in \Omega$$

Vocabulary

- $\mathbf{x} = (x_1, x_2, \ldots, x_N)^\top \in \mathbb{X}^N$ is the vector of variables or parameters of the optimization problem

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- the set $\Omega \subseteq \mathbb{X}^N$ is the constraint or feasible set. Often, Ω takes the form

  $$\Omega = \{\mathbf{x} \mid \mathbf{h}(\mathbf{x}) = \mathbf{0},\ \mathbf{g}(\mathbf{x}) \leq \mathbf{0}\}$$

  i.e., it is defined in terms of *functional constraints*.

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Nomenclature

- The space $\mathbb{X}$ can be:
  - finite or discrete: discrete (or combinatorial) optimization
  - continuous $\mathbb{X} = \mathbb{R}$: continuous optimization

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- the nature of f defines specific problems:
  - f linear: linear optimization
  - f quadratic: quadratic optimization
  - f convex and convex constraints: convex optimization
  - f non-differentiable, non-linear, etc.

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each category has its own resolution algorithms

Scope of this course

continuous optimization with and without constraints

$$\min_{\mathbf{x} \in \mathbb{R}^N} f(\mathbf{x}) \text{ subject to } \mathbf{x} \in \Omega$$

typical assumption: $f : \mathbb{R}^N \to \mathbb{R}$ is $\mathcal{C}^1$ (or at least, differentiable)

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Note: minimization vs. maximization

There are also maximization problems (e.g., maximizing the return of a stock portfolio)

$$\max_{\mathbf{x}\in\mathbb{R}^N} g(\mathbf{x}) \text{ subject to } \mathbf{x} \in \Omega$$

This problem is equivalent to the previous problem for $f(\mathbf{x}) = -g(\mathbf{x})$.
$\rightarrow$ In practice, we always reduce the problem to a minimization problem.

Typology of solutions

$$\min_{\mathbf{x} \in \mathbb{R}^N} f(\mathbf{x}) \text{ subject to } \mathbf{x} \in \Omega$$

solving this optimization problem means finding $\mathbf{x}^\star \in \Omega$ (i.e. satisfying the constraints) that minimizes the function f.

An optimization problem can have:

- no solution — e.g. $\min_{x \in \mathbb{R}} f(x) := -x^2$
- a unique solution
- a finite number of solutions
- an infinite number of solutions

when it exists, we call a solution $\mathbf{x}^\star$ a minimizer of f over Ω

Global and local minimizers

$$\min_{\mathbf{x}\in\mathbb{R}^N} f(\mathbf{x}) \text{ subject to } \mathbf{x}\in\Omega$$

Definition (Global minimizer)

A point $\mathbf{x}^\star \in \Omega$ is a *global minimizer* of f over Ω if $f(\mathbf{x}) \geq f(\mathbf{x}^\star)$ for all $\mathbf{x} \in \Omega \setminus \{\mathbf{x}^\star\}$.

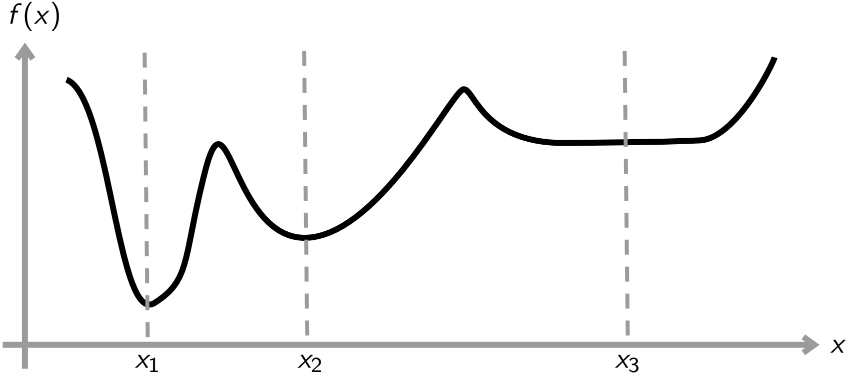
Definition (Local minimizer)

A point $\mathbf{x}^\star \in \Omega$ is a *local minimizer* of f over Ω if there exists $\varepsilon > 0$ such that $f(\mathbf{x}) \geq f(\mathbf{x}^\star)$ for all $\mathbf{x} \in \Omega \setminus \{\mathbf{x}^\star\}$ and $\|\mathbf{x} - \mathbf{x}^\star\| < \varepsilon$.

Remarks

- a global minimizer is a local minimizer, but the converse is not in general
- Replace "$\geq$" by "$>$" in definitions: strict (local, global) minimizer
- if $\mathbf{x}^\star$ is a (local, global) minimizer, then the value $f(\mathbf{x}^\star)$ is a (local, global) minimum

Example: unconstrained optimization in 1D



- $\mathbf{x}_1$ is a strict global minimizer
- $\mathbf{x}_2$ is a strict local minimizer
- $\mathbf{x}_3$ is a local minimizer

Example: constrained optimization in 2D

$$\min_{[x_1, x_2]^\top \in \mathbb{R}^2} (x_1 - 2)^2 + (x_2 - 1)^2 \text{ subject to } \begin{cases} x_1^2 - x_2 \leq 0 \\ x_1 + x_2 \leq 2 \end{cases}$$

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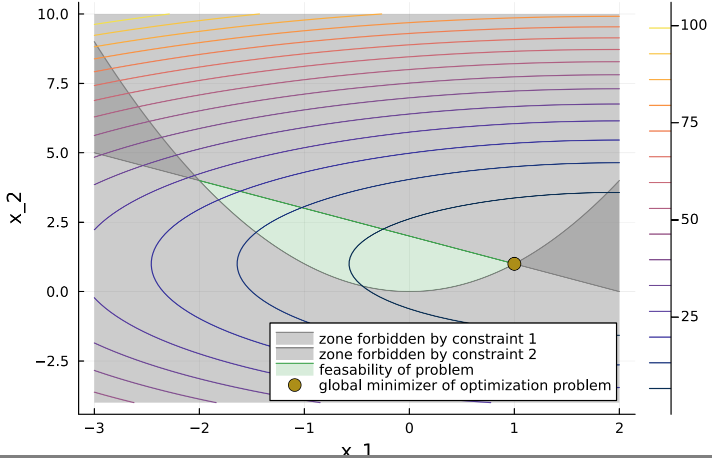

About notations [disgression]

Many names in the literature

- mathematical programming,
- mathematical optimization,
- numerical optimization,
- optimization

they all mean the field of study of *optimization problems*

About notations [disgression]

In the literature, you'll find many different equivalent notations for the same optimization problem

$$\min_{\mathbf{x}\in\mathbb{X}^N} f(\mathbf{x}) \text{ subject to } \mathbf{x}\in\Omega$$

can be simply written as

$$\min_{\mathbf{x}\in\Omega} f(\mathbf{x})$$

or as

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{x}\in\Omega \end{aligned}$$

sometimes, you'll find the notation

$$\arg\min_{\mathbf{x}\in\Omega} f(\mathbf{x})$$

to highlight our interest in finding *minimizers* of the problem.

Outline

Some standard optimization problems

Several optimization problems are so frequently encountered that they are given specific names

being able to recognize to which class belongs a given problem is important as resolution methods are usually problem dependent

Some important examples are

- Linear programming
- Quadratic programming
- Convex programming
- Multi-objective programming
- etc.

For each of these cases, we will review the standard form and give some examples.

Linear programming

Affine objective and constraints: this is a Linear Program (LP).

LP general form

$$\begin{aligned} \text{minimize} \quad & \mathbf{c}^\top \mathbf{x} + \mathbf{d} \\ \text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{b}, \\ & \mathbf{G}\mathbf{x} \leq \mathbf{h} \end{aligned}$$

Comments

- the $\mathbf{d}$ term does not affect the optimization problem – only the linear term $\mathbf{c}^\top \mathbf{x}$ affects the objective function;
- the feasible set is a polyhedron;
- LPs are frequently encountered in *operation research*;
- Solving LPs requires specific algorithms (outside of the scope of this course), such as Dantzig's simplex algorithm.

LP example: diet problem

Example from Boyd and Vanderberghe.

A healthy diet contains m different nutrients in quantities at least equal to $b_1, \ldots, b_M$. We can compose such a diet by choosing quantities of N different foods. One unit of food j contains a_{ij} of nutrient i and has a cost of c_j.

Question write the optimization problem corresponding to choosing the cheapest healthy diet.

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Solution The corresponding optimization problem is

$$\begin{aligned} \text{minimize} \quad & \mathbf{c}^\top \mathbf{x} \\ \text{subject to} \quad & \mathbf{A}\mathbf{x} \geq \mathbf{b}, \\ & \mathbf{x} \geq \mathbf{0} \end{aligned}$$

where $\mathbf{x} \in \mathbb{R}^N$ contains the (non-negative) quantities of each food.

Quadratic programming

When the objective function is (convex) quadratic and the constrains are affine, we obtain a Quadratic Program (QP).

QP general form

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^\top \mathbf{P}\mathbf{x} + \mathbf{q}^\top \mathbf{x} + \mathbf{r} \\ \text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{b}, \\ & \mathbf{G}\mathbf{x} \le \mathbf{h} \end{aligned}$$

where $\mathbf{P} \succeq \mathbf{0}$ (is positive semidefinite) (more on that later).

Comments

- Like in LPs, the feasible set is a polyhedron;
- QPs are fundamental for many fields, ranging from signal processing, parameter estimation, regression, machine learning, econometrics, etc.
- have a direct connection with least-squares problems (see session 3)

QP example: Gaussian maximum likelihood estimation (I)

We want to estimate the mean $\boldsymbol{\theta} \in \mathbb{R}^N$ of a Gaussian random variable $\mathcal{N}(\boldsymbol{\theta}, \boldsymbol{\Sigma})$, with known covariance matrix $\boldsymbol{\Sigma}$ from M i.i.d. measurements $\mathbf{y}_1, \ldots, \mathbf{y}_M \sim \mathcal{N}(\boldsymbol{\theta}, \boldsymbol{\Sigma})$. Recall that

$$p(\mathbf{y}_i; \boldsymbol{\theta}) = \frac{1}{(2\pi)^{N/2} |\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2} (\mathbf{y}_i - \boldsymbol{\theta})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{y}_i - \boldsymbol{\theta}) \right)$$

Maximum likelihood (ML) principle

$$\text{find } \boldsymbol{\theta}^\star = \arg\max_{\boldsymbol{\theta} \in \mathbb{R}^N} \mathcal{L}(\boldsymbol{\theta}; \mathbf{y}_1, \ldots, \mathbf{y}_M) := p(\mathbf{y}_1, \ldots, \mathbf{y}_M; \boldsymbol{\theta})$$

The function $\mathcal{L}(\boldsymbol{\theta}; \mathbf{y}_1, \ldots, \mathbf{y}_M)$ is called the *likelihood function*.

The goal of ML estimation is to find the parameter $\boldsymbol{\theta}$ for which the data $\mathbf{y}_1, \ldots, \mathbf{y}_M$ has the highest joint probability.

Exercise: write the corresponding optimization problem!

QP example: Gaussian maximum likelihood estimation (II)

Solution

First, since observations are i.i.d., $p(\mathbf{y}_1, \ldots, \mathbf{y}_M; \boldsymbol{\theta}) = \prod_{i=1}^{M} p(\mathbf{y}_i; \boldsymbol{\theta})$.

Second, observe that the ML principle is equivalent to

$$\text{find } \boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta} \in \mathbb{R}^N}{\arg\max}\, \mathcal{L}(\boldsymbol{\theta}; \mathbf{y}_1, \ldots, \mathbf{y}_M) = \underset{\boldsymbol{\theta} \in \mathbb{R}^N}{\arg\max} \log \mathcal{L}(\boldsymbol{\theta}; \mathbf{y}_1, \ldots, \mathbf{y}_M)$$

since the likelihood is positive (by definition) and log is monotone. Thus,

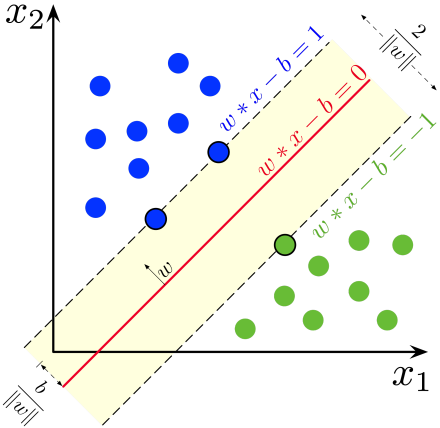
$$\boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta} \in \mathbb{R}^N}{\arg\max} -\frac{1}{2} \sum_{i=1}^{M} (\mathbf{y}_i - \boldsymbol{\theta})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{y}_i - \boldsymbol{\theta})$$

which can be rewritten as the (unconstrained) QP

$$\text{minimize} \quad \frac{1}{2} \boldsymbol{\theta}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\theta} - \frac{1}{M} \left(\sum_{i=1}^{M} \mathbf{y}_i \right)^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\theta}$$

QP example: support vector machines (SVMs)

SVMs are a supervised learning tool for classification and regression.



Idea: find the *maximum-margin* hyperplane that divides the data into two classes $\rightarrow$ one obtains a constrained QP.

More on this in TPs !

Convex programming

Linear programs and quadratic programs are convex problems.

In the next session, we will precisely define this notion and see why it is crucial for many optimization problems.

General form of a convex problem

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, M \\ & \mathbf{a}_i^\top \mathbf{x} = b_i, \quad i = 1, \ldots, P \end{aligned}$$

where f and $g_1, \ldots, g_M$ are *convex* functions.

When we will discuss constrained optimization problems, we will solely focus on convex optimization problems.

Multi-objective optimization (I)

Sometimes we are interested in optimization problems that involve multiple objective functions, say $F_1, F_2, \ldots, F_Q$. Multi-objective problems can be formulated as

$$\min_{\mathbf{x} \in \Omega} \quad [F_1(\mathbf{x}), F_2(\mathbf{x}), \ldots, F_Q(\mathbf{x})]$$

where $\Omega \subset \mathbb{R}^N$ is the feasible set.

A feasible point $\mathbf{x} \in \Omega$ is said to *Pareto dominate* another solution $\mathbf{y} \in \Omega$ if

- $F_i(\mathbf{x}) \leq F_i(\mathbf{y})$ for all $i = 1, \ldots, Q$
- $F_i(\mathbf{x}) < F_i(\mathbf{y})$ for at least one i.

A point $\mathbf{x}^{\text{po}}$ is said to be Pareto optimal is there does not exist another solution that dominates it. The set of such points is called the Pareto front or Pareto boundary.

Multi-objective optimization (II)

A typical transformation of the multi-objective optimization problem

$$\min_{\mathbf{x}\in\Omega} \quad [F_1(\mathbf{x}), F_2(\mathbf{x}), \ldots, F_Q(\mathbf{x})]$$

is the scalarization procedure

$$\min_{\mathbf{x}\in\Omega} \quad \lambda_1 F_1(\mathbf{x}) + \lambda_2 F_2(\mathbf{x}) + \ldots + \lambda_Q F_Q(\mathbf{x})$$

where $\lambda_1, \lambda_2, \ldots, \lambda_Q > 0$ are weights controlling the trade-offs between the Q objective terms.

Under certain conditions, solutions of the scalarized problem give Pareto optimal points (but not necessary all such points).

The notion of *regularization* can be interpreted in terms of multi-objective optimization. More in TPs!

Outline

Recap and take-home message

General form

$$\min_{\mathbf{x}\in\mathbb{R}^N} f(\mathbf{x}) \text{ subject to } \mathbf{x}\in\Omega$$

Which questions do we ask in optimization?

- Existence and uniqueness of a solution $\mathbf{x}^\star$
- Characterization of solutions: necessary or sufficient conditions for $\mathbf{x}^\star$ to be a solution
- Design an efficient way to compute $\mathbf{x}^\star$ numerically.
  - by a closed-form solution (not very often)
  - usually, by an algorithm which produces a sequence

$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(n)}, \ldots \xrightarrow[n\to\infty]{} \mathbf{x}^\star$$

- Characterize the properties of this algorithm: rate of convergence, numerical complexity, etc.