

An introduction to shape and topology optimization

Éric Bonnetier* and Charles Dapogny†

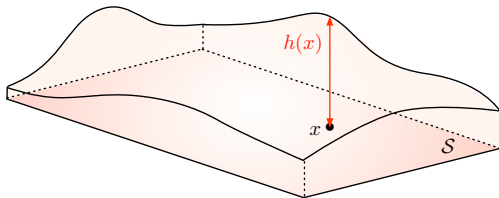
* Institut Fourier, Université Grenoble-Alpes, Grenoble, France

† CNRS & Laboratoire Jean Kuntzmann, Université Grenoble-Alpes, Grenoble, France

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Foreword

- In this lecture, we focus on **parametric optimization**, or **optimal control**:
 - The shape is described by a set h of **parameters**, lying in a **fixed vector space**.
 - The **state equations**, accounting for the physical behavior of the shape, depend on h in a “**simple**” way.
- Many key concepts and methods of the course can be exposed in this framework, with a minimum amount of technicality.



An elastic plate can be described by its height $h : S \rightarrow \mathbb{R}$ with respect to a fixed cross-section S .

Part II

Optimal control and parametric optimization problems

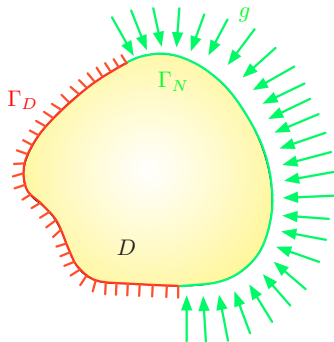
- 1 Parametric optimization problems
 - Presentation of the model problem
 - Non existence of optimal design
 - Calculation of the derivative of the objective function
 - The formal method of C ea
- 2 Numerical algorithms

A model problem involving the conductivity equation (I)

- We return to the problem of optimizing the **thermal conductivity** $h : D \rightarrow \mathbb{R}$.
- The **temperature** u_h is the solution in $H^1(D)$ to the “state”, conductivity equation:

$$\begin{cases} -\operatorname{div}(h\nabla u_h) &= f & \text{in } D, \\ u_h &= 0 & \text{on } \Gamma_D, \\ h \frac{\partial u_h}{\partial n} &= g & \text{on } \Gamma_N, \end{cases}$$

where $f \in L^2(D)$ and $g \in L^2(\Gamma_N)$.



The considered cavity

- The set \mathcal{U}_{ad} of **design variables** is:

$$\mathcal{U}_{\text{ad}} = \left\{ h \in L^\infty(D), \alpha \leq h(x) \leq \beta \text{ a.e. } x \in D \right\} \subset L^\infty(D),$$

where $0 < \alpha < \beta$ are fixed bounds.

A model problem involving the conductivity equation (II)

- We consider a problem of the form:

$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h), \text{ where } J(h) = \int_D j(u_h) \, dx,$$

and $j : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth function satisfying **growth conditions**:

$$\forall s \in \mathbb{R}, \quad |j(s)| \leq C(1 + |s|^2), \text{ and } j'(s) \leq C(1 + |s|).$$

- Many variants are possible, e.g. featuring **constraints** on h or u_h .
- In this simple setting,
 - the state u_h is evaluated on the **same** domain D , regardless of the actual value of the design variable $h \in \mathcal{U}_{\text{ad}}$;
 - the design variable h acts as a **parameter** in the coefficients of the state equation.
- Even in this case, the optimization problem has no (global) solution in general...

Part II

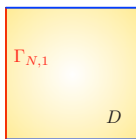
Optimal control and parametric optimization problems

- 1 Parametric optimization problems
 - Presentation of the model problem
 - **Non existence of optimal design**
 - Calculation of the derivative of the objective function
 - The formal method of C ea
- 2 Numerical algorithms

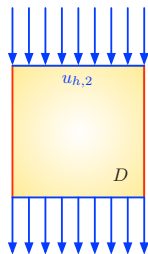
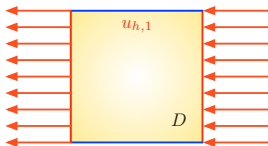
Non existence of optimal design (I)

- This counter-example is discussed in details in [All] §5.2.
- The defining domain is the unit square $D = (0, 1)^2$.
- We consider two physical situations:

$$\left\{ \begin{array}{ll} -\operatorname{div}(h\nabla u_{h,1}) = 0 & \text{in } D, \\ h \frac{\partial u_{h,1}}{\partial n} = \mathbf{e}_1 \cdot \mathbf{n} & \text{in } \Gamma_{N,1}, \\ h \frac{\partial u_{h,1}}{\partial n} = 0 & \text{in } \Gamma_{N,2}, \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{ll} -\operatorname{div}(h\nabla u_{h,2}) = 0 & \text{in } D, \\ h \frac{\partial u_{h,2}}{\partial n} = 0 & \text{in } \Gamma_{N,1}, \\ h \frac{\partial u_{h,2}}{\partial n} = \mathbf{e}_2 \cdot \mathbf{n} & \text{in } \Gamma_{N,2}. \end{array} \right.$$



$\Gamma_{N,2}$



(Left) Boundary conditions, (middle) boundary data for $u_{h,1}$; (right) boundary data for $u_{h,2}$.

Non existence of optimal design (II)

The optimization problem of interest in this example is:

$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h),$$

where the considered objective function is:

$$J(h) = \int_{\Gamma_{N,1}} \mathbf{e}_1 \cdot \mathbf{n} u_{h,1} \, ds - \int_{\Gamma_{N,2}} \mathbf{e}_2 \cdot \mathbf{n} u_{h,2} \, ds,$$

and the set \mathcal{U}_{ad} of admissible designs encompasses a **volume constraint**:

$$\mathcal{U}_{\text{ad}} = \left\{ h \in L^\infty(D), \quad \begin{array}{l} \alpha < h(x) < \beta \text{ a.e. } x \in D, \\ \int_D h \, dx = V_T \end{array} \right\}.$$

In other terms, one aims to

- **Minimize** the temperature difference between the left and right sides in **Case 1**.
- **Maximize** the temperature difference between the top and bottom sides in **Case 2**.

Non existence of optimal design (III)

Theorem 1.

The parametric optimization problem $\min_{h \in \mathcal{U}_{\text{ad}}} J(h)$ does not have a global solution.

Hint of the proof: The proof comprises three stages:

Step 1: One calculates a **lower bound** m on the values of $J(h)$ for $h \in \mathcal{U}_{\text{ad}}$:

$$\forall h \in \mathcal{U}_{\text{ad}}, J(h) \geq m.$$

Step 2: One proves that this lower bound is not attained by an element in \mathcal{U}_{ad} :

$$\forall h \in \mathcal{U}_{\text{ad}}, J(h) > m.$$

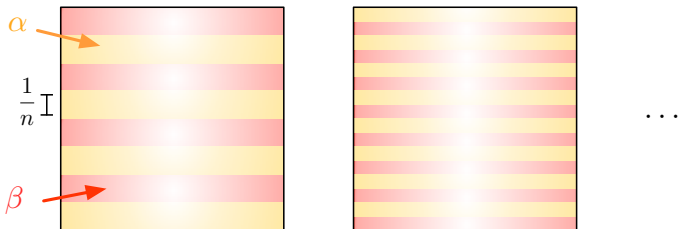
Step 3: One constructs a **minimizing sequence** of designs $h^n \in \mathcal{U}_{\text{ad}}$:

$$J(h^n) \xrightarrow{n \rightarrow \infty} m.$$

Hence, m is the infimum of $J(h)$ over \mathcal{U}_{ad} but it is not attained by any $h \in \mathcal{U}_{\text{ad}}$.

Non existence of optimal design (IV)

The minimizing sequence is constructed as a **laminate**, i.e. a succession of layers with maximum and minimum conductivities.



Two elements in a minimizing sequence h^n of conductivities.

Homogenization effect: *To get more optimized, designs tend to create very thin structures, at the microscopic level.*

Non existence of optimal design (V)

- In general, shape optimization problems, even under their simplest forms, do not have global solutions, for deep physical reasons.
- See [Mu] for many such examples of non existence of optimal design in optimal control problems.
- To ensure existence of an optimal shape, two techniques are usually employed:
 - **Relaxation**: the set \mathcal{U}_{ad} of admissible designs is **enlarged** so that it contains “microscopic designs”: this is the essence of the **Homogenization method** for optimal design [All2].
 - **Restriction**: the set \mathcal{U}_{ad} is restricted to, e.g. **more regular** designs.
- In practice, we shall be interested in the search of **local minimizers** of such problems, which are e.g. “close” to an initial design inspired by intuition.

Part II

Optimal control and parametric optimization problems

- 1 Parametric optimization problems
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Derivative of the objective function (I)

Let us return to our (further simplified) problem:

$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h),$$

where

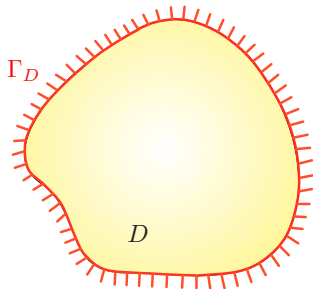
$$J(h) = \int_D j(u_h) \, dx,$$

the set of admissible designs is:

$$\mathcal{U}_{\text{ad}} = \left\{ h \in L^\infty(D), \alpha \leq h(x) \leq \beta \text{ a.e. } x \in D \right\},$$

and the **temperature** u_h is the solution in $H_0^1(D)$ to:

$$\begin{cases} -\operatorname{div}(h \nabla u_h) & = f & \text{in } D, \\ u_h & = 0 & \text{on } \partial D. \end{cases}$$



Remark Again, for simplicity, we omit constraints on h or u_h .

Derivative of the objective function (II)

To solve this program numerically, we intend to apply a **gradient-based algorithm**, of the form:

Initialization: Start from an initial design h^0 ,

For $n = 0, \dots$ **convergence:**

- 1 Calculate the **derivative** $J'(h^n)$ of the mapping $h \mapsto J(h)$ at $h = h^n$;
- 2 Select an appropriate **time step** $\tau^n > 0$;
- 3 Update the design as: $h^{n+1} = h^n - \tau^n J'(h^n)$.

- The cornerstone any such method is the calculation of the **derivative** of $J(h)$.
- This task is uneasy since $J(h)$ depends on h in a complicated way – via the solution u_h to a PDE whose coefficients depend on h .

Theorem 2.

The objective function

$$J(h) = \int_D j(u_h) \, dx$$

is Fréchet differentiable at any $h \in \mathcal{U}_{\text{ad}}$, and its derivative reads

$$\forall \hat{h} \in L^\infty(D), \quad J'(h)(\hat{h}) = \int_D (\nabla u_h \cdot \nabla p_h) \hat{h} \, dx,$$

where the **adjoint state** $p_h \in H_0^1(D)$ is the unique solution to the system:

$$\begin{cases} -\operatorname{div}(h \nabla p_h) = -j'(u_h) & \text{in } D, \\ p_h = 0 & \text{on } \partial D. \end{cases}$$

Derivative of the objective function (IV)

Proof: The proof is divided into three steps:

- 1 Using the **implicit function theorem**, we prove that the state mapping

$$\mathcal{U}_{\text{ad}} \ni h \mapsto u_h \in H_0^1(D)$$

is **Fréchet differentiable**, with derivative $\hat{h} \mapsto u'_h(\hat{h})$.

(Here the fact that all the u_h belong to a fixed functional space is handy)

- 2 We calculate the derivative of $J(h)$ by using the **chain rule**.
- 3 We give a more convenient structure to this derivative, introducing an **adjoint state** p_h to eliminate the occurrence of $u'_h(\hat{h})$.

Step 1: *Differentiability of $h \mapsto u_h$:*

For any $h \in \mathcal{U}_{\text{ad}}$, u_h is the unique solution in $H_0^1(D)$ to the variational problem:

$$\forall v \in H_0^1(D), \quad \int_D h \nabla u_h \cdot \nabla v \, dx = \int_D f v \, dx.$$

Derivative of the objective function (V)

Let

$$\mathcal{F} : \mathcal{U}_{\text{ad}} \times H_0^1(D) \rightarrow H^{-1}(D)$$

be the mapping defined by:

$$\mathcal{F}(h, u) : v \mapsto \int_D h \nabla u \cdot \nabla v \, dx - \int_D f v \, dx.$$

One verifies that

- \mathcal{F} is a mapping of class \mathcal{C}^1 ;
- For given $h \in \mathcal{U}_{\text{ad}}$, u_h is the unique solution u to the equation

$$\mathcal{F}(h, u) = 0.$$

- The differential of the partial mapping $u \mapsto \mathcal{F}(h, u)$ reads:

$$H_0^1(D) \ni \hat{u} \mapsto \left[v \mapsto \int_D h \nabla \hat{u} \cdot \nabla v \, dx \right] \in H^{-1}(D).$$

It is an isomorphism, owing to the **Lax-Milgram theorem**:

For all $g \in H^{-1}(D)$, there exists a unique $u \in H_0^1(D)$ s.t.

$$\forall v \in H_0^1(D), \int_D h \nabla u \cdot \nabla v \, dx = \langle g, v \rangle_{H^{-1}(D), H_0^1(D)}.$$

Derivative of the objective function (VI)

The **implicit function theorem** guarantees that the mapping $h \mapsto u_h$ is of class \mathcal{C}^1 .

To calculate the derivative $\hat{h} \mapsto u'_h(\hat{h})$, we return to the variational formulation for u_h :

$$\forall v \in H_0^1(D), \int_D h \nabla u_h \cdot \nabla v \, dx = \int_D f v \, dx.$$

Differentiating with respect to h in a direction $\hat{h} \in L^\infty(D)$ yields:

$$\int_D \hat{h} \nabla u_h \cdot \nabla v \, dx + \int_D h \nabla u'_h(\hat{h}) \cdot \nabla v \, dx = 0,$$

and so, for all $\hat{h} \in L^\infty(D)$, $u'_h(\hat{h})$ is the unique solution in $H_0^1(D)$ to:

$$\forall v \in H_0^1(D), \int_D h \nabla u'_h(\hat{h}) \cdot \nabla v \, dx = - \int_D \hat{h} \nabla u_h \cdot \nabla v \, dx.$$

Derivative of the objective function (VII)

Step 2: *Calculation of the derivative of $J(h)$:*

Since $h \mapsto u_h$ is of class \mathcal{C}^1 , the **chain rule** yields immediately:

$$\forall \hat{h} \in L^\infty(D), \quad J'(h)(\hat{h}) = \int_D j'(u_h) u'_h(\hat{h}) \, dx.$$

- This expression is **awkward**: the dependence $\hat{h} \mapsto J'(h)(\hat{h})$ is not explicit and it is difficult to find a **descent direction**, i.e. a vector $\hat{h} \in L^\infty(D)$ such that:

$$J'(h)(\hat{h}) < 0.$$

- Fortunately, the expression of $J'(h)$ can be simplified thanks to the introduction of the **adjoint state** p_h .

Derivative of the objective function (VIII)

Step 3: Reformulation of $J'(h)$ using an adjoint state:

The **adjoint state** p_h is the unique solution in $H_0^1(D)$ to the variational problem:

$$\forall v \in H_0^1(D), \int_D h \nabla p_h \cdot \nabla v \, dx = - \int_D j'(u_h) v \, dx,$$

to be compared with the variational formulation for $u'_h(\hat{h}) \in H_0^1(D)$:

$$\forall v \in H_0^1(D), \int_D h \nabla u'_h(\hat{h}) \cdot \nabla v \, dx = - \int_D \hat{h} \nabla u_h \cdot \nabla v \, dx.$$

Then, we calculate:

$$\begin{aligned} J'(h)(\hat{h}) &= \int_D j'(u_h) u'_h(\hat{h}) \, dx, \\ &= - \int_D h \nabla p_h \cdot \nabla u'_h(\hat{h}) \, dx, \\ &= - \int_D h \nabla u'_h(\hat{h}) \cdot \nabla p_h \, dx, \\ &= \int_D \hat{h} \nabla u_h \cdot \nabla p_h \, dx. \end{aligned}$$

where the last line uses the variational formulation of $u'_h(\hat{h})$ with p_h as test function.

About the adjoint state

- The adjoint state p_h satisfies

$$\begin{cases} -\operatorname{div}(h\nabla p_h) = -j'(u_h) & \text{in } D, \\ p_h = 0 & \text{on } \partial D. \end{cases}$$

It is therefore a “**virtual temperature**” driven by a source (or sink) equal to the rate of change of the integrand of $J(h)$ at the state described by u_h .

- From the last expression, one obviously obtains a **descent direction**:

$$\hat{h} = -\nabla u_h \cdot \nabla p_h \Rightarrow J'(h)(\hat{h}) < 0,$$

which can be interpreted as the power induced by the “virtual temperature” p_h .

- We shall see soon a second interpretation of p_h as the **Lagrange multiplier** associated to the PDE constraint if we formulate our optimization problem as:

$$\min_{(h,u)} \int_D j(u) \, dx \quad \text{s.t.} \quad \begin{cases} -\operatorname{div}(h\nabla u) = f & \text{in } D, \\ u = 0 & \text{on } \partial D. \end{cases}$$

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Optimal control and parametric optimization problems

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The formal method of Céa

The method of Céa is a **formal way** to calculate the derivative of $J(h)$. It **assumes** that the mapping $h \mapsto u_h$ is differentiable.

Let the **Lagrangian**

$$\mathcal{L} : \mathcal{U}_{\text{ad}} \times H_0^1(D) \times H_0^1(D) \rightarrow \mathbb{R}$$

be defined by:

$$\mathcal{L}(h, u, p) = \underbrace{\int_D j(u) \, dx}_{\text{Objective function at stake}} + \underbrace{\int_D h \nabla u \cdot \nabla p \, dx - \int_D f p \, dx}_{\text{Enforcement of the PDE constraint } -\Delta u = f \text{ with a Lagrange multiplier } p} .$$

In particular, for any $\hat{p} \in H_0^1(D)$,

$$J(h) = \mathcal{L}(h, u_h, \hat{p}).$$

For a given $h \in \mathcal{U}_{\text{ad}}$, we search for the saddle points (u, p) of $\mathcal{L}(h, \cdot, \cdot)$.

The formal method of Céa

- Imposing the partial derivative of \mathcal{L} with respect to p to vanish amounts to

$$\forall \hat{p} \in H_0^1(D), \int_D h \nabla u \cdot \nabla \hat{p} \, dx - \int_D f \hat{p} \, dx = 0;$$

this is the variational formulation for $u = u_h$.

- Imposing the partial derivative of \mathcal{L} with respect to u to vanish amounts to

$$\forall \hat{u} \in H_0^1(D), \int_D h \nabla p \cdot \nabla \hat{u} \, dx = - \int_D j'(u) \hat{u} \, dx;$$

since $u = u_h$, we recognize the variational formulation for $p = p_h$.

The formal method of Céa

- Recall that, for arbitrary $\hat{p} \in H_0^1(D)$,

$$J(h) = \mathcal{L}(h, u_h, \hat{p}).$$

- Since we have assumed that $h \mapsto u_h$ is differentiable, the **chain rule** yields:

$$J'(h)(\hat{h}) = \frac{\partial \mathcal{L}}{\partial h}(h, u_h, \hat{p})(\hat{h}) + \frac{\partial \mathcal{L}}{\partial u}(h, u_h, \hat{p})(u'_h(\hat{h})).$$

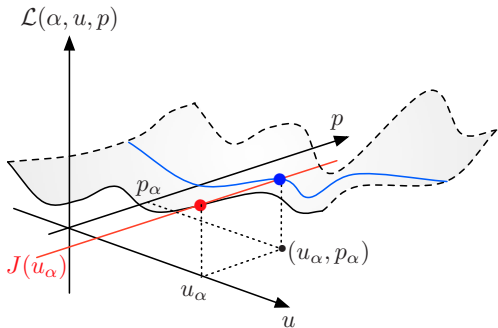
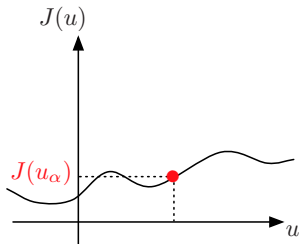
- Now taking $\hat{p} = p_h$, the last term in the above right-hand side vanishes:

$$J'(h)(\hat{h}) = \frac{\partial \mathcal{L}}{\partial h}(h, u_h, p_h)(\hat{h}).$$

- The above derivative is simply that of the mapping $h \mapsto \int_D h \nabla u \cdot \nabla p \, dx$ for given u, p . Hence:

$$J'(h)(\hat{h}) = \int_D \hat{h} \nabla u_h \cdot \nabla p_h \, dx.$$

The formal method of C ea: intuition



Physical intuition: The function $J(h)$ is "twisted" into the value $\mathcal{L}(h, u_h, p_h)$ at the parametrized saddle point $\mathcal{L}(h, \cdot, \cdot)$, which is easy to differentiate with respect to the parameter.

Part II

Optimal control and parametric optimization problems

- 1 Parametric optimization problems
- 2 **Numerical algorithms**
 - A refresher about the finite element method
 - A refresher about basic optimization methods
 - Numerical algorithms for parametric optimization

The finite element method: variational formulations (I)

- As a model problem, we consider the **Laplace equation**:

$$\text{Search for } u \in H_0^1(D) \text{ s.t. } \begin{cases} -\Delta u = f & \text{in } D, \\ u = 0 & \text{on } \partial D, \end{cases}$$

where $f \in L^2(D)$ is a given source.

- The associated **variational formulation** reads:

$$\text{Search for } u \in V \text{ s.t. } \forall v \in V, a(u, v) = \ell(v),$$

where

- The Hilbert space V is the Sobolev space $H_0^1(D)$;
 - $a(\cdot, \cdot)$ is the bilinear form on V given by: $a(u, v) = \int_D \nabla u \cdot \nabla v \, dx$;
 - $\ell(\cdot)$ is the linear form on V defined by: $\ell(v) = \int_D f v \, dx$.
- The above variational problem has a unique solution $u \in V$ owing to the **Lax-Milgram theorem**.

The finite element method: variational formulations (II)

- The **finite element method** consists in searching for an approximation u_h to h inside a **finite-dimensional** subspace $V_h \subset V$.
- The exact variational problem is replaced by:

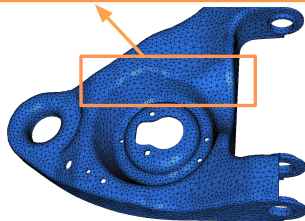
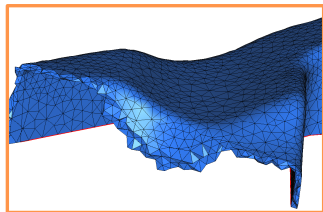
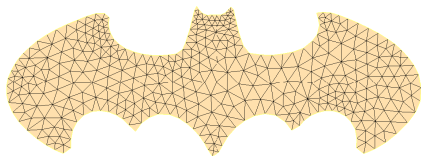
$$\text{Search for } u_h \in V_h \text{ s.t. } \forall v_h \in V_h, a(u_h, v_h) = \ell(v_h),$$

which is also well-posed owing to the Lax-Milgram theorem.

- The subscript h refers to the **sharpness** of the approximation: as $h \rightarrow 0$, it is expected that $V_h \approx V$ and $u_h \approx u$.

Meshing the physical domain (I)

In practice, the domain D is discretized by means of a **mesh** \mathcal{T} , i.e. a covering by **simplices** (triangles in 2d, tetrahedra in 3d).



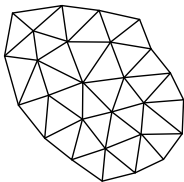
Meshing the physical domain (II)

A **mesh** \mathcal{T} is defined by the datum of:

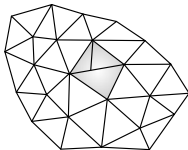
- A set of **vertices** $\{a_i\}_{i=1,\dots,N_V}$;
- A set of (open) **simplices** $\{T_j\}_{j=1,\dots,N_T}$, with vertices in $\{a_i\}$.

We also require that the mesh \mathcal{T} be:

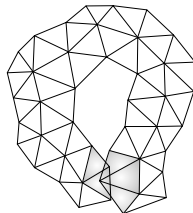
- **Valid**: For all simplices T_i, T_j with $i \neq j$, $T_i \cap T_j = \emptyset$.
- **Conforming**: For all simplices T_i, T_j , the intersection $\overline{T_i} \cap \overline{T_j}$ is either a vertex, or an edge, or a triangle (or a tetrahedron in 3d) of \mathcal{T} .



Valid, conforming mesh



Non conforming mesh



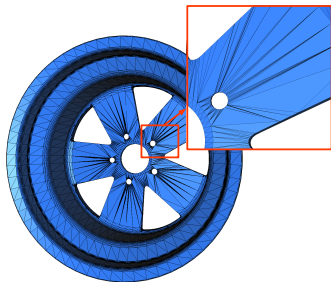
Invalid mesh

Meshing the physical domain (III)

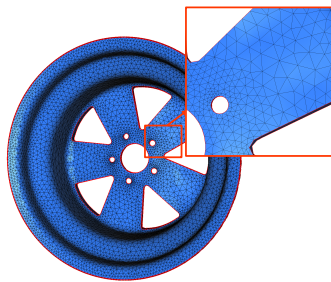
- It is often crucial in applications that \mathcal{T} has good **quality**, i.e. that its elements are close to equilateral.
- The quality of a simplex T , with edges a_j can be evaluated e.g. by the function:

$$Q(T) = \alpha \frac{\text{Vol}(T)}{\left(\sum_{j=1}^{d(d+1)/2} |a_j|^2 \right)^{\frac{d}{2}}},$$

where $\alpha \in \mathbb{R}$ is such that $Q(T) = 1$ if T is equilateral and $Q(T) = 0$ if T is flat.



Bad quality mesh, with nearly flat elements



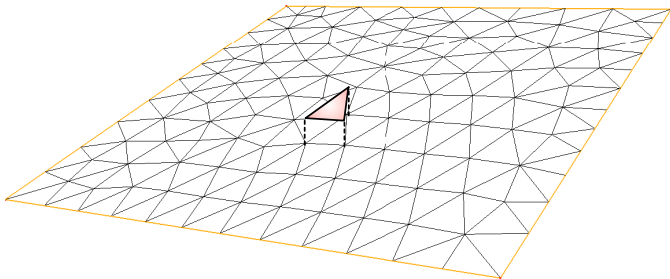
Good quality mesh, with almost regular elements

Construction of the finite element space V_h (I)

- In the finite element context, the mesh \mathcal{T}_h is labelled by the **size** h of its elements.
- A basis $\{\varphi_1, \dots, \varphi_{N_h}\}$ of the **finite element space** V_h is based on \mathcal{T}_h .

Example: the \mathbb{P}_0 Finite element method

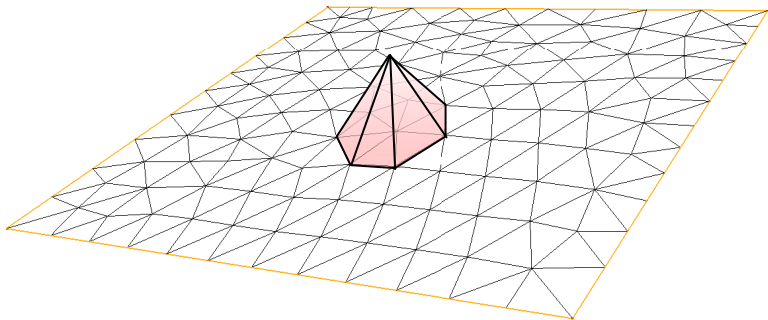
- N_h is the number N_T of simplices T_1, \dots, T_{N_h} in the mesh;
- For $i = 1, \dots, N_h$, φ_i is constant on each simplex $T \in \mathcal{T}_h$ and $\varphi_i(x) = 1$ on T_i and $\varphi_i(x) = 0$ for $x \notin T_i$.



Construction of the finite element space V_h (II)

Example: the \mathbb{P}_1 Finite element method

- N_h is the number N_V of vertices a_1, \dots, a_{N_h} of the mesh;
- For $i = 1, \dots, N_h$, φ_i is affine in restriction to each triangle $T \in \mathcal{T}_h$ and $\varphi_i(a_i) = 1$ and $\varphi_i(a_j) = 0$ for $j \neq i$.



The finite element method in a nutshell (I)

Introducing the (sought) decomposition of the (sought) function u_h on this basis:

$$u_h = \sum_{j=1}^{N_h} u_j \varphi_j,$$

the variational problem becomes an $N_h \times N_h$ **linear system**:

$$KU = F,$$

where

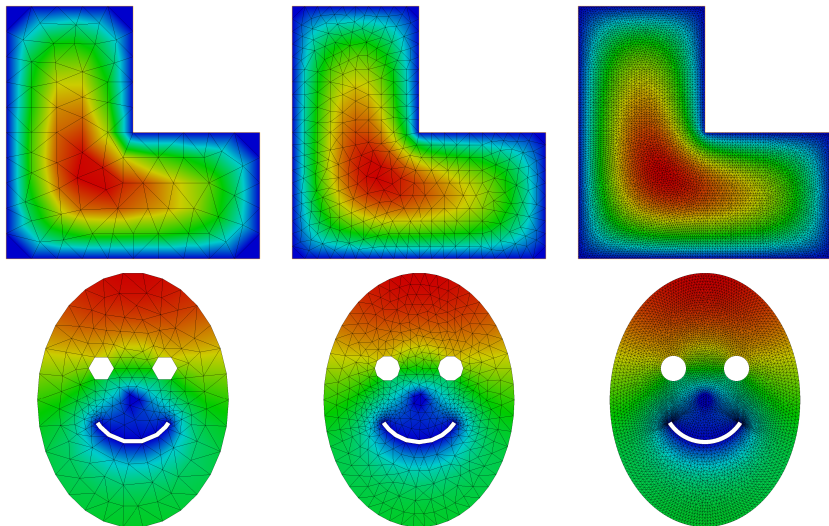
- $U = \begin{pmatrix} u_1 \\ \vdots \\ u_{N_h} \end{pmatrix}$ is the vector of unknowns,

- K is the **stiffness matrix**, defined by its entries:

$$K_{ij} = a(\varphi_j, \varphi_i), \quad i, j = 1, \dots, N_h;$$

- F is the **right-hand side** vector: $F_i = \ell(\varphi_i)$.

The finite element method in a nutshell (II)



Resolution of the Laplace equation with the finite element method on several domains D , using various meshes \mathcal{T} .

Some practical aspects about the finite element method

- In practice, the discrete finite element system

$$KU = F$$

is a large $N_h \times N_h$ linear system, which is **sparse**.

- In realistic examples, its resolution can only be achieved thanks to **iterative methods**, such as the **Conjugate Gradient** algorithm, **GMRES**, etc.
- The numerical efficiency of such methods depends on the **condition number** of the matrix K , which is directly related to the **quality** of the computational mesh.
- The resolution of this system can also take advantage of recent **Domain Decomposition methods**.
- In shape optimization algorithms, such systems have to be solved **multiple times**: this is the main source of computational burden.

Final remarks about the finite element method

- The Finite Element paradigm extends (with some work!) to various frameworks:
 - **Mixed variational formulations**, like in the case of the Stokes equations;
 - **Eigenvalue problems**;
 - **Non linear PDE**, such as the Navier-Stokes equations, or the non linear elasticity system.

- To go further, see the introductory and reference monographs [All] and [ErnGue].

Part II

Optimal control and parametric optimization problems

- 1 Parametric optimization problems
- 2 **Numerical algorithms**
 - A refresher about the finite element method
 - **A refresher about basic optimization methods**
 - Numerical algorithms for parametric optimization

Definition 1.

Let $(X, \|\cdot\|_X)$ be a *Banach space*. A real-valued function $F : X \rightarrow \mathbb{R}$ is *differentiable* at $u \in X$ if there exists a linear, continuous mapping $F'(u) : X \rightarrow \mathbb{R}$ such that:

$$F(u + v) = F(u) + F'(u)(v) + o(\|v\|), \text{ where } \frac{o(\|v\|_X)}{\|v\|_X} \xrightarrow{h \rightarrow 0} 0.$$

The linear mapping $F'(u) \in X^*$ is the *differential*, or *Fréchet derivative* of F at u .

Definition 2.

If in addition X is a Hilbert space $(H, \langle \cdot, \cdot \rangle_H)$, the *Riesz representation theorem* allows to identify the derivative $F'(u)$ with an element $\nabla F(u) \in H$:

$$\forall v \in H, F'(u)(v) = \langle \nabla F(u), v \rangle_H;$$

$\nabla F(u)$ is called the *gradient* of F at u .

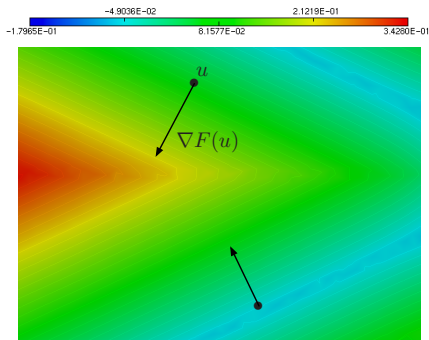
Refresher: differential and gradient (II)

Physical interpretation: If F is differentiable at $u \in H$, it holds, for “small” $\tau > 0$:

$$\begin{aligned} \forall \hat{u} \in H, \|\hat{u}\|_H \leq 1, \quad F(u + t\hat{u}) &\approx F(u) + \tau \langle \nabla F(u), \hat{u} \rangle_H, \\ &\leq F(u) + \tau \|\nabla F(u)\|_H, \end{aligned}$$

where equality holds if and only if $\hat{u} = \frac{\nabla F(u)}{\|\nabla F(u)\|_H}$ (Cauchy-Schwarz inequality).

$\Rightarrow \nabla F(u)$ (resp. $-\nabla F(u)$) is the best ascent (resp. descent) direction for F from u .



Some isolines of a function $F : \mathbb{R}^2 \rightarrow \mathbb{R}$ and the gradient $\nabla F(u) \in \mathbb{R}^2$ at some point $u \in \mathbb{R}^2$.

The gradient algorithm (I)

In a Hilbert space H , we consider the **unconstrained** minimization problem:

$$\min_{h \in H} J(h),$$

where $J(h)$ is a differentiable function.

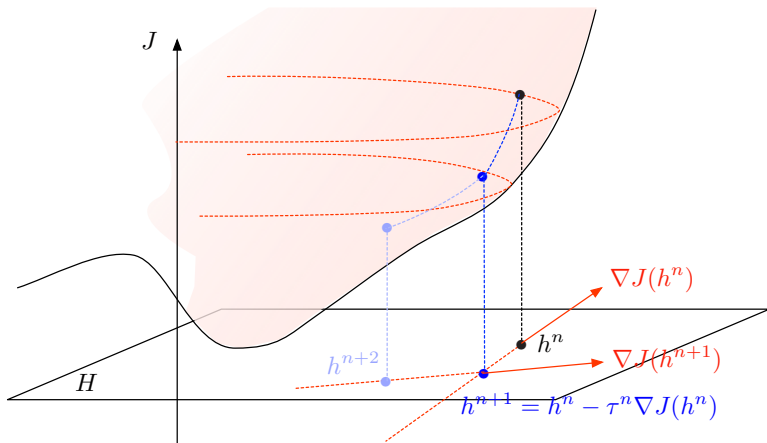
Initialization: Start from an initial design h^0 .

For $n = 0, \dots$ convergence:

- 1 Calculate the derivative $J'(h^n)$ of J at h^n and the gradient $\nabla J(h^n) \in H$; infer a descent direction $\hat{h}^n = -\nabla J(h^n)$.
- 2 Take a suitable small time step $\tau^n > 0$ such that:
$$J(h^n + \tau^n \hat{h}^n) < J(h^n).$$
- 3 The new iterate is $h^{n+1} = h^n + \tau^n \hat{h}^n$.

Return: h^n .

The gradient algorithm (II)



The gradient algorithm proceeds by successive steps in the negative direction of the gradient of $J(h)$.

The augmented Lagrangian algorithm (I) [NoWri]

- Let us now consider the **equality-constrained problem**

$$\min_{h \in H} J(h) \text{ s.t. } C(h) = 0,$$

where $J : H \rightarrow \mathbb{R}$ and $C : H \rightarrow \mathbb{R}$ are differentiable.

- One possibility is to replace this problem with the unconstrained one:

$$\min_{h \in H} J(h) + \ell C(h),$$

where $J(h)$ is **penalized** by the constraint $C(h)$, using a fixed weight $\ell > 0$.

- In practice, the “suitable” value ℓ^* for ℓ , i.e. that driving the optimization process to the desired level of constraint $C(h) = 0$, is estimated after a few trial and errors.
- This value ℓ^* can be interpreted as the **Lagrange multiplier** associated to the constraint $C(h) = 0$ at the obtained local minimum.

The augmented Lagrangian algorithm (II)

The **augmented Lagrangian algorithm** reduces the resolution of a constrained optimization problem to a series of **unconstrained** ones, with updated parameters.

Initialization: Start from an initial design h^0 , initial parameters ℓ^0, b^0 .

For $n = 0, \dots$ convergence:

- 1 Solve the **unconstrained** optimization problem:

$$\min_{h \in H} J(h) + \ell^n C(h) + \frac{b^n}{2} C(h)^2,$$

starting from h^n to obtain h^{n+1} .

- 2 Update the optimization parameters via:

$$\ell^{n+1} = \ell^n + b^n C(h^n), \text{ and } b^{n+1} = \begin{cases} \alpha b^n & \text{if } b < b_{\max}, \\ b^n & \text{otherwise.} \end{cases}$$

- ℓ^n and b^n are updated so that the constraint $C(h) = 0$ holds at convergence;
- ℓ^n converges to the optimal Lagrange multiplier for the constraint $C(h) = 0$;
- b^n is a weight for the quadratic penalization of the constraint function $C(h)$.

The augmented Lagrangian algorithm (III)

The following “pragmatic” version involves fewer (costly) evaluations of $J(h)$, $C(h)$, and the derivatives $J'(h)$, $C'(h)$.

Initialization: Start from an initial design h^0 , initial parameters ℓ^0 , b^0 .

For $n = 0, \dots$ convergence:

- 1 Calculate a descent direction \hat{h}^n for the functional:

$$h \mapsto \mathcal{L}(h, \ell^n, b^n) := J(h) + \ell^n C(h) + \frac{b^n}{2} C(h)^2.$$

- 2 Select a suitably small time step so that:

$$\mathcal{L}(h^n + \tau^n \hat{h}^n, \ell^n, b^n) < \mathcal{L}(h^n, \ell^n, b^n).$$

- 3 Update the design via:

$$h^{n+1} = h^n + \tau^n \hat{h}^n.$$

- 4 Update the optimization parameters via:

$$\ell^{n+1} = \ell^n + b^n C(h^{n+1}), \text{ and } b^{n+1} = \begin{cases} \alpha b^n & \text{if } b < b_{\max}, \\ b^n & \text{otherwise.} \end{cases}$$

Part II

Optimal control and parametric optimization problems

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- 2 Numerical algorithms
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Numerical algorithms (I)

We solve the optimization problem:

$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h), \text{ where } J(h) = \int_D j(u_h) \, dx + \ell \int_D h \, dx;$$

in there:

- The set \mathcal{U}_{ad} is: $\mathcal{U}_{\text{ad}} = \{h \in L^\infty(D), \alpha < h(x) < \beta \text{ a.e. } x \in D\}$;
- A **constraint** on the high values of h is added by a fixed **penalization**.

A basic **projected gradient algorithm** then reads:

Initialization: Start from an initial design h^0 ,

For $n = 0, \dots$ **convergence:**

- 1 Calculate the **state** u_{h^n} and the **adjoint** p_{h^n} at $h = h^n$;
- 2 Calculate the descent direction $\hat{h}^n = -\nabla u_{h^n} \cdot \nabla p_{h^n} - \ell$.
- 3 Select an appropriate time step $\tau^n > 0$;
- 4 Update the design as: $h^{n+1} = \min(\beta, \max(\alpha, h^n - \tau^n \hat{h}^n))$.

Numerical algorithms (II)

In practice,

- The domain D is equipped with a fixed mesh \mathcal{T} , composed e.g. of triangles.
- The optimized conductivity h is discretized on this mesh, e.g. as a \mathbb{P}_0 or \mathbb{P}_1 finite element function.
- For a given value of h , the solutions u_h and p_h to the state and adjoint equations are calculated by the **finite element method** on the mesh \mathcal{T} .

One first example: the optimal radiator (I)

We consider the problem:

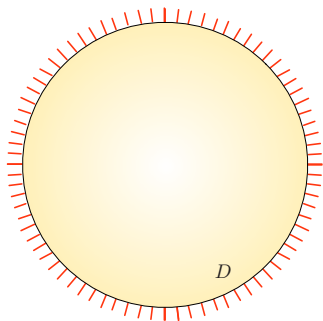
$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h), \text{ where } J(h) = \int_D u_h \, dx + \ell \int_D h \, dx,$$

the temperature $u_h \in H_0^1(D)$ is the solution to:

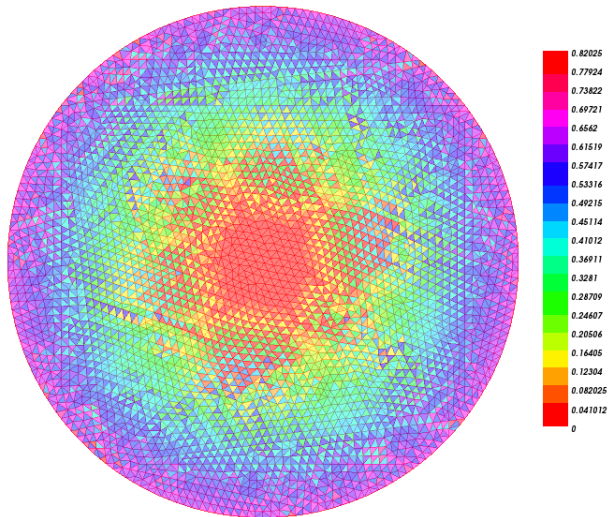
$$\begin{cases} -\operatorname{div}(h \nabla u_h) = 1 & \text{in } D, \\ u_h = 0 & \text{on } \partial D. \end{cases}$$

In other terms,

- The **mean temperature** inside D is minimized;
- A constraint on the high values of the conductivity is added by a **fixed penalization** of the objective function.



One first example: the optimal radiator (II)



Optimized density in the thermal radiator problem.

One first example: the optimal radiator (III)

- This oscillatory behavior is actually not surprising: the algorithm tries to reproduce the “homogenized” behavior of solutions.
- It is however highly undesirable in practice.
- One remedy consists in acting on the selected descent direction, by changing inner products, a general idea which fulfills many other purposes.
- Other solutions are presented later in the course.

Changing inner products (I)

- By definition of the Fréchet derivative, the following expansion holds:

$$J(h + \tau \hat{h}) = J(h) + \tau J'(h)(\hat{h}) + o(\tau),$$

and a **descent direction** for J from h is any $\hat{h} \in L^\infty(D)$ such that $J'(h)(\hat{h}) < 0$.

- The formula for the derivative

$$J'(h)(\hat{h}) = \int_D \hat{h} \nabla u_h \cdot \nabla p_h \, dx$$

makes it very natural to take as a descent direction the **$L^2(D)$ gradient** of $J'(h)$:

$$\hat{h} = -\nabla u_h \cdot \nabla p_h,$$

i.e. the gradient associated to the differential $J'(h)$ via the $L^2(D)$ dual pairing.

- This choice is actually awkward: ∇u_h and ∇p_h are **not very regular**, and nor is \hat{h} . In the theoretical framework, \hat{h} does not even belong to $L^\infty(D)$!
- Other, more adapted choices of a descent direction are possible, as **gradients** of $J'(h)$ obtained with other inner products than that of $L^2(D)$.

Changing inner products (II)

Let H be a Hilbert space with inner product $\langle \cdot, \cdot \rangle_H$.

Solve the following **identification problem**: Search for $V \in H$ such that:

$$\forall w \in H, \langle V, w \rangle_H = J'(h)(w) = \int_D w \nabla u_h \cdot \nabla p_h \, dx.$$

Then $-V$ is also a descent direction for $J(h)$, since for $\tau > 0$ small enough:

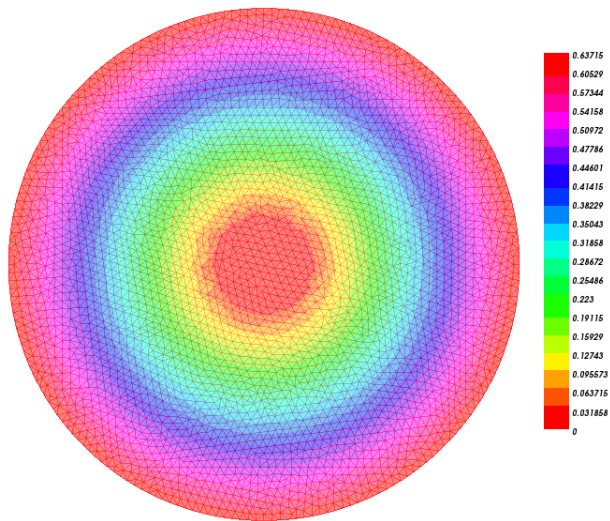
$$\begin{aligned} J(h - \tau V) &= J(h) - \tau J'(h)(V) + o(\tau) \\ &= J(h) - \tau \langle V, V \rangle_H + o(\tau) \\ &< J(h). \end{aligned}$$

Example: A descent direction which is **more regular** than that supplied by the $L^2(D)$ inner product is obtained with the choice:

$$H = H^1(D), \text{ and } \langle u, v \rangle_H = \int_D (\alpha^2 \nabla u \cdot \nabla v + uv) \, dx,$$

for α “small” (of the order of the mesh size).

The optimal radiator again



Optimized density for the thermal radiator problem using the “change of inner product” trick.

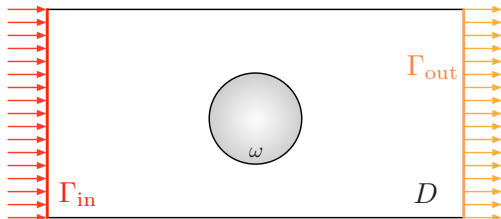
Another example: design of a “heat lens” (I)

As proposed in [Che], the problem

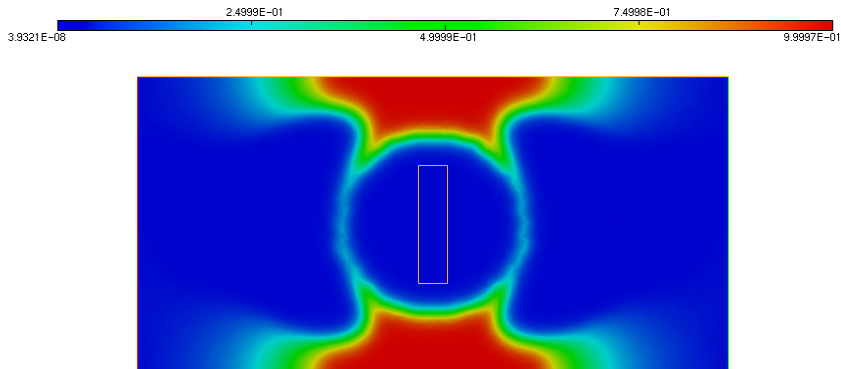
$$\min J(h) \text{ where } J(h) = \int_{\omega} \left| \alpha \frac{\partial u_h}{\partial x_1} \right|^2 dx + \ell \int_D h dx$$

is considered:

- The **horizontal heat flux** through a non optimizable region ω is minimized;
- A **penalization** on high values of the conductivity h is added.



Another example: design of a “heat lens” (II)



Optimized heat lens under a penalization of high values of the conductivity.

- The above strategy to impose a constraint on the amount of high conductivity material is very crude. Other constrained optimization algorithms may be used, such as the **Augmented Lagrangian algorithm**.
- This parametric optimization framework lends itself to the use of:
 - Quasi-Newton methods, such as the **Gauss-Newton** or the **BFGS** algorithms;
 - “True” second-order algorithms, based on the **Hessian** of the mapping $h \mapsto J(h)$.
- **Density-based methods** for **topology optimization problems** often rely on an adaptation of this parametric framework.

Technical appendix

The Lax Milgram theorem

In a **Hilbert space** H , let $a : H \times H \rightarrow \mathbb{R}$ be a bilinear form and $\ell : H \rightarrow \mathbb{R}$ be a linear form such that:

- a is **continuous**, i.e. there exists $M > 0$ such that:

$$\forall u, v \in H, |a(u, v)| \leq M \|u\|_H \|v\|_H.$$

- a is **coercive**, i.e. there exists $\alpha > 0$ such that:

$$\forall u \in H, \alpha \|u\|_H^2 \leq a(u, u).$$

- ℓ is **continuous** (i.e. ℓ belongs to the **dual space** H^*):

$$\|\ell\|_{H^*} := \sup_{\substack{v \in H \\ v \neq 0}} \frac{|\ell(v)|}{\|v\|_H} < \infty.$$

Theorem 3.

Under the above hypotheses, the variational problem

$$\text{Search for } u \in H \text{ s.t. for all } v \in H, a(u, v) = \ell(v)$$

has a unique solution $u \in H$, which depends continuously on ℓ :

$$\|u\|_H \leq \frac{M}{\alpha} \|\ell\|_{H^*}.$$

Fréchet and Gateaux derivatives

Several notions of **derivative** are available for a function $F : U \rightarrow V$ between two normed vector spaces $(U, \|\cdot\|_U)$ and $(V, \|\cdot\|_V)$.

Definition 3 (Fréchet differentiability).

- A function $F : U \rightarrow V$ is called **Fréchet differentiable** at some point $x \in U$ if there exists a linear, continuous mapping $L_x : U \rightarrow V$ such that:

$$F(x + v) = F(x) + L_x(v) + o(\|v\|_U), \text{ where } \frac{\|o(\|v\|_U)\|_V}{\|v\|_U} \xrightarrow{v \rightarrow 0} 0.$$

- The mapping $v \mapsto L_x(v)$ is denoted by $v \mapsto F'(x)(v)$, or $d_x F(v)$ and is called the **differential** or the **Fréchet derivative** of F at x .
- The function $F : U \rightarrow V$ is called **Gateaux differentiable** at $x \in U$ if for any direction $v \in U$, the following limit exists:

$$\lim_{\substack{t \rightarrow 0 \\ t > 0}} \frac{F(x + tv) - F(x)}{t}.$$

Remark: The notion of **Fréchet differentiability** is stronger than that of **Gateaux differentiability**, which is a generalization of **directional differentiability**.

Fréchet derivatives: the “chain rule”

The **chain rule** is a *fundamental result*, which supplies the **Fréchet derivative** of the **composite** $G \circ F$ of two functions

$$F : U \rightarrow V \text{ and } G : V \rightarrow W$$

between three normed vector spaces $(U, \|\cdot\|_U)$, $(V, \|\cdot\|_V)$ and $(W, \|\cdot\|_W)$.

Theorem 4 (Chain rule).

Let $x \in U$ be a point such that:

- F is Fréchet differentiable at x ;
- G is Fréchet differentiable at $F(x) \in V$.

Then, the composite function $G \circ F : U \rightarrow W$ is **Fréchet differentiable** at x , and its Fréchet derivative $v \mapsto (G \circ F)'(x)(v)$ is the linear mapping defined by:

$$\forall v \in U, (G \circ F)'(x)(v) = G'(F(x))(F'(x)(v)).$$

The implicit function theorem

The **implicit function theorem** is a key result, ensuring the **existence** and **smoothness** of a solution $u = u_\theta$ to a parametrized, non linear equation of the form:

$$\mathcal{F}(\theta, u) = 0,$$

where u is the unknown and θ is a “parameter”; see [La], Chap. I, Th. 5.9.

Theorem 5 (Implicit function theorem).

Let Θ, E, F be Banach spaces, $\mathcal{V} \subset \Theta$, $U \subset E$ be open sets. and $\mathcal{F} : \mathcal{V} \times U \rightarrow G$ be a function of class \mathcal{C}^p for $p \geq 1$. Let $(\theta_0, u_0) \in \mathcal{V} \times U$ be such that $\mathcal{F}(\theta_0, u_0) = 0$ and assume that:

*The differential $d_u \mathcal{F}(\theta_0, u_0) : F \rightarrow G$ is a linear **isomorphism**.*

Then there exist open subsets $\mathcal{V}' \subset \mathcal{V}$ of θ_0 in Θ and $U' \subset U$ of u_0 in E , and a mapping $g : \mathcal{V}' \rightarrow U'$ of class \mathcal{C}^p satisfying the properties:

- 1 $g(\theta_0) = u_0$,
- 2 For all $\theta \in \mathcal{V}'$, the equation $\mathcal{F}(\theta, u) = 0$ has a unique solution $u \in U'$, given by $u = g(\theta)$.

First-order necessary optimality conditions (I)

Let H be a Hilbert space, and let $J : H \rightarrow \mathbb{R}$ be a differentiable function; we consider the **unconstrained** minimization problem:

$$\min_{u \in H} J(u). \quad (UC)$$

Definition 4.

A point $u \in H$ is a **local minimizer** for (UC) if there exists an open neighborhood $V \subset H$ containing u such that:

$$\forall v \in V, J(u) \leq J(v).$$

Theorem 6.

Let u be a local minimize for (UC); then:

$$\nabla J(u) = 0.$$

First-order necessary optimality conditions (II)

Proof: Let $h \in H$ be given; by the definition of u , it holds for $t > 0$ small enough:

$$J(u + th) \geq J(u), \text{ and so } \frac{J(u + th) - J(u)}{t} \geq 0.$$

Letting $t \rightarrow 0$, the differentiability of J yields:

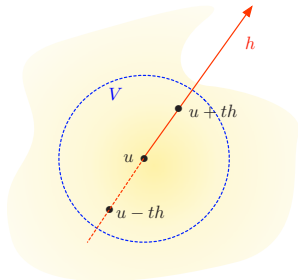
$$J'(u)(h) = \langle \nabla J(u), h \rangle \geq 0.$$

Replacing h by $-h$ in the previous argument yields the converse inequality

$$\langle \nabla J(u), h \rangle \leq 0,$$

which completes the proof. □

Remark The above proof uses in a crucial way that the point u in (UC) minimizes $J(v)$ (locally) in **any** direction $h \in H$.



□

First-order necessary optimality conditions (III)

Let H be a Hilbert space, and let $J : H \rightarrow \mathbb{R}$ and $C : H \rightarrow \mathbb{R}^p$ be differentiable functions; we consider the **equality-constrained** minimization problem:

$$\min_{h \in H} J(h) \text{ s.t. } C(h) = 0. \quad (\text{EC})$$

Definition 5.

A point $u \in H$ is a **local minimizer** for (EC) if there exists an open neighborhood $V \subset H$ containing u such that:

$$\forall v \in V \text{ s.t. } C(v) = 0, \quad J(u) \leq J(v).$$

Theorem 7 (First-order necessary optimality conditions).

Let u be a local minimizer for (EC), and assume that the gradients $\nabla C_1(u), \dots, \nabla C_p(u)$ are **linearly independent**. Then there exist **Lagrange multipliers** $\lambda_1, \dots, \lambda_p \in \mathbb{R}$ such that:

$$\nabla J(u) + \sum_{i=1}^p \lambda_i \nabla C_i(u) = 0.$$

First-order necessary optimality conditions (IV)

Hint of proof:

- The local optimality of u no longer implies that, for arbitrary $h \in H$ and t small enough,

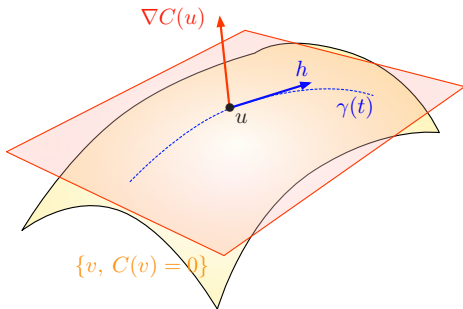
$$J(u + th) \geq J(u).$$

- Such an inequality can only be written with directions h in the **admissible space**:

$$K(u) := \{h \in H, \text{ there exists } \varepsilon > 0 \text{ and a curve } \gamma : [-\varepsilon, \varepsilon] \rightarrow H \text{ s.t.} \\ \gamma(0) = u, \gamma'(0) = h \text{ and } C(\gamma(t)) = 0 \text{ for } t > 0\}.$$

- $K(u)$ is a **vector space**, which rewrites, using the **implicit function theorem**:

$$K(u) = \bigcap_{i=1}^p \{\nabla C_i(u)\}^\perp.$$



First-order necessary optimality conditions (II)

- For any $h \in K(u)$, introducing a curve $\gamma(t)$ with the above properties:

$$J(\gamma(t)) \geq J(u), \text{ and so } \frac{J(\gamma(t)) - J(u)}{t} \geq 0.$$

Taking limits, it follows,

$$\langle \nabla J(u), h \rangle \geq 0.$$

Since $K(u)$ is a **vector space**, the same argument applies to $-h$, and so:

$$\langle \nabla J(u), h \rangle = 0.$$

- Hence, we have proved that

$$\forall h \in K(u) \quad \langle \nabla J(u), h \rangle = 0, \text{ that is } \nabla J(u) \in \left(\bigcap_{i=1}^p \{ \nabla C_i(u) \}^\perp \right)^\perp.$$

- Finally, using the general fact that, for arbitrary subsets $A_1, \dots, A_p \subset H$,

$$(\text{span} \{ A_i, i = 1, \dots, p \})^\perp = \bigcap_{i=1}^p A_i^\perp,$$

the desired result follows.

First-order necessary optimality conditions (III)

Interpretation (when $p = 1$): The above optimality condition implies that:

- Either $\nabla J(u) = 0$, which is the necessary first-order optimality condition for u to be an **unconstrained** minimizer of $J(v)$.
- Or $\lambda \neq 0$, and so,

$$\nabla C(u) = -\frac{1}{\lambda} \nabla J(u).$$

- “At first order”, a direction $h \in H$ such that $J(u + th) < J(u)$ for small $t > 0$, has a non zero coordinate along $\nabla J(u)$:
 $h = \alpha \nabla J(u) + v$, where $v \perp \nabla J(u), \alpha < 0$.
- Alternatively, h rewrites:.
 $h = \beta \nabla C(u) + w$, where $w \perp \nabla C(u), \beta \neq 0$.
- Hence, $C(u + th) \neq 0$, so that $u + th$ is not an admissible point in (EC).

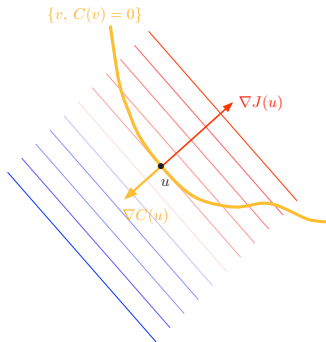













Illustration when $H = \mathbb{R}^2$, $p = 1$ and J is an affine function, whose isolines are depicted. At a local optimum u of (EC), $\nabla J(u)$ and $\nabla C(u)$ are aligned.

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