MsC in Data Sciences & Business Analytics

Optimization Course

Gif-sur-Yvette
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Summary

1. Introduction.
2. Unconstrained optimization.
   - Derivative-free algorithms.
   - Gradient-based algorithms.
   - Least squares algorithms.
3. Least-square problems.
4. Constrained optimization.
5. Global / discrete optimization.

Organization

8 courses:

- Course 1: lecture.
- Courses 2 to 8: 1h30 lecture and 1h30 practical session (matlab).
- Dec. 14, 2017: exam.

1. Introduction

General formulation (unconstrained)

Minimize $f(\boldsymbol{x})$.

Terminology:

- $\boldsymbol{x} \in \mathbb{R}^n$: variables.
- $f : \mathbb{R}^n \mapsto \mathbb{R}$: objective function (criterion).

Resolution:

- Existence and unicity of the solution?
- Which numerical algorithm?
- Algorithm complexity: computation time, memory storage.

General formulation (constrained)

Minimize $f(x)$ **subject to** $\begin{cases} g_i(x) \leq 0, & i = 1, \ldots, p \\ h_i(x) = 0, & i = 1, \ldots, q. \end{cases}$

Terminology:

- $x \in \mathbb{R}^n$: variables.
- $f : \mathbb{R}^n \mapsto \mathbb{R}$: objective function.
- $g_i : \mathbb{R} \mapsto \mathbb{R}$: inequality constraints.
- $h_i : \mathbb{R} \mapsto \mathbb{R}$: equality constraints.

Reformulation

Minimize $f(\boldsymbol{x})$ **subject to** $\boldsymbol{x} \in \mathcal{D}$.

Feasible set: $\mathcal{D} = \{\boldsymbol{x} \in \mathbb{R}^n, \, \boldsymbol{g}(\boldsymbol{x}) \leq \mathbf{0}_p, \, \boldsymbol{h}(\boldsymbol{x}) = \mathbf{0}_q\}$

- $\boldsymbol{g}(\boldsymbol{x}) = \begin{bmatrix} g_1(\boldsymbol{x}) \\ \vdots \\ g_p(\boldsymbol{x}) \end{bmatrix}$ gathers the p inequality constraints.
- $\boldsymbol{h}(\boldsymbol{x}) = \begin{bmatrix} h_1(\boldsymbol{x}) \\ \vdots \\ h_q(\boldsymbol{x}) \end{bmatrix}$ gathers the q equality constraints.

Example 1: Knapsack problem

Jo goes hitch hiking. The maximum weight allowed in his knapsack is W. Each article $i = 1, \ldots, n$ he can take weight w_i and has a usefulness u_i. What articles should be taken in the knapsack to maximize the usefulness?

Example. $W = 25$, and:

i	w_i	u_i
1	25.00	40
2	12.50	35
3	11.25	18
4	5.00	4
5	2.50	10
6	1.25	2

Mathematical formulation

1. What is the search space?

   $\boldsymbol{x} \in \mathcal{D} = \{0, 1\}^n$

   $x_i = 1 \Leftrightarrow$ bring article # i in the knapsack

2. What is the objective function?

   $$f(\boldsymbol{x}) = \sum_{i=1}^{n} w_i x_i$$

3. What constraints?

   $$\sum_{i=1}^{n} w_i x_i \leq W$$

$\Rightarrow$ *Combinatorial* (discrete) optimization problem.

Example 2: Traveling salesman problem

Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?

- Search space? $\mathcal{D}$: set of all permutations of $\{1, \ldots, n\}$.

$\Rightarrow$ *Combinatorial* (discrete) optimization problem.

Example 3: Ressource allocation: example

A factory produces two products P1 and P2 and has resources R1 (equipment), R2 (human), R3 (raw materials) in limited quantities.

P1 is sold for 6 euros per unit, P2 is sold for 4 euros per unit.

Example.

	P1	P2	Availability
R1	3	9	81
R2	4	5	55
R3	2	1	20
Profit	6	4	

Questions. Mathematical formulation? Feasible domain?

Example 3: Ressource allocation

- Bandwith allocation in wireless communication.
- Strategic planning: allocating scarce resources (*e.g.,* human resources) among the various projects or business units.
- *etc.*

Linear programming problems.

Example 4: Portfolio optimization

Choosing the proportions of various assets to be held in a portfolio, in such a way as to make the portfolio better than any other according to some criterion.

The criterion will combine considerations of:

- the expected value of the portfolio's rate of return
- the return dispersion
- other measures of financial risk.

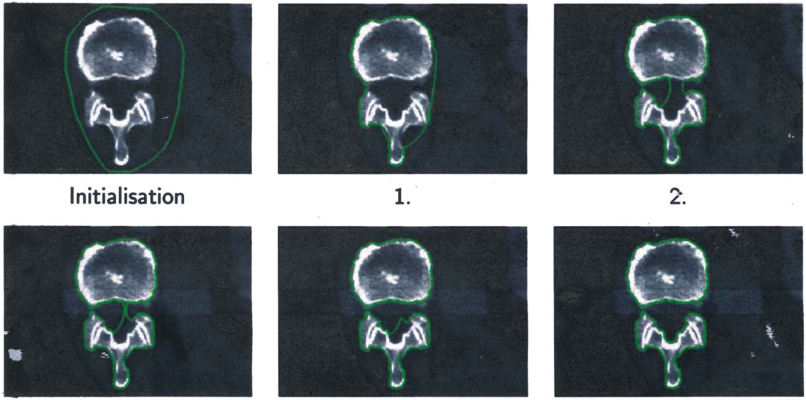
Example 5: Mechanical design of structures

Bridge topology optimization

- Minimize the total mass under rigidity constraints.
- Shape optimization: maximize the stability (oscillations due to car traffic, pedestrian or wind) of hanging bridges.

Example 6: Image segmentation using active contours

Contours actifs 2D *3/5*



Initialisation 1. 2.

3. 4. Résultat

Example 6: Image segmentation using active contours

A contour is defined as a parametric function $M = f(s)$.

- The contours lays in the contrast areas of the image.

  $\Rightarrow$ maximimize
  $$\int_s \|\nabla \boldsymbol{A}(f(s))\|_2^2 \, ds$$
  with respect to f.
- Find a smooth contour.

  $\Rightarrow$ constraint that the smoothness function R(f) is bounded.
- Formulation:

$$\min_f - \int_s \|\nabla \boldsymbol{A}(f(s))\|_2^2 \, ds \quad \text{subject to} \quad R(f) \leq A$$

Example 7: Image registration

$$\max_{T} S(I_t, T(I_s))$$

- T: geometrical transformation (translation, rotation, *etc.*).
- I_s: source image, I_t target image.
- S: measure of similarity.

Conclusion (part 1)

There is no generic numerical method to solve all kinds of problems!

The effectiveness of numerical optimization methods depends on:

- The differentiability of f.
- The possibility to compute efficiently its derivatives.
- The feasible set: discrete or continuous?
- The kinds of constraints (equalities / inequalities).
- The specific class of problem (linear programming, convex, *etc.*).
- The problem dimension.

Basic definitions

Local/global minimizers

$\boldsymbol{x}^\star \in \mathcal{D}$ is a global minimizer of f over $\mathcal{D}$ if $\forall \boldsymbol{x} \in \mathcal{D}$, $f(\boldsymbol{x}) \geq f(\boldsymbol{x}^\star)$.

$\boldsymbol{x} \in \mathcal{D}$ is a local minimizer of f over $\mathcal{D}$ if there exists a neighborhood $\mathcal{V}(\boldsymbol{x})$ of $\boldsymbol{x}$ such $\forall \boldsymbol{y} \in \mathcal{V}(\boldsymbol{x}) \cap \mathcal{D}$, $f(\boldsymbol{y}) \geq f(\boldsymbol{x})$.

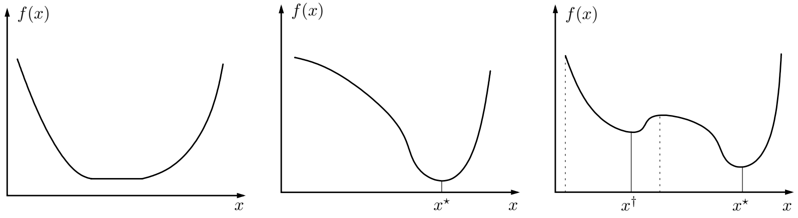
The minimum of f over $\mathcal{D}$ is the value $\min\limits_{\boldsymbol{x} \in \mathcal{D}} f(\boldsymbol{x})$.

Unimodality / multimodality

f is unimodal if f possesses a unique local minimizer.
Otherwise, f is multimodal.

Remark.

- Strict convexity $\Rightarrow$ unimodality.
- Convexity $\Rightarrow$ all local minimizers are global minimizers.



convex but multimodal — nonconvex but unimodal — nonconvex and multimodal

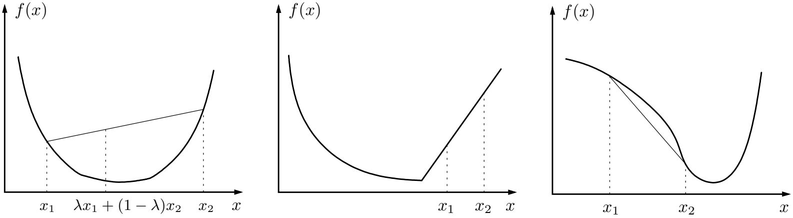
Convexity

f is convex if for any $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathcal{D}$, and any $\lambda \in [0, 1]$,

$$f(\lambda \boldsymbol{x}_1 + (1-\lambda)\boldsymbol{x}_2) \;\leq\; \lambda f(\boldsymbol{x}_1) + (1-\lambda) f(\boldsymbol{x}_2)$$

f is strictly convex if for any $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathcal{D}$, and any $\lambda \in]0, 1[$,

$$f(\lambda \boldsymbol{x}_1 + (1-\lambda)\boldsymbol{x}_2) < \lambda f(\boldsymbol{x}_1) + (1-\lambda) f(\boldsymbol{x}_2)$$



strictly convex | convex | nonconvex

Convexity: specific cases

Linear programming.

- $f(\boldsymbol{x}) = \boldsymbol{c}^T \boldsymbol{x} = \sum_i c_i x_i$ is convex.

Quadratic programming.

- $f(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2 = \sum_i (y_i - \boldsymbol{a}_i^T \boldsymbol{x})^2$ is convex.

- $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}^T \boldsymbol{x} = \frac{1}{2} \sum_i \sum_j a_{ij} x_j x_j - \sum_i b_i x_i$ is convex when $\boldsymbol{H}$ is symmetric positive semedefinite.

Iterative algorithms

Iterative algorithms.

Solve the minimization with an iterative algorithm which generates a sequence of iterates x_0, x_1, ..., x_n.

Convergence.

The sequence of iterates x_n converges to the solution $x^\star$ of the minimization problem.

- Global convergence: valid for all $x_0 \in \mathcal{D}$.
- Local convergence: valid for x_0 in a neighborhood of $x^\star$.

Rate of convergence

- Linear convergence: $\dfrac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^\star\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^\star\|} \leq r$ for k sufficiently large.
- Quadratic convergence: $\dfrac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^\star\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^\star\|^2} \leq r$ for k sufficiently large.
- Super-linear convergence: $\displaystyle\lim_{k\to\infty} \frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^\star\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^\star\|} = 0$.

Linear programming

Canonical form:

Minimize $\boldsymbol{c}^T \boldsymbol{x}$ subject to $\begin{cases} \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \\ \boldsymbol{x} \geq \boldsymbol{0} \end{cases}$

Standard form:

Minimize $\boldsymbol{c}^T \boldsymbol{x}$ subject to $\boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{b}$

Remarks:

- Set $\boldsymbol{z} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{0}$. Standard form $\Rightarrow$ Canonical form.
- No closed-form solution.

Resolution:

- The simplex algorithm.
- Integer linear programming (discrete case).

Linear least squares

Given $\boldsymbol{y} \in \mathbb{R}^m$ and $\boldsymbol{A} \in \mathbb{R}^{m\times n}$, find $\boxed{\boldsymbol{x}^\star \in \arg\min_{\boldsymbol{x}} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2}$

$\boldsymbol{x}^\star$ is a solution of

$$\begin{aligned} & \nabla_{\boldsymbol{x}} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2 = \mathbf{0} \\ \Leftrightarrow\ & 2\boldsymbol{A}^T(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}) = \mathbf{0} \\ \Leftrightarrow\ & \boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{y} \end{aligned}$$

If $m \geq n$ and $\boldsymbol{A}$ is full column rank: $\boldsymbol{x}^\star = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}$.

Otherwise:

- infinity of solutions.
- Generalized inverse: solution having the minimum ℓ_2-norm:

Example. Find the best coefficients (a, b) of a linear model so as to reproduce at best observations y_i at times t_i.

Example. Data fitting using a polynom of degree p.

Quadratic programming

Given $\boldsymbol{c} \in \mathbb{R}^n$, $\boldsymbol{Q} \in \mathbb{R}^{n\times n}$, $\boldsymbol{A} \in \mathbb{R}^{p\times n}$,

Minimize $\frac{1}{2}\boldsymbol{x}^T Q \boldsymbol{x} + \boldsymbol{c}^T \boldsymbol{x}$ **subject to** $A\boldsymbol{x} \leq \boldsymbol{b}$.

- p: number of constraints.
- j-th constraint: $\boldsymbol{a}_i^T \boldsymbol{x} \leq b_i$.
- Q is positive semi-definite $\implies$ convex problem.
- Q is positive definite: strictly convex problem.

Nonlinear least squares

Given $\boldsymbol{y} \in \mathbb{R}^m$ and $\boldsymbol{\varphi} : \mathbb{R}^n \mapsto \mathbb{R}^m$,

$$\textbf{Minimize } \|\boldsymbol{y} - \boldsymbol{\varphi}(\boldsymbol{x})\|_2^2$$

- No closed form solution
- Specific algorithms taking the structure of the problem into account (Levenberg-Marquardt)

Example

Given a set of points (x_i, y_i), $i = 1, \ldots, N$, approximate the set of points using a parametric curve $y = \varphi(x; \boldsymbol{\theta})$.

Example: $\varphi(x; \alpha_1, \alpha_2, \tau_1, \tau_2) = \alpha_1 \exp(x/\tau_1) + \alpha_2 \exp(x/\tau_2)$

with $\boldsymbol{\theta} = \{\alpha_1, \alpha_2, \tau_1, \tau_2\}$.

1. Formulate the problem as an optimization problem.
2. Call the appropriate Matlab function.

cf. Matlab simulations.

2. Unconstrained local optimization

Working assumptions

$f : \mathbb{R}^n \to \mathbb{R}$ is $\mathcal{C}^1$ or $\mathcal{C}^2$.

Definitions.

- Gradient of criterion $f(\boldsymbol{x})$: $\nabla f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \dots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} \in \mathbb{R}^n$

- Hessian of criterion $f(\boldsymbol{x})$:

$$\boldsymbol{H}(\boldsymbol{x}) = \nabla^2 f(\boldsymbol{x}) = \begin{bmatrix} \dots & \dots & \dots \\ \dots & \frac{\partial^2 f}{\partial x_i \, \partial x_j} & \dots \\ \dots & \dots & \dots \end{bmatrix} \in \mathbb{R}^{n \times n}$$

Existence of a local minimizer

Theorem. Given $\mathcal{U}$ a closed subset of $\mathbb{R}^n$, and a continuous function $f : \mathcal{U} \subset \mathbb{R}^n \to \mathbb{R}$.

- If $\mathcal{U}$ is bounded,
- or if $\lim\limits_{\substack{\|\boldsymbol{x}\| \to \infty \\ \boldsymbol{x} \in \mathcal{U}}} f(\boldsymbol{x}) = +\infty$ [coercivity],

then f admits a local minimum on $\mathcal{U}$.

Line search strategy

An iterative algorithm generates a sequence $\boldsymbol{x}_0$, $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_n$.

How to move from $\boldsymbol{x}_k$ to $\boldsymbol{x}_{k+1}$?

- Use the information about function f at $\boldsymbol{x}_k$.
- Possibly use information from earlier iterates $\boldsymbol{x}_{k-1}$, $\boldsymbol{x}_{k-2}$, *etc.*

Line search.

- Choose a direction $\boldsymbol{d}_k$.
- Solve (approximately) the 1D minimization problem:

$$\min_{t>0} f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$$

- Set $\boxed{\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + t\boldsymbol{d}_k}$

Feasible direction

$\boldsymbol{d}$ is a feasible direction at $\boldsymbol{x} \in \mathcal{D}$ if

$$\exists A > 0, \forall t \in [0, A], \boldsymbol{x} + t\boldsymbol{d} \in \mathcal{D}$$

Descent direction

- $\boldsymbol{d}$ is a descent direction of f at $\boldsymbol{x} \in \mathcal{D}$ if

$$\exists A > 0,\ \forall t \in [0, A],\ f(\boldsymbol{x} + t\boldsymbol{d}) \leq f(\boldsymbol{x})$$

- First order Taylor expansion:

$$f(\boldsymbol{x} + t\boldsymbol{d}) = f(\boldsymbol{x}) + t\boldsymbol{d}^T \nabla f(\boldsymbol{x}) + o(t)$$

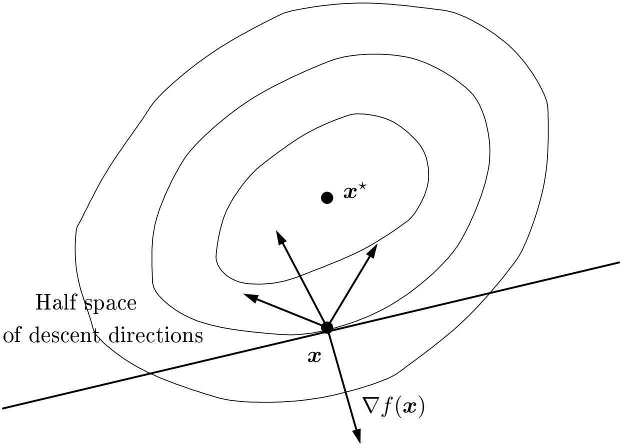
- $\boldsymbol{d}$ is a descent direction $\Longleftrightarrow \boldsymbol{d}^T \nabla f(\boldsymbol{x}) < 0$

  $\Longrightarrow$ Half space of descent directions.

Descent directions and level sets

Level sets: $\mathcal{L}_z = \{\boldsymbol{x} \in \mathbb{R}^n,\ f(\boldsymbol{x}) = z\}$.

Descent directions:



Derivatives

First order Taylor expansion:

$$f(\boldsymbol{x} + t\boldsymbol{d}) = f(\boldsymbol{x}) + t\boldsymbol{d}^T \nabla f(\boldsymbol{x}) + o(t)$$

Second order Taylor expansion:

$$f(\boldsymbol{x} + \boldsymbol{h}) = f(\boldsymbol{x}) + \boldsymbol{h}^T \nabla f(\boldsymbol{x}) + \frac{1}{2}\boldsymbol{h}^T \boldsymbol{H}(\boldsymbol{x})\boldsymbol{h} + o(\|\boldsymbol{h}\|^2)$$

$$f(\boldsymbol{x} + t\boldsymbol{d}) = f(\boldsymbol{x}) + t\boldsymbol{d}^T \nabla f(\boldsymbol{x}) + \frac{t^2}{2}\boldsymbol{d}^T \boldsymbol{H}(\boldsymbol{x})\boldsymbol{d} + o(t^2)$$

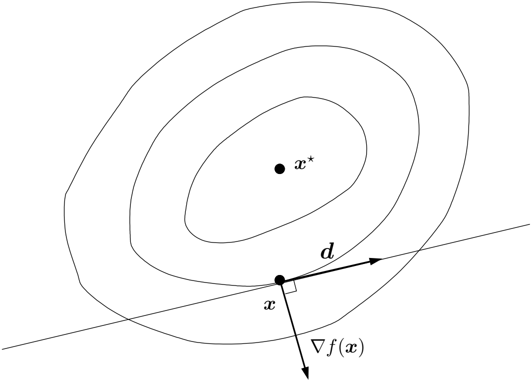
Directional derivative in the direction $\boldsymbol{d}$:

$$\begin{aligned} f'(\boldsymbol{x};\boldsymbol{d}) &= \lim_{t\to 0} \frac{f(\boldsymbol{x}+t\boldsymbol{d}) - f(\boldsymbol{x})}{t} \\ &= \boldsymbol{d}^T \nabla f(\boldsymbol{x}) \end{aligned}$$

Derivatives

If $\boldsymbol{d}$ is tangent to the level set, then $f'(\boldsymbol{x};\boldsymbol{d}) = \boldsymbol{d}^T \nabla f(\boldsymbol{x}) = 0$.

$\nabla f(\boldsymbol{x})$ is thus orthogonal to the level set.



Necessary condition for a local minimizer

Problem. Find $\boldsymbol{x}^\star \in \arg\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x})$

Note. $\max_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x}) = -\min_{\boldsymbol{x}\in\mathbb{R}^n}(-f(\boldsymbol{x}))$

Theorem. If f admits a local minimum at $\boldsymbol{x}^\star$, then $\nabla f(\boldsymbol{x}^\star) = 0$.

Proof. Show that $f'(\boldsymbol{x}^\star; \boldsymbol{d}) = \boldsymbol{d}^T \nabla f(\boldsymbol{x}^\star) = 0 \ \forall \boldsymbol{d}$.

Remark. The condition is necessary but not sufficient.

Sufficient condition for a local minimizer

Theorem. If $\nabla f(\boldsymbol{x}^\star) = 0$ and $\boldsymbol{H}(\boldsymbol{x}^\star) > 0$, then f admits a local minimum at $\boldsymbol{x}^\star$.

Positive definiteness. $\boldsymbol{H}(\boldsymbol{x}^\star) > 0 \Leftrightarrow \forall \boldsymbol{d} \neq \mathbf{0},\ \boldsymbol{d}^T \boldsymbol{H}(\boldsymbol{x}^\star)\boldsymbol{d} > 0$.

Proof. Show that $\forall \boldsymbol{d},\ f(\boldsymbol{x}^\star + t\boldsymbol{d}) > f(\boldsymbol{x}^\star)$ for $|t|$ sufficiently small.

Descent algorithms

Choose $\boldsymbol{x}_0$.

For $k \geq 0$,

- Find a descent direction $\boldsymbol{d}_k$
- Find a step $t_k > 0$.
- Compute $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + t_k \boldsymbol{d}_k$.

Choice 1. Constant step $t_k = t$, $\forall k$.

Choice 2. 1D minimisation: $t_k = \arg\min_{t>0} f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$.

Descent algorithms

Descent: $\forall k,\ f(\boldsymbol{x}_{k+1}) < f(\boldsymbol{x}_k)$.

Stopping conditions:

- $f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) < \varepsilon_1$.
- $\|\boldsymbol{x}_{k+1} - \boldsymbol{x}_k\|_2 < \varepsilon_2$.
- $\|\nabla f(\boldsymbol{x}_k)\|_2 < \varepsilon_3$.
- $k = K_{\text{max}}$.

Choice of the initial solution

- Unimodal criterion: any value of $\boldsymbol{x}_0$ should work (theoretically...)

Gradient based algorithms

The gradient algorithm.

- Choose $\boldsymbol{x}_0$.
- For $k \geq 0$, do $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k - t_k \nabla f(\boldsymbol{x}_k)$.

  $\Rightarrow$ Constant step: $t_k = t$, $\forall k$.
  $\Rightarrow$ 1D minimization: $t_k \approx \arg\min_{t>0} f(\boldsymbol{x}_k - t\nabla f(\boldsymbol{x}_k))$.

The conjugate gradient algorithm.

- Choose $\boldsymbol{x}_0$.
- For $k \geq 0$, do $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k - t_k \nabla f(\boldsymbol{x}_k) + \beta_k(\boldsymbol{x}_k - \boldsymbol{x}_{k-1})$.

Convergence rate is much faster!

Gradient algorithm

Remark.

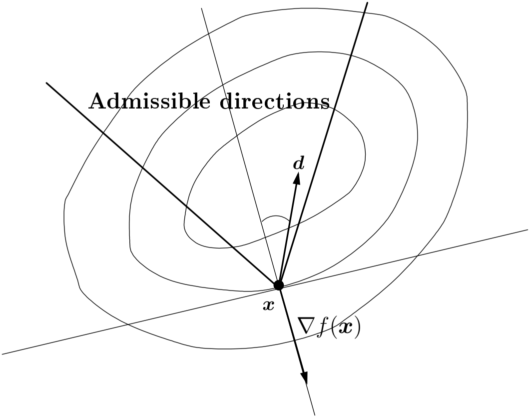
If the step is chosen as

$$t_k = \arg\min_{t>0} f(\boldsymbol{x}_k - t\nabla f(\boldsymbol{x}_k))$$

then forall k, $\nabla f(\boldsymbol{x}_k)$ and $\nabla f(\boldsymbol{x}_{k+1})$ are orthogonal (slow convergence, zigzag phenomenon).

$\Rightarrow$ Linear convergence.

Choice of descent direction



Impose that $|\mathrm{Angle}(\boldsymbol{d}_k, -\nabla f(\boldsymbol{x}_k))| \leq \frac{\pi}{2} - \mu$.

Line minimization

How to compute $\quad t_k \approx \arg\min_{t>0} f(\boldsymbol{x}_k - t\nabla f(\boldsymbol{x}_k)) \quad$?

- Steepest descent: exact minimization.
- Constant step $t_k = t$.
  - Risk of small steps.
  - Does not guarantee that $f(\boldsymbol{x}_k + t\boldsymbol{d}_k) < f(\boldsymbol{x}_k)\ \forall k$.
    $\Rightarrow$ Reajust $t = t/2$.
- Dichotomy, golden section.
- Quadratic approximation of $\phi : t \to f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$.
- Quadratic or cubic approximation of ϕ from the knowledge of $\phi'(0)$.
- Armijo and Wolfe's rules: ensure that t is "acceptable" (sufficient decrease of f, sufficiently large step t).

Line minimization: example

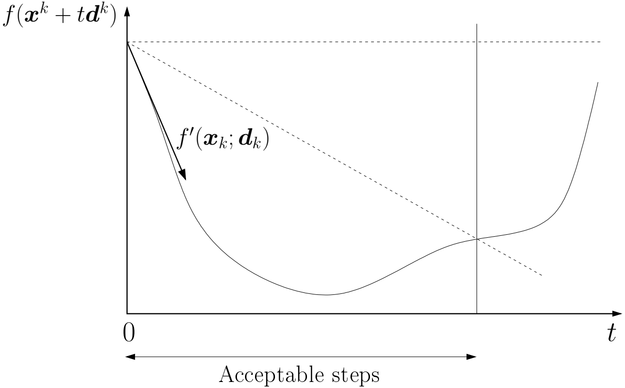
Quadratic interpolator.

Let $\phi(t) := f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$.

Approximate $\phi(t) \approx q(t) = at^2 + bt + c$.

1. Compute $\phi(0) = f(\boldsymbol{x}_k)$.
2. Compute $\phi'(0) = \boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k)$.
3. Compute $\phi(t_0) = f(\boldsymbol{x}_k + t_0\boldsymbol{d}_k)$ for some t_0.
4. Find the quadratic interpolator: compute a, b, c.
5. Minimize $q(t) \quad \Rightarrow t_k$.

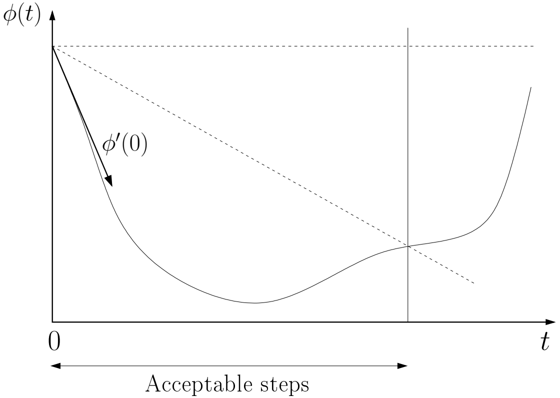
Step selection: Armijo's rule



Choose t such that $\quad f(\boldsymbol{x}_k + t\boldsymbol{d}_k) \leq f(\boldsymbol{x}_k) + c_1\, t\, f'(\boldsymbol{x}_k; \boldsymbol{d}_k)$

with $0 < c_1 < 1$.

Step selection: Armijo's rule

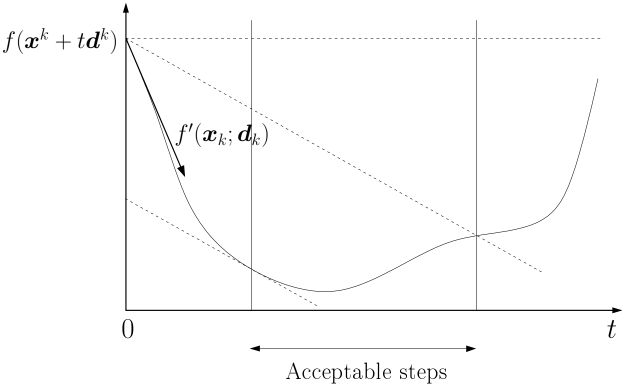


Let $\phi(t) := f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$.

Armijo's condition rewrites $\quad \phi(t) \leq \phi(0) + c_1\, t\, \phi'(0)$

with $\phi'(0) = f'(\boldsymbol{x}_k; \boldsymbol{d}_k) = \nabla f(\boldsymbol{x}_k)^T \boldsymbol{d}_k$.

Step selection: Wolfe's rule



Choose t such that $$\begin{cases} \phi(t) \leq \phi(0) + c_1\, t\, \phi'(0) \\ \phi'(t) \geq c_2\, \phi'(0) \ \text{ with } \ 0 < c_2 < c_1 < 1 \end{cases}$$

Step selection: Wolfe's rule

Choose t such that $\begin{cases} \phi(t) \leq \phi(0) + c_1\, t\, \phi'(0) \\ \phi'(t) \geq c_2\, \phi'(0) \ \text{ with } \ 0 < c_2 < c_1 \end{cases}$

Rewriting:

Choose t such that

$$\begin{cases} f(\boldsymbol{x}_k + t\boldsymbol{d}_k) & \leq \ f(\boldsymbol{x}_k) + c_1\, t\, \nabla f(\boldsymbol{x}_k)^T \boldsymbol{d}_k \\ \nabla f(\boldsymbol{x}_k + t\boldsymbol{d}_k)^T \boldsymbol{d}_k & \geq c_2\, \nabla f(\boldsymbol{x}_k)^T \boldsymbol{d}_k \ \text{ with } \ 0 < c_2 < c_1 \end{cases}$$

Conjugate gradient algorithm

Conjugate gradient.

For $k \geq 0$,

$$\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \beta_k \boldsymbol{d}_k \quad \text{with} \quad \boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k) + \beta_k \boldsymbol{d}_{k-1}.$$

- Fletcher-Reeves: $\beta_k^{\text{FR}} = \dfrac{\|\nabla f(\boldsymbol{x}_k)\|^2}{\|\nabla f(\boldsymbol{x}_{k-1})\|^2}$
- Polak-Ribière: $\beta_k^{\text{PR}} = \dfrac{[\nabla f(\boldsymbol{x}_k)]^T(\nabla f(\boldsymbol{x}_k) - \nabla f(\boldsymbol{x}_{k-1}))}{\|\nabla f(\boldsymbol{x}_{k-1})\|^2}$

Subspace optimization (memory gradient).

$$\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k) + \sum_{\ell=1}^{m} \omega_\ell \boldsymbol{d}_{k-\ell} \quad \text{with} \quad \omega_\ell > 0.$$

Use of second order derivatives

Idea.

1. Replace f by its quadratic approximation at point $\boldsymbol{x}_k$:

$$f(\boldsymbol{x}_k + \boldsymbol{d}) \approx f(\boldsymbol{x}_k) + \boldsymbol{d}^T \nabla f(\boldsymbol{x}_k) + \frac{1}{2}\boldsymbol{d}^T \boldsymbol{H}(\boldsymbol{x}_k)\boldsymbol{d}$$

2. Minimize the quadratic approximation: $\boldsymbol{d}_k = -[\boldsymbol{H}(\boldsymbol{x}_k)]^{-1}\boldsymbol{g}_k$

Works only if $\boldsymbol{H}(\boldsymbol{x}_k) > 0$.

Convex optimization

Newton algorithm.

- Choose $\boldsymbol{x}_0$.
- For $k \geq 0$, do $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k - t_k[\boldsymbol{H}(\boldsymbol{x}_k)]^{-1}\nabla f(\boldsymbol{x}_k)$.

\+ Fast (superlinear) convergence.
– Costly, not suited to large scale applications.

Adaptations

Newton direction: solve $\boldsymbol{H}(\boldsymbol{x}_k)\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k)$.

Truncated Newton direction: solve $\boldsymbol{H}(\boldsymbol{x}_k)\boldsymbol{d}_k \approx -\nabla f(\boldsymbol{x}_k)$:

find $\boldsymbol{d}_k$ s.t. $\|\boldsymbol{H}(\boldsymbol{x}_k)\boldsymbol{d}_k + \nabla f(\boldsymbol{x}_k)\| \leq \eta_k \|\nabla f(\boldsymbol{x}_k)\|$ for $0 < \eta_k < 1$.

Modified Newton direction: when H_k is not invertible, solve

$$[\boldsymbol{H}(\boldsymbol{x}_k) + \lambda_k \boldsymbol{I}_n]\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k)$$

for $\lambda_k > 0$.

Quasi-Newton methods

Idea: Approximate $\boldsymbol{H}(\boldsymbol{x}_k)$, $\boldsymbol{H}(\boldsymbol{x}_k)^{-1}$, or $\boldsymbol{H}(\boldsymbol{x}_k)^{-1}\nabla f(\boldsymbol{x}_k)$ without computing second order derivatives.

Notations:

- $\boldsymbol{g}_k := \nabla f(\boldsymbol{x}_k)$.
- $\boldsymbol{H}_k$: approximation of $\boldsymbol{H}(\boldsymbol{x}_k)$.
- $\boldsymbol{B}_k$: approximation of $[\boldsymbol{H}(\boldsymbol{x}_k)]^{-1}$.

First order Taylor expansion:

$$\nabla f(\boldsymbol{x}_{k+1} + \boldsymbol{h}) = \nabla f(\boldsymbol{x}_{k+1}) + \boldsymbol{H}_{k+1}\boldsymbol{h} + o(\|\boldsymbol{h}\|)$$

$\Rightarrow$ Choose $\boldsymbol{H}_{k+1}$ such that $\boldsymbol{g}_{k+1} - \boldsymbol{g}_k = \boldsymbol{H}_{k+1}(\boldsymbol{x}_{k+1} - \boldsymbol{x}_k)$.

$\Leftrightarrow$ Choose $\boldsymbol{B}_{k+1}$ such that $\boldsymbol{B}_{k+1}(\boldsymbol{g}_{k+1} - \boldsymbol{g}_k) = \boldsymbol{x}_{k+1} - \boldsymbol{x}_k$.

Quasi-Newton algorithm

BFGS algorithm (Broyden, Fletcher, Goldfarb, Shanno):

$\boldsymbol{B}_0 = \boldsymbol{I}_n$ and:

$$\boldsymbol{B}_{k+1} = \boldsymbol{B}_k + \left(1 + \frac{\boldsymbol{p}_k^T \boldsymbol{B}_k \boldsymbol{p}_k}{\boldsymbol{s}_k^T \boldsymbol{p}_k}\right) \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{s}_k^T \boldsymbol{p}_k} - \frac{\boldsymbol{s}_k \boldsymbol{p}_k^T \boldsymbol{B}_k + \boldsymbol{B}_k \boldsymbol{p}_k \boldsymbol{s}_k^T}{\boldsymbol{s}_k^T \boldsymbol{p}_k}$$

with:

- $\boldsymbol{s}_k := \boldsymbol{x}_{k+1} - \boldsymbol{x}_k$.
- $\boldsymbol{p}_k := \nabla f(\boldsymbol{x}_{k+1}) - \nabla f(\boldsymbol{x}_k)$.

Notes.

- $\boldsymbol{B}_k$ is symmetric.
- For strictly convex f, BFGS preserves positive definiteness of $\boldsymbol{B}_k$.

Quasi-Newton algorithm

DFP algorithm (Davidson, Fletcher, Powell):

$\boldsymbol{B}_0 = \boldsymbol{I}_n$ and:

$$\boldsymbol{B}_{k+1} = \boldsymbol{B}_k + \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{s}_k^T \boldsymbol{p}_k} - \frac{\boldsymbol{B}_k \boldsymbol{p}_k \boldsymbol{p}_k^T \boldsymbol{B}_k}{\boldsymbol{p}_k^T \boldsymbol{B}_k \boldsymbol{p}_k}$$

Quasi-Newton algorithm

Choose $\boldsymbol{x}_0$.

Set $\boldsymbol{B}_0 = \boldsymbol{I}_n$.

For $k = 0, 1, 2, \ldots,$

- $\boldsymbol{d}_k = -\boldsymbol{B}_k \boldsymbol{g}_k$.
- $t_k = \arg\min_{t>0} f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$.
- $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + t_k \boldsymbol{d}_k$.
- $\boldsymbol{B}_{k+1} = \boldsymbol{B}_k + \ldots$ (BFGS rule).

End.

L-BFGS algorithm

Large scale problems, *e.g.,* image processing.

Avoid to store the Hessian matrix ($n(n+1)/2$ coefficients).

Recursively update $\boldsymbol{B}_k \boldsymbol{g}_k$.

Matlab implementation: run fminunc

1. Write a Matlab function containing the variables x (here, called z) as the first input and at least one ouput (objective value f):

```
function [f,g] = myobj1(z,beta)

x=z(1);
y=z(2);

f = (y-sin(beta*x)-0.1*x*x)^2;
g(1) = -2*(beta*cos(beta*x)+0.2*x)*(y-sin(beta*x)-0.1*x*x);
g(2) = 2*(y-sin(beta*x) -0.1*x*x);
```

- Name of the file: same as the name of the function (here, `myobj1.m`).
- At least one output (`f`), gradient output `g` is optional.
- Recommendation: to speed up the optimization process, provide `g` as output when computation of `g` is possible.

Matlab implementation: run fminunc

2. Run the Matlab solver . This is another Matlab file, *e.g.,* `runfminunc.m`:

```
clear all; % clear memory
close all; % close figures

beta = 2;

options = optimoptions('fminunc');
options = optimoptions(options,'Display','iter',...
   'MaxFunctionEvaluations',1000,'StepTolerance',1e-10,...
   'SpecifyObjectiveGradient',true,'CheckGradients',true);

% Initial solution
x0=[10;10];

% Compute initial objective value
fprintf('x0=(%.2f,%.2f), f=%f\n',x0(1),x0(2),...
        myobj1(x0,beta));
```

```
% Run optimization solver
xsol = fminunc(@(x)myobj1(x,beta),x0,options);

fprintf('Final solution=(%.2f,%.2f), f=%f\n',...
        xsol(1),xsol(2), myobj1(xsol,beta));

% 2D and 3D display

x=0:.1:6;
y=-1:.1:5;

% Pixel coordinates:
[xx,yy]=meshgrid(x,y);

zz=zeros(size(xx));
for i=1:length(xx(:)),
  zz(i)=myobj1([xx(i),yy(i)],beta);
end;
```

```matlab
% 2D image
figure(1);
imagesc(x,y,zz);
colorbar;
axis xy
xlabel('x'); ylabel('y');

% 3D surface
figure(2);
mesh(x,y,zz);
colormap pink
shading flat
xlabel('x'); ylabel('y');
```

3. Least squares problems

Least squares problems

- Goal: $$\min_{\boldsymbol{x}\in\mathbb{R}^n} \left\{ f(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{F}(\boldsymbol{x})\|_2^2 = \frac{1}{2}\sum_{j=1}^{p} F_j^2(\boldsymbol{x}) \right\}$$

- Residual vector $\boldsymbol{F} : \mathbb{R}^n \mapsto \mathbb{R}^p$:

$$\boldsymbol{F}(\boldsymbol{x}) = \begin{bmatrix} F_1(\boldsymbol{x}) \\ \vdots \\ F_p(\boldsymbol{x}) \end{bmatrix}$$

- $\boldsymbol{F}$ linear with respect to $\boldsymbol{x}$?

  Linear least squares *vs* nonlinear least squares.

Example 1

Predict the parameter of the model which best agrees with a time observation:

- y_j: observation at time t_j.
- p observations.
- $\phi(t;\boldsymbol{x}) = x_1 + t x_2 + t^2 x_3$.

$$\Rightarrow \quad \min_{\boldsymbol{x}\in\mathbb{R}^n} \sum_{j=1}^{p} \left[\phi(t_j;\boldsymbol{x}) - y_j\right]^2.$$

- Linear *vs* nonlinear least-squares?
  - $\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{J}\boldsymbol{x} - \boldsymbol{y}$?

Linear least-squares: $\min_{\boldsymbol{x}\in\mathbb{R}^n} \left\{ f(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{F}(\boldsymbol{x})\|_2^2 = \frac{1}{2}\|\boldsymbol{J}\boldsymbol{x} - \boldsymbol{y}\|_2^2 \right\}$

with:

$$\boldsymbol{F}(\boldsymbol{x}) = \begin{bmatrix} x_1 + t_1 x_2 + t_1^2 x_3 - y_1 \\ x_1 + t_2 x_2 + t_2^2 x_3 - y_2 \\ \vdots \\ x_1 + t_p x_2 + t_p^2 x_3 - y_p \end{bmatrix} \in \mathbb{R}^p$$

$$= \begin{bmatrix} 1 & t_1 & t_1^2 \\ 1 & t_2 & t_2^2 \\ \vdots & \vdots & \vdots \\ 1 & t_p & t_p^2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{bmatrix}$$

$$= \boldsymbol{J}\boldsymbol{x} - \boldsymbol{y}$$

- Linear least-squares problem: $\min_{x \in \mathbb{R}^n} \left\{ f(x) = \frac{1}{2} \|Jx - y\|_2^2 \right\}$

- Gradient: $\nabla f(x) = J^T(Jx - y)$.

- Solution:

$$\begin{aligned} \nabla f(x^\star) = \mathbf{0} \quad &\Longleftrightarrow \quad J^T(Jx^\star - y) = \mathbf{0} \\ &\Longleftrightarrow \quad (J^T J)x^\star = J^T y \quad \text{(normal equations).} \\ &\Longleftrightarrow \quad x^\star = (J^T J)^{-1} J^T y. \end{aligned}$$

Example 2

Predict the parameter of the model which best agrees with a time observation:

- y_j: observation at time t_j.
- P observations.
- $\phi(t;\boldsymbol{x}) = x_1 + t x_2 + t^2 x_3 + x_4 e^{-x_5 t}$.

$$\Rightarrow \quad \min_{\boldsymbol{x}\in\mathbb{R}^n} \sum_{j=1}^{P} \left[\phi(t_j;\boldsymbol{x}) - y_j\right]^2.$$

- Nonlinear least-squares

Nonlinear least-squares: $\displaystyle \min_{\boldsymbol{x}\in\mathbb{R}^n} \left\{ f(\boldsymbol{x}) = \frac{1}{2}\|F(\boldsymbol{x})\|_2^2 \right\}$

with:

$$\boldsymbol{F}(x_1, x_2, x_3, x_4, x_5) = \begin{bmatrix} F_1(x_1, x_2, x_3, x_4, x_5) \\ F_2(x_1, x_2, x_3, x_4, x_5) \\ \vdots \\ F_p(x_1, x_2, x_3, x_4, x_5) \end{bmatrix}$$

$$= \begin{bmatrix} x_1 + t_1 x_2 + t_1^2 x_3 + x_4 e^{-x_5 t_1} - y_1 \\ x_1 + t_2 x_2 + t_2^2 x_3 + x_4 e^{-x_5 t_2} - y_2 \\ \vdots \\ x_1 + t_p x_2 + t_p^2 x_3 + x_4 e^{-x_5 t_p} - y_p \end{bmatrix} \in \mathbb{R}^p$$

Nonlinear least-squares

- Objective function: $f(\boldsymbol{x}) = \dfrac{1}{2} \displaystyle\sum_{j=1}^{p} F_j^2(\boldsymbol{x})$.
- Partial derivatives: $\dfrac{\partial f}{\partial x_i}(\boldsymbol{x}) = \displaystyle\sum_{j=1}^{p} \dfrac{\partial F_j}{\partial x_i}(\boldsymbol{x}) \, F_j(\boldsymbol{x})$
- Gradient:

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial F_1}{\partial x_1}(\boldsymbol{x}) & \frac{\partial F_2}{\partial x_1}(\boldsymbol{x}) & \dots & \frac{\partial F_p}{\partial x_1}(\boldsymbol{x}) \\ \frac{\partial F_1}{\partial x_2}(\boldsymbol{x}) & \frac{\partial F_2}{\partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial F_p}{\partial x_2}(\boldsymbol{x}) \\ \vdots & \vdots & \vdots & \\ \frac{\partial F_1}{\partial x_p}(\boldsymbol{x}) & \frac{\partial F_2}{\partial x_p}(\boldsymbol{x}) & \dots & \frac{\partial F_p}{\partial x_p}(\boldsymbol{x}) \end{bmatrix} \begin{bmatrix} F_1(\boldsymbol{x}) \\ F_2(\boldsymbol{x}) \\ \vdots \\ F_p(\boldsymbol{x}) \end{bmatrix}$$

Gradient and Jacobian

Jacobian $\boldsymbol{J}(\boldsymbol{x})$ is a matrix of size $p \times n$ whose rows identify with $\nabla F_j(\boldsymbol{x})$:

$$\boldsymbol{J}(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial F_1}{\partial x_1}(\boldsymbol{x}) & \frac{\partial F_1}{\partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial F_1}{\partial x_n}(\boldsymbol{x}) \\ \frac{\partial F_2}{\partial x_1}(\boldsymbol{x}) & \frac{\partial F_2}{\partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial F_2}{\partial x_n}(\boldsymbol{x}) \\ \vdots & \vdots & \vdots & \\ \frac{\partial F_p}{\partial x_1}(\boldsymbol{x}) & \frac{\partial F_p}{\partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial F_p}{\partial x_n}(\boldsymbol{x}) \end{bmatrix}$$

$$\boxed{\nabla f(\boldsymbol{x}) = \left[\boldsymbol{J}(\boldsymbol{x})\right]^T \boldsymbol{F}(\boldsymbol{x})}.$$

Second order derivatives

- Partial derivatives: $\dfrac{\partial f}{\partial x_i} = \displaystyle\sum_{k=1}^{p} \dfrac{\partial F_k}{\partial x_i} F_k$

- Second order derivatives:

$$\frac{\partial^2 f}{\partial x_i \, \partial x_j} = \sum_{k=1}^{p} \frac{\partial F_k}{\partial x_i} \frac{\partial F_k}{\partial x_j} + \sum_{k=1}^{p} F_k \frac{\partial^2 F_k}{\partial x_i \, \partial x_j}.$$

- Hessian of f: $\boldsymbol{H}(\boldsymbol{x}) = \nabla^2 f(\boldsymbol{x}) = \begin{bmatrix} \cdots & \cdots & \cdots \\ \cdots & \frac{\partial^2 f}{\partial x_i \, \partial x_j} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} \in \mathbb{R}^{n \times n}$

$$\Longrightarrow \boxed{\boldsymbol{H}(\boldsymbol{x}) = \boldsymbol{J}(\boldsymbol{x})^T \boldsymbol{J}(\boldsymbol{x}) + \sum_{k=1}^{p} \boldsymbol{F}_k \boldsymbol{H}_k}$$

Gauss-Newton method

The gradient and Hessian of $f(\boldsymbol{x}) = \dfrac{1}{2}\sum_{j=1}^{p} F_j^2(\boldsymbol{x})$ read:

$$\nabla f(\boldsymbol{x}) = \left[\boldsymbol{J}(\boldsymbol{x})\right]^T \boldsymbol{F}(\boldsymbol{x})$$

$$\boldsymbol{H}(\boldsymbol{x}) = \boldsymbol{J}(\boldsymbol{x})^T \boldsymbol{J}(\boldsymbol{x}) + \sum_{k=1}^{p} \boldsymbol{F}_k \boldsymbol{H}_k$$

1. Approximate $\boldsymbol{H} \approx \boldsymbol{J}(\boldsymbol{x})^T \boldsymbol{J}(\boldsymbol{x})$.
2. Compute descent direction by solving

$$[\boldsymbol{J}(\boldsymbol{x}_k)^T \boldsymbol{J}(\boldsymbol{x}_k)]\boldsymbol{d}_k = -\boldsymbol{J}(\boldsymbol{x}_k)^T \boldsymbol{F}(\boldsymbol{x}_k)$$

3. Line search:

$$\min_{t>0} f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$$

Gauss-Newton method

Validity.

- When residuals are small ($\boldsymbol{F}(\boldsymbol{x}) \approx \mathbf{0}$).
- When $F_j(\boldsymbol{x})$ are nearly linear.

Advantages.

- Numerical cost is cheap (no calculation of second order derivatives).
- When $\boldsymbol{J}(\boldsymbol{x}_k)$ has full rank and $\nabla f(\boldsymbol{x}) \neq \mathbf{0}$, $\boldsymbol{d}_k$ is a descent direction for f.

The Levenberg-Marquardt method

1. Approximate $\boldsymbol{H} \approx \boldsymbol{J}(\boldsymbol{x})^T \boldsymbol{J}(\boldsymbol{x}) + \lambda \boldsymbol{I}_n$ for some $\lambda \geq 0$.
2. Compute descent direction by solving
$$[\boldsymbol{J}(\boldsymbol{x}_k)^T \boldsymbol{J}(\boldsymbol{x}_k) + \lambda_k \boldsymbol{I}_n] \boldsymbol{d}_k = -\boldsymbol{J}(\boldsymbol{x}_k)^T \boldsymbol{F}(\boldsymbol{x}_k)$$
3. Line search:
$$\min_{t>0} f(\boldsymbol{x}_k + t\boldsymbol{d}_k)$$

Comments.

- Case where $J(\boldsymbol{x})$ is rank-deficient, or nearly so.
- $\lambda_k = 0$: Gauss-Newton method.
- $\lambda_k \to \infty$: the gradient algorithm (slower but numerically accurate).
- There are automatic strategies for tuning λ_k.

Matlab implementation: run lsqnonlin

1. Write a Matlab function containing the variables x as the first input and at least one ouput (residual vector $\boldsymbol{F}(\boldsymbol{x})$):

```
function [F,J] = residuals(x,t,y)

% residual vector
F = y-x(1)*exp(-t/x(2)); % same size as y

% Jacobian matrix of size (length(t) x length(x))
% Column 1:  derivative of F_i = y_i - x_1 exp(-t_i/x_2) w.r.t.  x_1
% Column 2:  derivative of F_i = y_i - x_1 exp(-t_i/x_2) w.r.t.  x_2
J = [-exp(-t/x(2)), -x(1)/(x(2)*x(2))*t.*exp(-t./x(2))];
```

- Name of the file: `residuals.m`.
- At least one output (`F`), Jacobian output `J` is optional.
- Recommendation: to speed up the optimization process, provide `J` as output when computation of `J` is easy.

Matlab implementation: run lsqnonlin

2. Run the Matlab solver. This is another Matlab file, *e.g.,* `fit_expo.m`:

```
% load data t and y, defined as column vectors
figure(1), clf, plot(t,y,'o','linewidth',2); grid on;

% Initial parameter values
x_init = [10,10];

opt = optimoptions('lsqnonlin');
opt = optimoptions(opt,'Display','iter');

% If Jacobian is provided as output of function "residuals"
opt = optimoptions(opt,'SpecifyObjectiveGradient',true);

% for debug only, checks that the Jacobian computation
% is correct:
% opt = optimoptions(opt,'CheckGradients',true);
```

```
% Run optimization solver

x = lsqnonlin(@(x)(residuals(x,t,y)),x_init,[],[],opt);

disp('Solution:'); fprintf('%.2f ',x'); disp(' ');

% Plot prediction of data y using model x1 exp(-t/x2)
figure(1), hold on,
plot(t,x(1)*exp(-t/x(2)),'-r','linewidth',2);

% One could also plot the prediction of data y
% using the initial parameters x_init which is less accurate

% plot(t,x_init(1)*exp(-t/x_init(2)),'-g','linewidth',2);
```

4. Constrained local optimization

Constrained minimization

Minimize $f(\boldsymbol{x})$ **subject to** $\begin{cases} g_i(\boldsymbol{x}) \leq 0, & i = 1, \ldots, p \\ h_j(\boldsymbol{x}) = 0, & j = 1, \ldots, q. \end{cases}$

Case of linear constraints:

- Each constraint reads $g_i(\boldsymbol{x}) = \boldsymbol{a}_i^T \boldsymbol{x} - b_i = \sum_{k=1}^{n} a_i(k) x(k) - b_i$.
- Matrix form: $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} - \boldsymbol{b} \leq \mathbf{0}_p$ with $\boldsymbol{A} \in \mathbb{R}^{p \times n}$.
- Similarly, write $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{C}\boldsymbol{x} - \boldsymbol{d}$.

- Matlab: $\boldsymbol{A}$, $\boldsymbol{b}$, $\boldsymbol{C}$, $\boldsymbol{d}$ are provided as inputs of fmincon.
- Case of lower ($x_k \geq \ell_k$) and upper bounds ($x_k \leq u_k$): compute corresponding $\boldsymbol{a}_i$ and b_i.

Constrained minimization

Minimize $f(x)$ **subject to** $\begin{cases} g_i(x) \leq 0, & i = 1, \ldots, p \\ h_j(x) = 0, & j = 1, \ldots, q. \end{cases}$

Case of nonlinear constraints (Matlab):

- Write a function

  ```
  [g,h] = function mycon(x);
  ```

  returning the values of $g_i(x)$ and $h_i(x)$ for all nonlinear constraints.

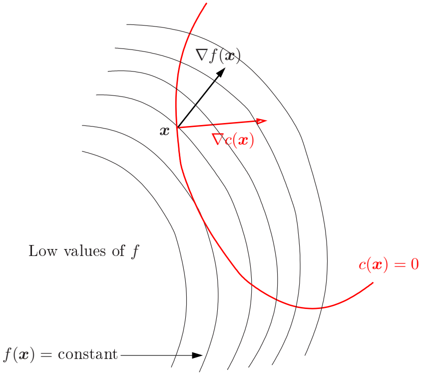
- Provide this function as input of `fmincon`.

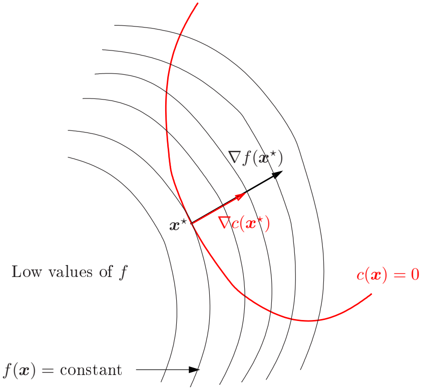
Existence of a minimizer

We will assume that functions f, g_i and h_j are twice differentiable.

If the feasible set $\mathcal{D} = \{\boldsymbol{x} \in \mathbb{R}^n,\, \boldsymbol{g}(\boldsymbol{x}) \leq \mathbf{0}_p,\, \boldsymbol{h}(\boldsymbol{x}) = \mathbf{0}_q\}$ is non-empty and bounded, then there exists a minimizer.

Case of 1 equality constraint $c(\boldsymbol{x}) = 0$





At the optimal point $\boldsymbol{x}^\star$, $\boxed{\nabla f(\boldsymbol{x}^\star) = \lambda \nabla c(\boldsymbol{x}^\star)}$ for some λ.

Generalization for q equality constraints

Problem with equality constraints only:

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} \quad f(\boldsymbol{x}) \quad \text{s.t.} \quad \begin{cases} h_1(\boldsymbol{x}) = 0 \\ h_2(\boldsymbol{x}) = 0 \\ \quad \vdots \\ h_q(\boldsymbol{x}) = 0 \end{cases}$$

Define the Lagrangian function for $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{\lambda} \in \mathbb{R}^q$:

$$\boxed{\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) - \lambda_1 h_1(\boldsymbol{x}) - \ldots - \lambda_q h_q(\boldsymbol{x})}$$

$\boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_q \end{bmatrix}$ are Lagrange multipliers.

First order optimality conditions

Lagrangian: $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) - \sum_{i=1}^{q} \lambda_i h_i(\boldsymbol{x})$

If $\boldsymbol{x}^\star$ is a local minimizer of f, then there exists $\boldsymbol{\lambda}^\star$ such that:

$$\left\{ \begin{array}{l} \nabla_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}^\star, \boldsymbol{\lambda}^\star) = \mathbf{0}_n \\ \\ \nabla_{\boldsymbol{\lambda}} \mathcal{L}(\boldsymbol{x}^\star, \lambda^\star) = \mathbf{0}_q \end{array} \right. \iff \left\{ \begin{array}{l} \nabla f(\boldsymbol{x}^\star) = \sum_{i=1}^{q} \lambda_i^\star \nabla h_i(\boldsymbol{x}^\star) \\ \\ h_1(\boldsymbol{x}^\star) = \ldots = h_q(\boldsymbol{x}^\star) = 0 \end{array} \right.$$

Example: $\min_{\boldsymbol{x} \in \mathbb{R}^2} \; (x_1^2 + x_2^2) \quad \text{s.t.} \quad x_1 + x_2 = 1$

1. Graphical representation.
2. Write the optimality conditions.
3. Solve the system.

Inequality constrained problems

Problem.

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \; f(\boldsymbol{x}) \quad \text{s.t.} \quad \begin{cases} g_1(\boldsymbol{x}) \leq 0 \\ g_2(\boldsymbol{x}) \leq 0 \\ \quad\vdots \\ g_p(\boldsymbol{x}) \leq 0 \end{cases}$$

Definition.

The i-th constraint is active at $\boldsymbol{x}$ if $g_i(\boldsymbol{x}) = 0$.

The i-th constraint is inactive at $\boldsymbol{x}$ if $g_i(\boldsymbol{x}) < 0$.

Lagrangian function

Problem with inequality constraints only:

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad f(\boldsymbol{x}) \quad \text{s.t.} \quad \begin{cases} g_1(\boldsymbol{x}) \geq 0 \\ g_2(\boldsymbol{x}) \geq 0 \\ \quad\vdots \\ g_p(\boldsymbol{x}) \geq 0 \end{cases}$$

Define the Lagrangian function for $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{\lambda} \in \mathbb{R}_+^p$:

$$\boxed{\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) - \lambda_1 g_1(\boldsymbol{x}) - \ldots - \lambda_p g_p(\boldsymbol{x})}$$

$$\boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_p \end{bmatrix} \geq \mathbf{0} \qquad \text{are Lagrange multipliers.}$$

Lagrangian function (bis)

Modified Problem:

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad f(\boldsymbol{x}) \quad \text{s.t.} \quad \begin{cases} g_1(\boldsymbol{x}) & \leq & 0 \\ g_2(\boldsymbol{x}) & \leq & 0 \\ & \vdots & \\ g_p(\boldsymbol{x}) & \leq & 0 \end{cases}$$

Define the Lagrangian function for $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{\lambda} \in \mathbb{R}_+^p$:

$$\boxed{\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \lambda_1 g_1(\boldsymbol{x}) + \ldots + \lambda_p g_p(\boldsymbol{x})}$$

$$\boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_p \end{bmatrix} \geq \mathbf{0} \quad \text{are Lagrange multipliers.}$$

Karush-Kuhn-Tucker (KKT) conditions

If $\boldsymbol{x}^\star$ is a local solution of

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \text{ s.t. } \boldsymbol{g}(\boldsymbol{x}) \geq \mathbf{0}_p$$

then there exists $\boldsymbol{\lambda}^\star$ such that:

$$\begin{cases} \nabla_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}^\star, \lambda^\star) = \mathbf{0}_n \iff \nabla f(\boldsymbol{x}^\star) = \sum_{i=1}^{p} \lambda_i^\star \nabla g_i(\boldsymbol{x}^\star) \\ \forall i,\ g_i(\boldsymbol{x}^\star) \geq 0 \\ \forall i,\ \lambda_i^\star \geq 0 \\ \forall i,\ \lambda_i^\star g_i(\boldsymbol{x}^\star) = 0 \end{cases}$$

$$\left(\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) - \sum_{i=1}^{p} \lambda_i g_i(\boldsymbol{x}) \right)$$

Karush-Kuhn-Tucker (KKT) conditions

If $\boldsymbol{x}^\star$ is a local solution of

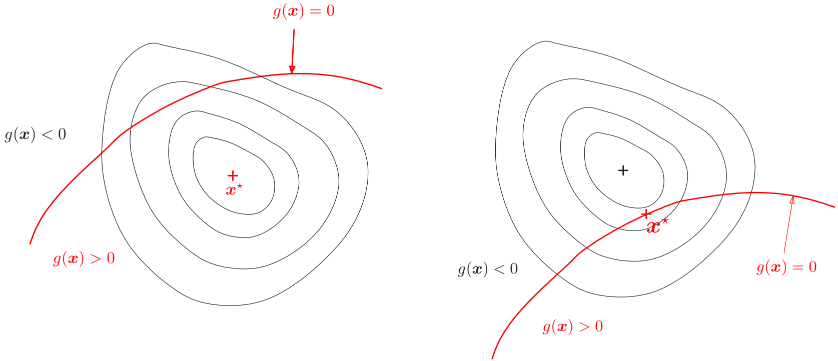
$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \ \text{ s.t. } \ \boldsymbol{g}(\boldsymbol{x}) \leq \mathbf{0}_p$$

then there exists $\boldsymbol{\lambda}^\star$ such that:

$$\begin{cases} \nabla_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}^\star, \boldsymbol{\lambda}^\star) = \mathbf{0}_n \iff \nabla f(\boldsymbol{x}^\star) = -\sum_{i=1}^{p} \lambda_i^\star \nabla g_i(\boldsymbol{x}^\star) \\ \forall i,\ g_i(\boldsymbol{x}^\star) \leq 0 \\ \forall i,\ \lambda_i^\star \geq 0 \\ \forall i,\ \lambda_i^\star g_i(\boldsymbol{x}^\star) = 0 \end{cases}$$

$$\Big(\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \sum_{i=1}^{p} \lambda_i g_i(\boldsymbol{x}) \Big)$$

Case of 1 inequality constraint $g(x) \geq 0$



Inactive constraint: $g(x^\star) > 0$

$\lambda^\star = 0$

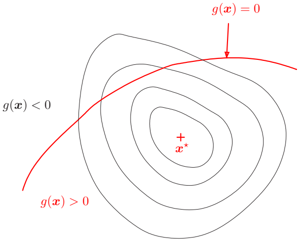
$(\lambda^\star g(x^\star) = 0)$

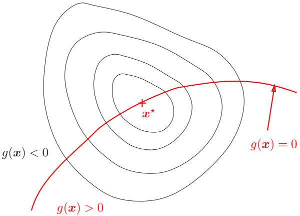
Active constraint: $g(x^\star) = 0$

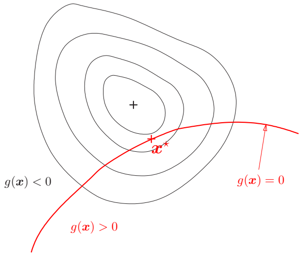
$\lambda^\star > 0$

$(\lambda^\star g(x^\star) = 0)$

Inequality constraints







Inactive	Weakly active	Active
$\lambda^\star = 0$	$\lambda^\star = 0$	$\lambda^\star > 0$
$g(\boldsymbol{x}^\star) > 0$	$g(\boldsymbol{x}^\star) = 0$	$g(\boldsymbol{x}^\star) = 0$

Examples

Example 1: $$\min_{\boldsymbol{x}\in\mathbb{R}^2} \; x_1^2 + x_2^2 \quad \text{s.t.} \quad \begin{cases} x_1 \geq 0 \\ x_2 \geq 0 \\ x_1 + 2x_2 \geq 1. \end{cases}$$

Example 2: [Nocedal & Wright, 2006, p. 329]

$$\min_{\boldsymbol{x}\in\mathbb{R}^2} \; \left(x_1 - \frac{3}{2}\right)^2 + \left(x_2 - \frac{1}{8}\right)^4 \quad \text{s.t.} \quad \begin{cases} x_2 \leq 1 - x_1 \\ x_2 \geq -1 - x_1 \\ x_2 \geq x_1 - 1 \\ x_2 \leq x_1 + 1 \end{cases}$$

1. Graphical representation.
2. Write the optimality conditions.
3. Solve the system.

Necessary condition for a local minimizer

First order optimality condition.

If $\boldsymbol{x}^\star$ is local minimizer, then $\boldsymbol{x}^\star$ satisfies the KKT conditions.

Second order optimality condition.

- Let $\mathcal{A}(\boldsymbol{x})$ denote the set of active constraints at $\boldsymbol{x}$
- Let $\mathcal{F}(\boldsymbol{x})$ denote the set of feasible directions at $\boldsymbol{x}$.
- Let $\mathcal{C}(\boldsymbol{x},\boldsymbol{\lambda}) = \{\boldsymbol{w} \in \mathcal{F}(\boldsymbol{x}) \mid [\nabla g_i(\boldsymbol{x})]^T \boldsymbol{w} = 0 \, \forall i \in \mathcal{A}(\boldsymbol{x}) \text{ with } \lambda_i > 0.\}$

If $\boldsymbol{x}^\star$ satisfies the KKT conditions and

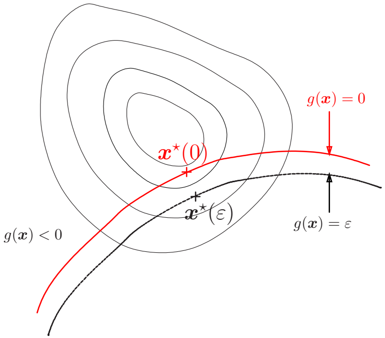
$$\forall \boldsymbol{w} \in \mathcal{C}(\boldsymbol{x}^\star,\boldsymbol{\lambda}^\star)\backslash\{\mathbf{0}\},\ \boldsymbol{w}^T \nabla_{\boldsymbol{xx}} \mathcal{L}(\boldsymbol{x}^\star,\boldsymbol{\lambda}^\star)\boldsymbol{w} > 0$$

then $\boldsymbol{x}^\star$ is a strict local minimizer of the inequality constrained problem.

Interpretation of Lagrange multipliers

For $\varepsilon > 0$, let $\boldsymbol{x}^\star(\varepsilon) = \arg\min_{\boldsymbol{x}} f(\boldsymbol{x}) \ \texttt{s.t.} \ g(\boldsymbol{x}) \geq \varepsilon$.

Let $f^\star(\varepsilon) = f(\boldsymbol{x}^\star(\varepsilon))$. Then, $\boxed{\lambda^\star \|\nabla g(\boldsymbol{x}^\star)\| = \frac{\partial f^\star}{\partial \varepsilon}(\varepsilon = 0)}$.



General case: inequality and equality constraints

Problem: $\min_{\boldsymbol{x}\in\mathbb{R}^n} \; f(\boldsymbol{x}) \;$ s.t. $\begin{cases} g_i(\boldsymbol{x}) \geq 0, & i = 1,\ldots,p \\ h_j(\boldsymbol{x}) = 0, & j = 1,\ldots,q. \end{cases}$

Define the Lagrangian function for $\boldsymbol{x} \in \mathbb{R}^n$, $\boldsymbol{\lambda} \in \mathbb{R}_+^p$, $\boldsymbol{\mu} \in \mathbb{R}^q$:

$$\boxed{\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\mu}) = f(\boldsymbol{x}) - \sum_{i=1}^{p} \lambda_i g_i(\boldsymbol{x}) - \sum_{i=1}^{q} \mu_j h_j(\boldsymbol{x})}$$

So, $\nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\mu}) = \nabla f(\boldsymbol{x}) - \sum_{i=1}^{p} \lambda_i \nabla g_i(\boldsymbol{x}) - \sum_{j=1}^{q} \mu_j \nabla h_j(\boldsymbol{x})$

KKT conditions

Problem: $\min_{\boldsymbol{x}\in\mathbb{R}^n} \; f(\boldsymbol{x}) \;$ s.t. $\begin{cases} g_i(\boldsymbol{x}) \geq 0, & i = 1, \ldots, p \\ h_j(\boldsymbol{x}) = 0, & j = 1, \ldots, q. \end{cases}$

If $\boldsymbol{x}^\star$ is a local minimizer, then there exists $\boldsymbol{\lambda}^\star$ and $\mu^\star$ such that:

$$\begin{cases} \nabla_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}^\star, \boldsymbol{\lambda}^\star, \boldsymbol{\mu}^\star) = \mathbf{0}_n \\ \forall i, \; g_i(\boldsymbol{x}^\star) \geq 0 \\ \forall j, \; h_j(\boldsymbol{x}^\star) = 0 \\ \forall i, \; \lambda_i^\star \geq 0 \\ \forall i, \; \lambda_i^\star \, g_i(\boldsymbol{x}^\star) = 0 \end{cases}$$

Example

$$\min_{\boldsymbol{x}\in\mathbb{R}^2} \; (4x_1^2 + 2x_2^2) \;\text{ s.t. }\; \begin{cases} 3x_1 + x_2 = 8 \\ 2x_1 + 4x_2 \leq 15 \end{cases}$$

- $\mathcal{L}(x_1, x_2, \lambda, \mu) = 4x_1^2 + 2x_2^2 + \lambda(2x_1 + 4x_2 - 15) - \mu(3x_1 + x_2 - 8)$.
- $\frac{\partial \mathcal{L}}{\partial x_1}(x_1, x_2, \lambda, \mu) = 8x_1 + 2\lambda - 3\mu$.
- $\frac{\partial \mathcal{L}}{\partial x_2}(x_1, x_2, \lambda, \mu) = 4x_2 + 4\lambda - \mu$.
- KKT conditions: $$\begin{cases} 8x_1 + 2\lambda - 3\mu = 0 \\ 4x_2 + 4\lambda - \mu = 0 \\ 3x_1 + x_2 = 8 \\ 2x_1 + 4x_2 \leq 15 \\ \lambda \geq 0 \\ \lambda\,(2x_1 + 4x_2 - 15) = 0 \end{cases}$$

$$\left\{\begin{array}{rcl} 8x_1+2\lambda-3\mu &=& 0\\ 4x_2+4\lambda-\mu &=& 0\\ 3x_1+x_2 &=& 8\\ 2x_1+4x_2 &\leq& 15\\ \lambda &\geq& 0\\ \lambda\,(2x_1+4x_2-15) &=& 0 \end{array}\right. \Longrightarrow \left\{\begin{array}{rcl} 8x_1-12x_2 &=& 10\lambda\\ 3x_1+x_2 &=& 8\\ 2x_1+4x_2 &\leq& 15\\ \lambda &\geq& 0\\ \lambda\,(2x_1+4x_2-15) &=& 0 \end{array}\right.$$

- Assume $2x_1+4x_2=15$. $3x_1+x_2=8$ implies that $x_1=\frac{17}{10}$, $x_2=\frac{29}{10}$. So, $\lambda=\frac{8x_1-12x_2}{10}=-\frac{212}{100}<0$. Contradiction!
- So, $\lambda=0$. The KKT conditions become:

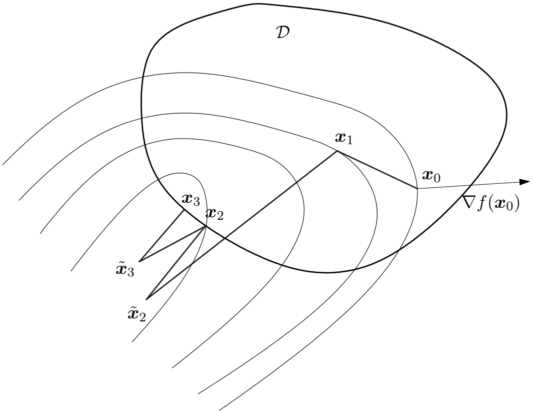
$$\left\{\begin{array}{rcl} \lambda &=& 0\\ \mu &=& \frac{8x_1}{3}\\ \mu &=& 4x_2\\ 3x_1+x_2 &=& 8\\ 2x_1+4x_2 &\leq& 15 \end{array}\right. \Longrightarrow \left\{\begin{array}{rcl} \lambda &=& 0\\ \mu &=& \frac{8x_1}{3}\\ x_1 &=& \frac{3}{2}x_2\\ \frac{11}{2}x_2 &=& 8\\ 2x_1+4x_2 &\leq& 15 \end{array}\right.$$

$$\Longrightarrow \left\{\begin{array}{rcl} \lambda &=& 0\\ \mu &=& \frac{8x_1}{3}\\ x_1 &=& \frac{24}{11}\\ x_2 &=& \frac{16}{11}\\ \text{Constraint}\quad \frac{112}{11} &\leq& 15\ \text{(OK)} \end{array}\right.$$

Gradient projection algorithm

Principle.

1. Line minimization: $\tilde{\boldsymbol{x}}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$.
2. Projection onto convex set: $\boldsymbol{x}_{k+1} = \texttt{proj}(\tilde{\boldsymbol{x}}_{k+1}, \mathcal{D})$.



Other approaches

Interior point approaches.

Example: Replace $\min_{\boldsymbol{x} \geq \mathbf{0}} f(\boldsymbol{x})$ by $\min_{\boldsymbol{x} \in \mathbb{R}^n} \left\{ f(\boldsymbol{x}) - \xi \sum_{i=1}^{n} \log x_i \right\}$.

Constrained minimization is replaced by the unconstrainted minimization of the augmented criterion.

"Exterior" approaches, *e.g.,* quadratic penalty, ADMM.

Example: Replace $\min_{\boldsymbol{x} \geq \mathbf{0}} f(\boldsymbol{x})$ by

$$\min_{\boldsymbol{x}, \boldsymbol{p} \geq \mathbf{0}} \{ \mathcal{K}(\boldsymbol{x}, \boldsymbol{p}; \xi) = f(\boldsymbol{x}) + \xi \|\boldsymbol{x} - \boldsymbol{p}\|^2 \} \text{ with } \xi \to \infty$$

Repeat:

- Minimize $\mathcal{K}$ with respect to $\boldsymbol{x}$ (unconstrained).
- Minimize $\mathcal{K}$ with respect to $\boldsymbol{p}$ (easy): $p_i = \max(x_i, 0)$.

Special case: linear programming

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \ \boldsymbol{c}^T\boldsymbol{x} \ \text{ s.t. } \begin{cases} \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \\ \boldsymbol{x} \geq \mathbf{0} \end{cases}$$

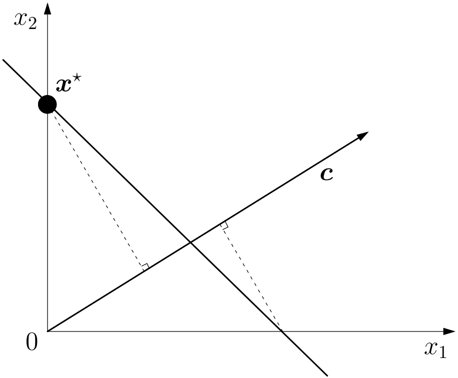
- $\boldsymbol{c} \in \mathbb{R}^n$ with $\boldsymbol{c} \geq \mathbf{0}_n$.
- $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ with $m \leq n$.

Example:

$$\min_{\boldsymbol{x}\in\mathbb{R}^4} \ x_1 + 2x_2 + 3x_3 + 4x_4 \quad \text{s.t.} \quad \begin{cases} x_1 + x_2 + x_3 + x_4 & = & 1 \\ x_1 + x_3 - 3x_4 & = & \frac{1}{2} \\ \boldsymbol{x} & \geq & \mathbf{0}. \end{cases}$$

- Rewrite the problem in matrix form.
- The solution $\boldsymbol{x}$ has two zero coordinates.

Interpretation in terms of orthogonal projections



The solution $x^\star$ has at least ($n - m$) zero coordinates.

Case $n = 2$, $m = 1$: solution has at least one 0 coordinate.

Case $n = 3$, $m = 1$: solution has at least two 0 coordinates.

Case $n = 3$, $m = 2$: solution has at least one 0 coordinate.

Principle of the simplex algorithm

1. Decompose $\boldsymbol{A} = [\boldsymbol{A}_B, \boldsymbol{A}_N]$ with $\boldsymbol{A}_B$ of size $m \times m$, and $\boldsymbol{A}_N$ of size $m \times (n-m)$.

2. Set $\boldsymbol{x}^B = \begin{bmatrix} \mathbf{x}_B \\ \mathbf{0}_{n-m} \end{bmatrix}$ with $\mathbf{x}_B = \boldsymbol{A}_B^{-1}\boldsymbol{b}$ ([1]).

3. $\boldsymbol{x}^B$ is a feasible point if $\mathbf{x}_B \geq \mathbf{0}_m$. The objective function is equal to $f(\boldsymbol{x}^B) = \boldsymbol{c}_B^T \boldsymbol{A}_B^{-1}\boldsymbol{b}$.

4. The simplex algorithm searches for the best decomposition $\boldsymbol{A} = [\boldsymbol{A}_B, \boldsymbol{A}_N]$. The subset B is updated at each iteration in such a way that $f(\boldsymbol{x}^B)$ is decreasing.

---

[1] assuming that the rank of $\boldsymbol{A}$ equals m and that $\boldsymbol{A}_B$ is invertible

Special case: quadratic programming (QP)

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} \quad \mathcal{Q}(\boldsymbol{x}) = \frac{1}{2} \boldsymbol{x}^T \boldsymbol{H} \boldsymbol{x} + \boldsymbol{g}^T \boldsymbol{x} \quad \text{s.t.} \quad \begin{cases} \boldsymbol{a}_i^T \boldsymbol{x} = b_i, \ i \in \mathcal{E} \\ \boldsymbol{a}_i^T \boldsymbol{x} \geq b_i, \ i \in \mathcal{I} \end{cases}$$

- $\boldsymbol{H}$ is symmetric.
- $\boldsymbol{H}$ is symmetric positive semedefinite ($\boldsymbol{x}^T \boldsymbol{H} \boldsymbol{x} \geq 0, \ \forall \boldsymbol{x}$)
  $\Rightarrow$ there exists a minimizer.
- $\boldsymbol{H}$ is symmetric positive definite ($\boldsymbol{x}^T \boldsymbol{H} \boldsymbol{x} > 0, \ \forall \boldsymbol{x} \neq \mathbf{0}$)
  $\Rightarrow$ there exists a unique minimizer.

QP with equality constraints

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \mathcal{Q}(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell}^T\boldsymbol{x} \quad \text{s.t.} \;\; \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$$

1. Assume([2]) that $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ has rank m. Let $\boldsymbol{A} = [\boldsymbol{A}_1, \boldsymbol{A}_2]$ with $\boldsymbol{A}_1 \in \mathbb{R}^{m\times n}$ invertible, and let $\boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix}$. $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ rereads $\boldsymbol{A}_1\boldsymbol{x}_1 + \boldsymbol{A}_2\boldsymbol{x}_2 = \boldsymbol{b}$, so $\boldsymbol{x}_1 = \boldsymbol{A}_1^{-1}(\boldsymbol{b} - \boldsymbol{A}_2\boldsymbol{x}_2)$.

   $\Rightarrow$ Solve unconstrained problem $\displaystyle\min_{\boldsymbol{x}_2} \;\; \mathcal{Q}(\boldsymbol{A}_1^{-1}(\boldsymbol{b} - \boldsymbol{A}_2\boldsymbol{x}_2), \boldsymbol{x}_2)$.

2. KKT conditions with $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = \dfrac{1}{2}\boldsymbol{x}^T\boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell}^T\boldsymbol{x} - \boldsymbol{\lambda}^T(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})$:

   Solve system

$$\begin{cases} \boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell} - \boldsymbol{A}^T\boldsymbol{\lambda} = \mathbf{0} \\ \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \end{cases} \iff \begin{bmatrix} \boldsymbol{H} & -\boldsymbol{A}^T \\ \boldsymbol{A} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -\boldsymbol{\ell} \\ \boldsymbol{b} \end{bmatrix}$$

[2] without loss of generality

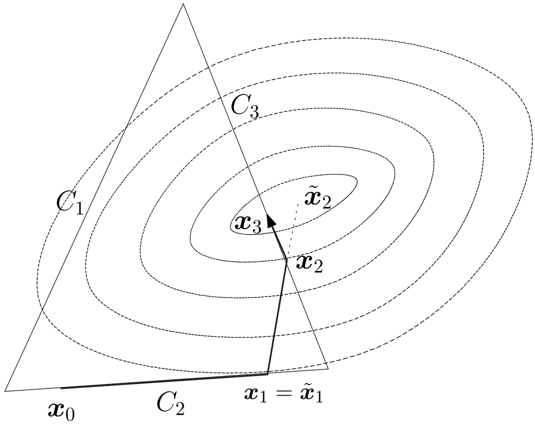
QP with inequality constraints

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \mathcal{Q}(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell}^T\boldsymbol{x} \quad \text{s.t. } \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{b}$$

Principle of the active-set algorithm.

1. Solve a sequence of QP problems with equality constraints.
2. Use a mechanism to add or remove active constraints.

The active set $\mathcal{A}(\boldsymbol{x}) = \{i : \boldsymbol{a}_i^T\boldsymbol{x} = b_i\}$ is defined as the set of active constraints at $\boldsymbol{x}$.



From a feasible point $\boldsymbol{x}_k$:

1. Solve QP with equality constraints on $\mathcal{A}(\boldsymbol{x}_k)$ only $\Rightarrow \tilde{\boldsymbol{x}}_{k+1}$.
2. If $\tilde{\boldsymbol{x}}_{k+1}$ is feasible, set $\boldsymbol{x}_{k+1} \leftarrow \tilde{\boldsymbol{x}}_{k+1}$. Compute the Lagrange multipliers $\{\lambda_i,\ i \in \mathcal{A}(\boldsymbol{x}_k)\}$. If some $\lambda_i < 0$, set $\mathcal{A}(\boldsymbol{x}_{k+1}) \leftarrow \mathcal{A}(\boldsymbol{x}_k) \backslash \{\arg\min_{i \in \mathcal{A}(\boldsymbol{x}_k)} \lambda_i\}$ and go back to step 1. Else, STOP.
3. Otherwise, set $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \alpha_k(\tilde{\boldsymbol{x}}_{k+1} - \boldsymbol{x}_k)$ with the maximum possible value of $\alpha_k \in]0, 1[$. Compute $\mathcal{A}(\boldsymbol{x}_{k+1})$ and go back to step 1.

Step 1

QP: $\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \mathcal{Q}(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell}^T\boldsymbol{x} \quad \text{s.t.} \;\; \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{b}$

QP with equality constraints: here, the inequality constraints are removed.

Define $\boldsymbol{A}_{\mathcal{A}} = \boldsymbol{A}(\mathcal{A}, :)$ and $\delta = \boldsymbol{x} - \boldsymbol{x}_k$ the descent direction.

$$\boxed{\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \mathcal{Q}(\boldsymbol{x}) \quad \text{s.t.} \;\; \boldsymbol{A}_{\mathcal{A}}\boldsymbol{x} = \boldsymbol{b}_{\mathcal{A}}}$$

$$\Leftrightarrow \quad \min_{\boldsymbol{\delta}\in\mathbb{R}^n} \quad \mathcal{Q}(\boldsymbol{x}_k + \boldsymbol{\delta}) = \mathcal{Q}(\boldsymbol{x}_k) + \mathcal{Q}(\boldsymbol{\delta}) + \boldsymbol{x}_k^T\boldsymbol{H}^T\boldsymbol{\delta} \quad \text{s.t.} \;\; \boldsymbol{A}_{\mathcal{A}}\boldsymbol{\delta} = \mathbf{0}$$

$$\Leftrightarrow \quad \min_{\boldsymbol{\delta}\in\mathbb{R}^n} \quad \frac{1}{2}\boldsymbol{\delta}^t\boldsymbol{H}\boldsymbol{\delta} + (\boldsymbol{H}\boldsymbol{x}_k + \boldsymbol{\ell})^T\boldsymbol{\delta} \quad \text{s.t.} \;\; \boldsymbol{A}_{\mathcal{A}}\boldsymbol{\delta} = \mathbf{0}.$$

Step 2: check KKT conditions for QP

Lagrangian of $\min_{\boldsymbol{x}\in\mathbb{R}^n} \mathcal{Q}(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell}^T\boldsymbol{x} \quad \text{s.t. } \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{b}$:

$$\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell}^T\boldsymbol{x} - \boldsymbol{\lambda}^T\boldsymbol{A}\boldsymbol{x} + \boldsymbol{\lambda}^T\boldsymbol{b}$$

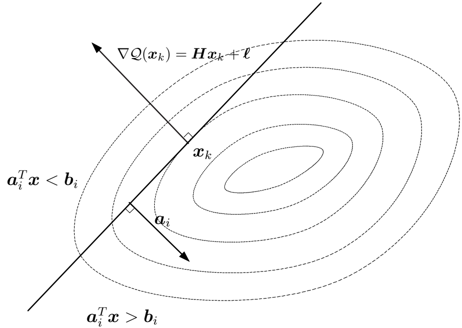
KKT conditions with $\boldsymbol{x} = \boldsymbol{x}_{k+1} \Rightarrow$

$$\left\{ \begin{aligned} \boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell} - \boldsymbol{A}^T\boldsymbol{\lambda} &= \mathbf{0} \\ \boldsymbol{A}_{\mathcal{A}}\boldsymbol{x} &= \boldsymbol{b}_{\mathcal{A}} \\ \boldsymbol{\lambda}_{\mathcal{A}} &\geq \mathbf{0} \\ \boldsymbol{A}_{\overline{\mathcal{A}}}\boldsymbol{x} &\geq \boldsymbol{b}_{\overline{\mathcal{A}}} \\ \boldsymbol{\lambda}_{\overline{\mathcal{A}}} &= \mathbf{0} \end{aligned} \right.$$

$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{A}_{\mathcal{A}} \\ \boldsymbol{A}_{\overline{\mathcal{A}}} \end{bmatrix}$ implies that $\boldsymbol{A}^T\boldsymbol{\lambda} = \left[\boldsymbol{A}_{\mathcal{A}}^T, \boldsymbol{A}_{\overline{\mathcal{A}}}^T\right] \begin{bmatrix} \boldsymbol{\lambda}_{\mathcal{A}} \\ \mathbf{0} \end{bmatrix} = \boldsymbol{A}_{\mathcal{A}}^T\boldsymbol{\lambda}_{\mathcal{A}}$.

So, the KKT condition becomes $\boxed{\boldsymbol{\lambda}_{\mathcal{A}} = \left[\boldsymbol{A}_{\mathcal{A}}^T\right]^{\dagger}(\boldsymbol{H}\boldsymbol{x} + \boldsymbol{\ell}) \geq \mathbf{0}}$

Case of an active-set with one constraint

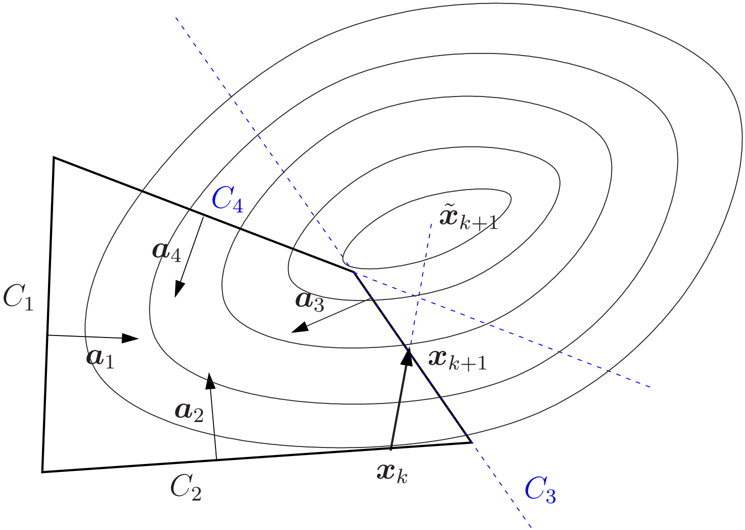


When $\mathcal{A} = \{i\}$ contains only one constraint, $\boldsymbol{a}_i$ is colinear with $\nabla\mathcal{Q}(\boldsymbol{x}_k) = \boldsymbol{H}\boldsymbol{x}_k + \boldsymbol{\ell}$, and

$$\lambda_i = \left[\boldsymbol{A}_{\mathcal{A}}^T\right]^\dagger (\boldsymbol{H}\boldsymbol{x}_k + \boldsymbol{\ell}) = [\boldsymbol{a}_i]^\dagger (\boldsymbol{H}\boldsymbol{x}_k + \boldsymbol{\ell}) = \frac{1}{\|\boldsymbol{a}_i\|^2}\, \boldsymbol{a}_i^T(\boldsymbol{H}\boldsymbol{x}_k + \boldsymbol{\ell}).$$

$\lambda_i < 0$ means that the i-th constraint may be removed

Step 3: illustration



Step 3: compute $\boldsymbol{x}_k + \alpha_k(\tilde{\boldsymbol{x}}_{k+1} - \boldsymbol{x}_k)$

It is easy to check that $\boldsymbol{x}_k + \alpha(\tilde{\boldsymbol{x}}_{k+1} - \boldsymbol{x}_k)$ is feasible when

$$\forall i \notin \mathcal{A}(\boldsymbol{x}_k) \;\text{ such that }\; \boldsymbol{a}_i^T(\tilde{\boldsymbol{x}}_{k+1} - \boldsymbol{x}_k) < 0,\ \alpha \leq \frac{\boldsymbol{b}_i - \boldsymbol{a}_i^T \boldsymbol{x}_k}{\boldsymbol{a}_i^T(\tilde{\boldsymbol{x}}_{k+1} - \boldsymbol{x}_k)}$$

So,

$$\boxed{\alpha_k = \min_{\substack{i \notin \mathcal{A}(\boldsymbol{x}_k) \\ \boldsymbol{a}_i^T(\tilde{\boldsymbol{x}}_{k+1} - \boldsymbol{x}_k) < 0}} \frac{\boldsymbol{b}_i - \boldsymbol{a}_i^T \boldsymbol{x}_k}{\boldsymbol{a}_i^T(\tilde{\boldsymbol{x}}_{k+1} - \boldsymbol{x}_k)}}$$

Sequential Quadratic Programming (SQP)

Solve a constrained problem $\min_{\boldsymbol{x}\in\mathbb{R}^n} \; f(\boldsymbol{x}) \quad \text{s.t.} \quad \begin{cases} g_1(\boldsymbol{x}) \geq 0 \\ \vdots \\ g_p(\boldsymbol{x}) \geq 0 \end{cases}$

Repeat:

1. Replace *f* by its quadratic approximation around $\boldsymbol{x}_k$:

$$f(\boldsymbol{x}_k + \boldsymbol{\delta}) \approx \mathcal{Q}_k(\boldsymbol{\delta}) = f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \boldsymbol{\delta} + \frac{1}{2}\boldsymbol{\delta}^T \nabla^2 \mathcal{L}(\boldsymbol{x}_k, \boldsymbol{\lambda}_k)\boldsymbol{\delta}$$

2. Replace g_j by their linear approximation around $\boldsymbol{x}_k$:

$$g_j(\boldsymbol{x}_k + \boldsymbol{\delta}) \approx g_j(\boldsymbol{x}_k) + \nabla g_j(\boldsymbol{x}_k)^T \boldsymbol{\delta}$$

3. Solve the quadratic problem

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \; \mathcal{Q}_k(\boldsymbol{\delta}) \quad \text{s.t.} \quad \begin{cases} g_1(\boldsymbol{x}_k) + \nabla g_j(\boldsymbol{x}_k)^T \boldsymbol{\delta} \geq 0 \\ \vdots \\ g_p(\boldsymbol{x}_k) + \nabla g_p(\boldsymbol{x}_k)^T \boldsymbol{\delta} \geq 0 \end{cases}$$

in a “trust region”, *i.e.,* a neighborhood of $\boldsymbol{x}_k$.

5. Global optimization (recall definitions pp. 17-18)

Goal of global minimization

- Local algorithms: the numerical solution $\hat{x}$ depends on the initial solution x_0.
- Global optimization:
  - less sensitive to initialization.
  - escape from "poor valleys".
  - often relies on the simulation of random variables: stochastic algorithms.

In practice

- First try local solvers with different initial solutions!
- Choose global optimization algorithms when the local optimization output strongly depends on the initial solution.
- Never choose global optimization algorithms when the problem is unimodal (especially for convex problems, including quadratic problems).
- Expectations: find a local minimizer which is not too “poor”. Generally, global algorithms do not guarantee to find the global minimizer in a finite number of iterations.

Definitions

An algorithm is deterministic if the rules do not depend on random draws. For a given input $\boldsymbol{x}_0$, the algorithm will always produce the same iterates $\boldsymbol{x}_k$, and the same output $\hat{\boldsymbol{x}}$.

An algorithm is stochastic if random variables are generated during the iterations. Run the algotihm twice with the same input $\boldsymbol{x}_0$: the algorithm will not produce the same iterates $\boldsymbol{x}_k$, nor the same output $\hat{\boldsymbol{x}}$.

- Idea: explore different valleys where $f(\boldsymbol{x})$ is low as effectively as possible.
- Iterates are realizations of a random process.
- Define a probalility density function.

Choice of a global optimization solver

Depends on:

- the size of the problem (number of variables).
- the number of local valleys.
- the time available for numerical computation.

By increasing level of complexity and computation time:

1. Random exploration with independent draws.
2. Interval optimization (deterministic).
3. Particle Swarm Optimization (PSO), Genetic Algorithm (GA).
4. Simulated Annealing.

Independent drawing of random variables

- Generate random points $\boldsymbol{x}_k \in \mathcal{D}$.
- Evaluate $f(\boldsymbol{x}_k)$.
- Select the point corresponding to the lowest value of $f(\boldsymbol{x}_k)$.

$\hat{f} = +\infty$.

For $k = 1, \ldots, K$,

  Randomly generate $\boldsymbol{x}_k \in \mathcal{D}$

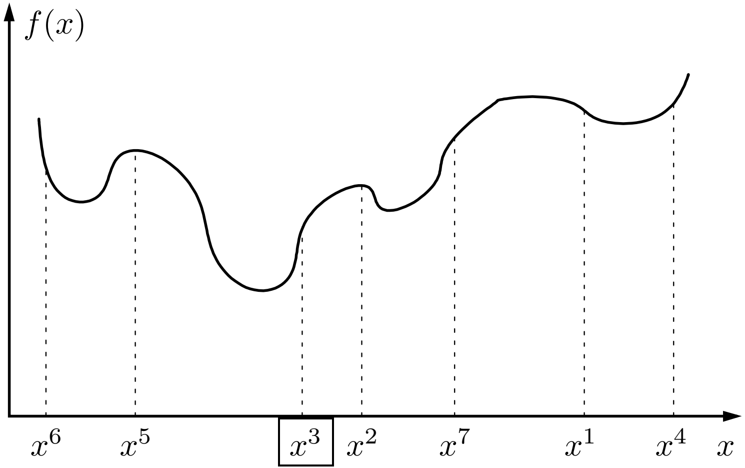
  If $f(\boldsymbol{x}_k) < \hat{f}$,

    $\hat{\boldsymbol{x}} = \boldsymbol{x}_k$ and $\hat{f} = f(\boldsymbol{x}_k)$

  End

End

Independent drawing of random variables



Hybrid approach: independent drawing + local optimization

$\hat{f} = +\infty$.

For $k = 1, \ldots, K$,

  Randomly generate $\boldsymbol{x}_k \in \mathcal{D}$

  Compute $\boldsymbol{y}_k = \text{Local\_Optim}(f; \boldsymbol{x}_k)$

  If $f(\boldsymbol{y}_k) < \hat{f}$,

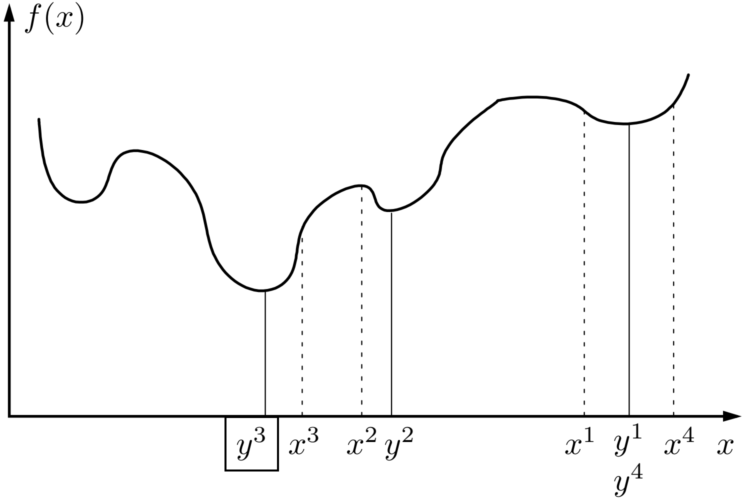
    $\hat{\boldsymbol{x}} = \boldsymbol{y}_k$ and $\hat{f} = f(\boldsymbol{y}_k)$

  End

End

Note: $\boldsymbol{y}_k$ is the a local minimizer in the valley containing $\boldsymbol{x}_k$.

Hybrid approach



Random drawing: which probability distribution?

$\hat{f} = +\infty$.

For $k = 1, \ldots, K$,

  Randomly generate $\boldsymbol{x}_k \in \mathcal{D}$

  If $f(\boldsymbol{x}_k) < \hat{f}$,

    $\hat{\boldsymbol{x}} = \boldsymbol{x}_k$ and $\hat{f} = f(\boldsymbol{x}_k)$

  End

End For

- Effectiveness strongly depends on the choice of the probability distribution.
- Uniform distribution on $\mathcal{D}$? (easy to simulate).
- More specific distribution if prior knowledge is available on the global minimizer $x^\star$?

Interval optimization

- A real number is represented by an interval, *e.g.,* π is replaced by the interval [3.14159, 3.14160].
- In 2D, an interval is a rectangle $[x_1^-, x_1^+] \times [x_2^-, x_2^+]$ with two lower bounds and two upper bounds.
- In nD, an interval is a cube $[x_1^-, x_1^+] \times [x_2^-, x_2^+] \times \cdots \times [x_n^-, x_n^+]$ of $\mathbb{R}^n$.
- Evaluate the objective function on an interval, that is, evaluate the image of an interval by function f. Examples:

$$
\begin{aligned}
[-2, 3] + [5, 7] &= [3, 10] \\
[-3, 2] * [-3, 2] &= [-6, 9] \\
[-3, 2]^2 &= [0, 9] \\
\exp([-2, 3]) &= [\exp(-2), \exp(3)] \\
\sin([0, 2\pi/3]) &= [0, 1] \\
[-3, 4] - [-3, 4] &= [-7, 7] \\
\ln([-2, -1]) &= \emptyset
\end{aligned}
$$

Evaluation of a function on an interval

- Decompose the function as a combination of simple fonctions, and evaluate each simple function.

- Example with $f(x) = x^2 + 2x + 4$:

$$\begin{aligned} f([-3, 4]) &= [-3, 4]^2 + 2 * [-3, 4] + [4, 4] \\ &= [0, 16] + [-6, 8] + [4, 4] = [-2, 28]. \end{aligned}$$

  means that $\forall x \in [-3, 4]$, $f(x) \in [-2, 28]$.

- Remark: the bounds -2 and 28 are not necessarily reached!

- Interval bisection: cut the interval in 2 sub-intervals, $[-3, 0.5]$ and $[0.5, 4]$ and evaluate each sub-interval.

Bisection: 2D example

We evaluate $f([x_1^-, x_1^+] \times [x_2^-, x_2^+]) = [-20, 200]$.
Then, the rectangle is split into 4 rectangles:

- $\mathcal{P}_{11} = \left[x_1^-, \frac{x_1^- + x_1^+}{2}\right] \times \left[x_2^-, \frac{x_2^- + x_2^+}{2}\right]$,
- $\mathcal{P}_{12} = \left[x_1^-, \frac{x_1^- + x_1^+}{2}\right] \times \left[\frac{x_2^- + x_2^+}{2}, x_2^+\right]$,
- $\mathcal{P}_{21} = \left[\frac{x_1^- + x_1^+}{2}, x_1^+\right] \times \left[x_2^-, \frac{x_2^- + x_2^+}{2}\right]$;
- $\mathcal{P}_{22} = \left[\frac{x_1^- + x_1^+}{2}, x_1^+\right] \times \left[\frac{x_2^- + x_2^+}{2}, x_2^+\right]$

and f is re-evaluated on each rectangle:

	$\left[x_2^-, \frac{x_2^- + x_2^+}{2}\right]$	$\left[\frac{x_2^- + x_2^+}{2}, x_2^+\right]$
$\left[x_1^-, \frac{x_1^- + x_1^+}{2}\right]$	$f(\mathcal{P}_{11}) = [32, 100]$	$f(\mathcal{P}_{12}) = [-14, 28]$
$\left[\frac{x_1^- + x_1^+}{2}, x_1^+\right]$	$f(\mathcal{P}_{21}) = [-10, 2]$	$f(\mathcal{P}_{22}) = [2, 3]$

Bisection: 2D example

	$\left[x_2^-, \frac{x_2^-+x_2^+}{2}\right]$	$\left[\frac{x_2^-+x_2^+}{2}, x_2^+\right]$
$\left[x_1^-, \frac{x_1^-+x_1^+}{2}\right]$	X	$f(\mathcal{P}_{12}) = [-14, 28]$
$\left[\frac{x_1^-+x_1^+}{2}, x_1^+\right]$	$f(\mathcal{P}_{21}) = [-10, 2]$	$f(\mathcal{P}_{22}) = [2, 3]$

Conclusion:

- $\mathcal{P}_{11}$ cannot contain a global minimizer.
- $\mathcal{P}_{12}$, $\mathcal{P}_{21}$ and $\mathcal{P}_{22}$ are candidates to contain a global minimizer.
- Make bisection of $\mathcal{P}_{12}$, $\mathcal{P}_{21}$ and $\mathcal{P}_{22}$ and re-evaluate f on the new (smaller) intervals.

Interval optimization

Principle.

- Handle of list of candidate intervals $\{\mathcal{P}_i\}$.
- Evaluate $[f_i^-, f_i^+] = f(\mathcal{P}_i)$.
- Update $\bar{f} = \min_i f_i^+$.
- Simplification of the list: remove $\mathcal{P}_i$ from the list when $f_i^- > \bar{f}$.

Branch and bound philosophy.

- All intervals are tested (bisection + evaluation of f), but some which cannot lead to the solution are deleted.
- The algorithm works for problems of dimension $n \leq 100$.
- The algorithm output is a list of candidate intervals and an upper bound $\bar{f}$ of $\min f(\boldsymbol{x})$.
- The global minimizers are guaranteed to be in one of the intervals in the list.

Evolutionary algorithms

- Particle Swarm Optimization.
- Genetic Algorithm.

Principle.

Evolutionary algorithms make an exploration of the feasible domain $\mathcal{D}$ using several variables in parallel.

Local optimization algorithm.

- 1 variable $\boldsymbol{x}$.
- Iteration k: $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + t_k \boldsymbol{d}_k$.

Evolutionary algorithms.

- N variables $\boldsymbol{x}^1, \dots, \boldsymbol{x}^N \in \mathbb{R}^n$.
- Iteration k: jointly update $\{\boldsymbol{x}_{k+1}^1, \dots, \boldsymbol{x}_{k+1}^N\}$ from $\{\boldsymbol{x}_k^1, \dots, \boldsymbol{x}_k^N\}$.

Evolutionary algorithms

Find a strategy with several variables (individuals, agents, particles) to explore “interesting valleys”. The number of variables N is fixed.

The update of the $\boldsymbol{x}_k^i$ depends on:

1. a local descent move (knowledge of $\nabla f(\boldsymbol{x}_k^i)$).
2. the introduction of random moves to avoid convergence towards a local minimizer.
3. the objective values for other variables $\boldsymbol{x}_k^j$ ($j \neq i$).

Heuristic algorithms, no guarantee of convergence towards a global minimizer.

Simple to implement, several parameters to tune, can work for large dimension n.

Genetic algorithms

Artificial intelligence: simulate the evolution of a population of N individuals according to Darwin's theory:

1. Natural selection: the most adapted individuals tend to live longer and to reproduce more easily.
2. Evolution: some novel species randomly appear.

Sketch of algorithm:

Set $k \leftarrow 0$.
Initialize $\boldsymbol{x}_0^1, \boldsymbol{x}_0^2, \ldots, \boldsymbol{x}_0^N \in \mathbb{R}^n$
For $k = 0, \ldots, K$,
    Select $N/2$ variables (the others are removed);
    Reproduction (mutations, crossbreed);
    Evaluate children;
    Replace some parents by their children.
End For

Genetic algorithms

Initialization.

x_0^i: uniform distribution on $\mathcal{D}$?

Selection:

1. *$N/2$-elitism*: keep the $N/2$ best variables (corresponding to the lowest values of $f(x)$).
2. *Tournament selection*:

   Repeat:
   - Choose q variables randomly;
   - Select the best as parent.

   until the number of parents is equal to $N/2$.

Remark.

- $N/2$-elitism may induce premature convergence towards a local minimizer.
- Tournament selection will tend to explore unlikely valleys.

Genetic algorithms

Crossbreed between variables x_i^k and x_j^k:

Generate a new position

$$x = \alpha_{ij} x_k^i + (1 - \alpha_{ij}) x_k^j$$

where α_{ij} is uniformly drawn on the line joining x_i^k and x_j^k. For instance, choose $\alpha_{ij} \in [-\varepsilon,\ 1 + \varepsilon]$.

Mutation of x_k^i:

$$x = x_k^i + \varepsilon_i \text{ with } \varepsilon_i \sim \mathcal{N}(\mathbf{0}, \sigma^2 I)$$

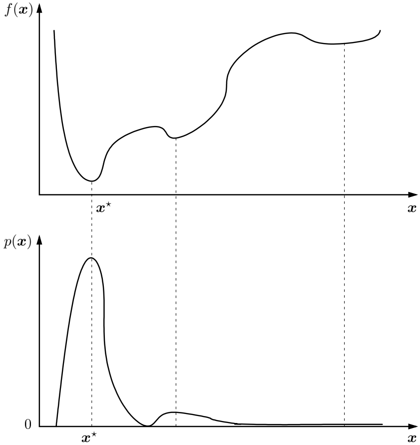
Overall parameters.

- N, σ, q (tournament selection), initial conditions.
- Tradeoff exploration (low q, large σ, large N) *vs* local convergence.

Monte Carlo based methods (simulated annealing...)

Minimize $f(\boldsymbol{x}) \iff$ Maximize $p(\boldsymbol{x}) = \frac{1}{Z}\exp(-f(\boldsymbol{x}))$.

$Z = \int_{\mathcal{D}} \exp(-f(\boldsymbol{x}))\, d\boldsymbol{x}$ is chosen to have a probability distribution.



Monte Carlo based methods

Minimize $f(\boldsymbol{x}) \iff$ Maximize $p(\boldsymbol{x}) = \frac{1}{Z} \exp(-f(\boldsymbol{x}))$.

- Draw samples $\boldsymbol{x}_k$ of the probability distribution $p(\boldsymbol{x})$.
- For large dimension problems, and when Z is unknown, we can make use of Markov chains.
- MCMC methods (*Markov chain Monte Carlo*) create a long Markov chain $\{\ldots, \boldsymbol{X}^k, \ldots\}$ whose samples are asymptotically distributed according to pdf $p(\boldsymbol{x})$.

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