OPTIMAL DESIGN OF STRUCTURES (MAP 562)

CHAPTER III

PREREQUISITES OF OPTIMIZATION

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Definitions

Let V be a Banach space, i.e., a normed vector space which is complete (any Cauchy sequence is converging in V).
Let $K \subset V$ be a non-empty subset. Let $J : V \to \mathbb{R}$. We consider

$$\inf_{v \in K \subset V} J(v).$$

Definition

An element u is called a local minimizer of J on K if

$$u \in K \quad \text{and} \quad \exists \delta > 0 \text{ s.t. } \forall v \in K \,, \; \|v - u\| < \delta \Rightarrow J(v) \geq J(u) \,.$$

An element u is called a global minimizer of J on K if

$$u \in K \quad \text{and} \quad J(v) \geq J(u) \quad \forall v \in K \,.$$

(difference: theory $\leftrightarrow$ global / numerics $\leftrightarrow$ local)

Definition

A *minimizing sequence* *of a function* J *on the set* K *is a sequence* $(u^n)_{n\in\mathbb{N}}$ *such that*

$$u^n \in K \ \forall\, n \quad \text{and} \quad \lim_{n\to+\infty} J(u^n) = \inf_{v\in K} J(v).$$

By definition of the infimum value of J on K there always exist minimizing sequences !

Optimization in finite dimension $V = \mathbb{R}^N$

Theorem

Let K be a non-empty closed subset of $\mathbb{R}^N$ and J a (lower semi-) continuous function from K to $\mathbb{R}$ satisfying the so-called "infinite at infinity" property, i.e.,

$$\forall (u^n) \text{ sequence in } K\ , \quad \lim_{n\to+\infty} \|u^n\| = +\infty \Rightarrow \lim_{n\to+\infty} J(u^n) = +\infty\ .$$

Then there exists at least one minimizer of J on K. Furthermore, from each minimizing sequence of J on K one can extract a subsequence which converges to a minimum of J on K.

Idea of the proof

The sets $\{u \in K, J(u) \leq c\}$ are closed and bounded, hence compact in finite dimension $\Rightarrow$ minimizing sequences admit converging subsequences. By continuity, such a limit is a global minimizer.

Optimization in infinite dimension

Difficulty: a continuous function on a closed bounded set does not necessarily attain its minimum !

Counter-example of non-existence: let $H^1(0,1)$ be the usual Sobolev space with its norm $\|v\| = \left(\int_0^1 \left(v'(x)^2 + v(x)^2\right) dx\right)^{1/2}$. Let

$$J(v) = \int_0^1 \Big((|v'(x)| - 1)^2 + v(x)^2 \Big) dx \, .$$

One can check that J is continuous and "infinite at infinity". Nevertheless the minimization problem

$$\inf_{v \in H^1(0,1)} J(v)$$

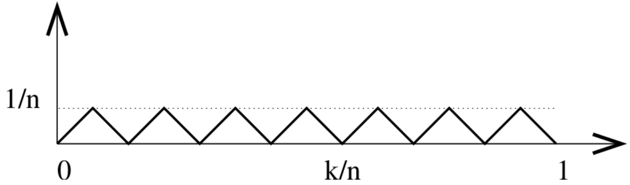
does not admit a minimizer.

Proof

There exists no $v \in H^1(0,1)$ such that $J(v) = 0$ but, still,

$$\left(\inf_{v \in H^1(0,1)} J(v) \right) = 0,$$

since, upon defining the sequence u^n such that $(u^n)' = \pm 1$,



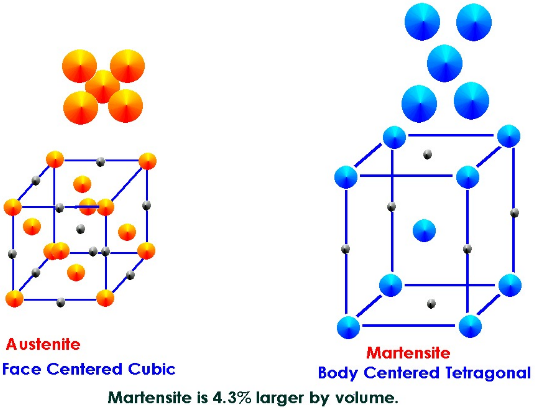
we check that $J(u^n) = \int_0^1 u^n(x)^2 dx = \frac{1}{4n} \to 0$.
We clearly see in this example that the minimizing sequence u^n is "oscillating" more and more and is not compact in $H^1(0,1)$ (although it is bounded in the same space).

A parenthesis in material sciences

The non-existence of minimizers for minimization problems is observed in material sciences !

The Ball-James theory (1987).

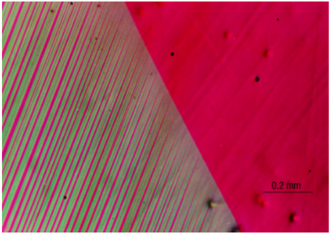
Co-existence of several crystalline phases: austenite and martensite.

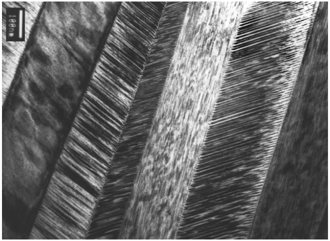


J. Ball and R. James proposed the following mechanism: to sustain the applied forces, the alloy has a tendency to coexist under different phases which minimize the energy.

$\Rightarrow$ **non-converging minimizing sequence forming microscopic patterns !**

Cu-Al-Ni alloy (courtesy of YONG S. CHU)





Convexity

To obtain the existence of minimizers we add a convexity assumption.

Definition

A set $K \subset V$ is said to be **convex** *if, for any $x, y \in K$ and for any $\theta \in [0,1]$, $\theta x + (1-\theta)y$ belongs to K.*

Definition

A function J, defined from a non-empty convex set $K \in V$ into $\mathbb{R}$ is **convex** *on K if*

$$J(\theta u + (1-\theta)v) \leq \theta J(u) + (1-\theta)J(v) \quad \forall\, u, v \in K \;,\; \forall\, \theta \in [0,1] \,.$$

Furthermore, J is **strictly convex** *if the inequality is strict whenever $u \neq v$ and $\theta \in]0,1[$.*

Existence result

Theorem

Let K be a non-empty closed convex set in a reflexive Banach space V, and J a convex continuous function on K, which is "infinite at infinity" in K, i.e.,

$$\forall (u^n) \textit{ sequence in } K \; , \; \lim_{n \to +\infty} \|u^n\| = +\infty \Longrightarrow \lim_{n \to +\infty} J(u^n) = +\infty \; .$$

Then, there exists a minimizer of J in K.

Remarks:

1. V reflexive Banach space $\Leftrightarrow (V')' = V$ (V' is the topological dual of V). Hence Hilbert spaces are reflexive.
2. The proof relies on compactness arguments for weak topologies.

Uniqueness

Proposition. If J is strictly convex, then there exists at most one minimizer of J.

Proposition. If J is convex on the convex set K, then any local minimizer of J on K is a global minimizer.

Remark. For convex functions there is no difference between local and global minimizers.

Remark. Convexity and reflexivity are not the only tools to prove existence of minimizers. The general argument relies on (weak) compactness of minimizing sequences and (weak) lower semicontinuity of J.

Differentiability

Definition

Let V be a normed vector space. A function J, defined from a neighborhood of $u \in V$ into $\mathbb{R}$, is said to be differentiable in the sense of Fréchet at u if there exists a continuous linear functional on V, $L \in V'$, such that

$$J(u+w) = J(u) + L(w) + o(w) \quad , \quad \text{with} \quad \lim_{w \to 0} \frac{|o(w)|}{\|w\|} = 0 \, .$$

We call L the differential (or derivative) of J at u and we denote it by $L = J'(u)$, or $L(w) = \langle J'(u), w \rangle_{V',V}$.

- If V is a Hilbert space then its dual V' can be identified with V itself by the Riesz representation theorem. Thus, there exists a unique $p \in V$, called gradient of J, such that $\langle p, w \rangle = L(w)$. We write by abuse of notation $p = J'(u)$.
- We use this identification $V = V'$ if $V = \mathbb{R}^n$ or $V = L^2(\Omega)$.
- Linear, bilinear functions and compositions of differentiable functions are differentiable.

Directional derivatives

A weaker notion of derivative is the following.

Definition

Let V be a normed vector space. A function J, defined from a neighborhood of $u \in V$ into $\mathbb{R}$, is said to admit a derivative in the direction w at u if the function

$$t \mapsto J(u + tw)$$

has a derivative in 0*. We denote* $j'(0) = J'(u; w)$*.*

Lemma. If J is differentiable at u then it admits derivatives in any directions and

$$\langle J'(u), w \rangle_{V',V} = J'(u; w) \qquad \forall w \in V.$$

A basic example to remember

Consider the variational formulation

$$\text{find } u \in V \text{ such that } a(u, w) = L(w) \quad \forall\, w \in V$$

where a is a symmetric coercive continuous bilinear form and L is a continuous linear functional.
Define the energy

$$J(v) = \frac{1}{2} a(v, v) - L(v)$$

Lemma. u is the unique minimizer of J

$$J(u) = \min_{v \in V} J(v)$$

Proof. We first compute

$$J(\theta u + (1 - \theta v)) - \theta J(u) - (1 - \theta) J(v) = -\frac{\theta(1 - \theta)}{2} a(u - v, u - v).$$

Hence J is strictly convex.

Then we check that the necessary and sufficient optimality condition $J'(u) = 0$ is equivalent to the variational formulation.

Computing the directional derivative is simpler than computing $J'(v)$!

We define $j(t) = J(u + tw)$

$$j(t) = \frac{t^2}{2} a(w,w) + t\Big(a(u,w) - L(w)\Big) + J(u)$$

and we differentiate $t \to j(t)$ (a polynomial of degree 2 !)

$$j'(t) = ta(w,w) + \Big(a(u,w) - L(w)\Big).$$

By definition, $j'(0) = \langle J'(u), w \rangle_{V',V}$, thus

$$\langle J'(u), w \rangle_{V',V} = a(u,w) - L(w).$$

It is not obvious to deduce a formula for $J'(u)$...
but it is enough, most of the time, to know $\langle J'(u), w \rangle_{V',V}$.

Examples: here we use the "usual" scalar product in L^2 (somehow canonical: distributions)

1. $J(v) = \int_\Omega \left(\frac{1}{2}v^2 - fv\right) dx$ with $v \in V = L^2(\Omega)$

$$\langle J'(u), w\rangle_{V',V} = \int_\Omega (uw - fw)\, dx.$$

Thus

$$J'(u) = u - f \ \in L^2(\Omega) \text{ (identified with its dual)}$$

2. $J(v) = \int_\Omega \left(\frac{1}{2}|\nabla v|^2 - fv\right) dx$ with $v \in V = H_0^1(\Omega)$

$$\langle J'(u), w\rangle_{V',V} = \int_\Omega (\nabla u \cdot \nabla w - fw)\, dx.$$

Therefore, after formal integration by parts,

$$J'(u) = -\Delta u - f \ \in H^{-1}(\Omega) = \left(H_0^1(\Omega)\right)'$$

(not identified with its dual)

Explanation. The L^2 scalar product does not endow $H_0^1(\Omega)$ with a Hilbert structure.
If instead of the L^2 scalar product we rather use the "true" H^1 scalar product, then we identify $J'(u)$ with a different function.
From the derivative

$$\langle J'(u), w\rangle_{V',V} = \int_\Omega (\nabla u \cdot \nabla w - fw)\, dx,$$

using the H^1 scalar product $\langle \phi, w\rangle = \int_\Omega (\nabla \phi \cdot \nabla w + \phi w)\, dx$, we infer

$$-\Delta J'(u) + J'(u) = -\Delta u - f, \quad J'(u) \in H_0^1(\Omega).$$

Here we identify $H_0^1(\Omega)$ with its dual. To get the gradient from the directional derivative we must solve a BVP.

Remarks. In case 1 we can restrict to $H^1(\Omega)$ and use the H^1 scalar product, too, to get a different gradient.

Optimality conditions

Theorem (Euler inequality)

Let $u \in K \subset V$ with K convex. We assume that J is differentiable at u. If u is a local minimizer of J in K, then

$$\langle J'(u), v - u \rangle_{V',V} \geq 0 \quad \forall\, v \in K \,.$$

If $u \in K$ satisfies this inequality and if J is convex, then u is a global minimizer of J in K.

Remarks.

- If u belongs to the interior of K, we deduce the Euler equation $J'(u) = 0$.
- The Euler inequality is usually just a necessary condition. It becomes necessary and sufficient for convex functions.

Minimization with equality constraints

Consider

$$\inf_{v \in V,\ F(v)=0} J(v)$$

with $F(v) = (F_1(v), ..., F_M(v))$ differentiable from V into $\mathbb{R}^M$.

Definition

We call **Lagrangian** *of this problem the function*

$$\mathcal{L}(v,\mu) = J(v) + \sum_{i=1}^{M} \mu_i F_i(v) = J(v) + \mu \cdot F(v) \qquad \forall (v,\mu) \in V \times \mathbb{R}^M.$$

The new variable $\mu \in \mathbb{R}^M$ is called **Lagrange multiplier** *for the constraint $F(v) = 0$.*

Lemma. The constrained minimization problem is equivalent to

$$\inf_{v \in V,\ F(v)=0} J(v) = \inf_{v \in V} \sup_{\mu \in \mathbb{R}^M} \mathcal{L}(v,\mu).$$

Stationarity of the Lagrangian

Theorem

Assume that J and F are continuously differentiable in a neighborhood of $u \in V$ such that $F(u) = 0$. If u is a local minimizer and if the vectors $\big(F_i'(u)\big)_{1 \leq i \leq M}$ are linearly independent, then there exist Lagrange multipliers $\lambda_1, \ldots, \lambda_M \in \mathbb{R}$ such that

$$\frac{\partial \mathcal{L}}{\partial v}(u, \lambda) = J'(u) + \lambda \cdot F'(u) = 0 \quad \text{and} \quad \frac{\partial \mathcal{L}}{\partial \mu}(u, \lambda) = F(u) = 0 \, .$$

Minimization with inequality constraints

Consider

$$\inf_{v \in V,\ F(v) \leq 0} J(v)$$

where $F(v) \leq 0$ means that $F_i(v) \leq 0$ for $1 \leq i \leq M$, with $F_1, \ldots, F_M$ differentiable from V to $\mathbb{R}$.

Definition

Let u be such that $F(u) \leq 0$. The set

$$I(u) = \{i \in \{1, \ldots, M\} \ s.t.\ F_i(u) = 0\}$$

is called the set of active constraints at u. The inequality constraints are said to be qualified at $u \in K$ if the vectors $(F_i'(u))_{i \in I(u)}$ are linearly independent.

Definition

We call Lagrangian of the previous problem the function

$$\mathcal{L}(v,\mu) = J(v) + \sum_{i=1}^{M} \mu_i F_i(v) = J(v) + \mu \cdot F(v) \qquad \forall (v,\mu) \in V \times (\mathbb{R}_+)^M.$$

The new **non-negative** *variable $\mu \in (\mathbb{R}_+)^M$ is called Lagrange multiplier for the constraint $F(v) \leq 0$.*

Lemma. The constrained minimization problem is equivalent to

$$\inf_{v \in V,\ F(v) \leq 0} J(v) = \inf_{v \in V} \sup_{\mu \in (\mathbb{R}_+)^M} \mathcal{L}(v,\mu).$$

Stationarity of the Lagrangian

Theorem

We assume that the constraints are qualified at u satisfying $F(u) \leq 0$. If u is a local minimizer, then there exist Lagrange multipliers $\lambda_1, \ldots, \lambda_M \geq 0$ such that

$$J'(u) + \sum_{i=1}^{M} \lambda_i F_i'(u) = 0 \,, \quad \lambda_i \geq 0 \,, \quad \underbrace{\lambda_i = 0 \text{ if } F_i(u) < 0}_{\Leftrightarrow \lambda_i F_i(u) = 0} .$$

This condition is indeed the stationarity of the Lagrangian since

$$\frac{\partial \mathcal{L}}{\partial v}(u, \lambda) = J'(u) + \lambda \cdot F'(u) = 0,$$

and the condition $\lambda \geq 0$, $F(u) \leq 0$, $\lambda \cdot F(u) = 0$ is equivalent to the Euler inequality for the **maximization** with respect to μ in the closed convex set $(\mathbb{R}_+)^M$

$$\frac{\partial \mathcal{L}}{\partial \mu}(u, \lambda) \cdot (\mu - \lambda) = F(u) \cdot (\mu - \lambda) \leq 0 \quad \forall \mu \in (\mathbb{R}_+)^M .$$

Interpreting the Lagrange multipliers

Define the Lagrangian for the minimization of $J(v)$ under the equality constraint $F(v) + c = 0$

$$\mathcal{L}(v, \mu, c) = J(v) + \mu \cdot (F(v) + c) .$$

We study the sensitivity of the minimal value with respect to variations of c.

Let $u(c)$ and $\lambda(c)$ be the minimizer and the optimal Lagrange multiplier. We assume that they are differentiable with respect to c. Then

$$\nabla_c \Big(J(u(c)) \Big) = \lambda(c).$$

λ gives the derivative of the minimal value with respect to c without any further calculation ! Indeed

$$\nabla_c \Big(J(u(c)) \Big) = \nabla_c \Big(\mathcal{L}(u(c), \lambda(c), c) \Big) = \frac{\partial \mathcal{L}}{\partial c}(u(c), \lambda(c), c) = \lambda(c)$$

because

$$\frac{\partial \mathcal{L}}{\partial v}(u(c), \lambda(c), c) = 0 \quad , \quad \frac{\partial \mathcal{L}}{\partial \mu}(u(c), \lambda(c), c) = 0 .$$

Duality and saddle point

Definition

Let $\mathcal{L}(v,q)$ be a Lagrangian. We call $(u,p) \in U \times P$ a saddle point (or mountain pass, or min-max) of $\mathcal{L}$ in $U \times P$ if

$$\forall\, q \in P \qquad \mathcal{L}(u,q) \le \mathcal{L}(u,p) \le \mathcal{L}(v,p) \quad \forall\, v \in U\,.$$

For $v \in U$ and $q \in P$, define $\mathcal{J}(v) = \sup_{q\in P} \mathcal{L}(v,q)$ and $\mathcal{G}(q) = \inf_{v\in U} \mathcal{L}(v,q)$. We call primal problem and dual problem, respectively

$$(\mathcal{P}) \qquad \inf_{v\in U} \mathcal{J}(v) = \inf_{v\in U} \sup_{q\in P} \mathcal{L}(v,q)\,,$$

$$(\mathcal{D}) \qquad \sup_{q\in P} \mathcal{G}(q) = \sup_{q\in P} \inf_{v\in U} \mathcal{L}(v,q)\,.$$

Example. $U = V$, $P = \mathbb{R}^M$ or $\mathbb{R}^M_+$, and $\mathcal{L}(v,q) = J(v) + q \cdot F(v)$. In this case $\mathcal{J}(v) = J(v)$ if $F(v) = 0$ and $\mathcal{J}(v) = +\infty$ otherwise, while there is no constraints for the dual problem (except $q \in P$).

Lemma (weak duality). It always holds true that

$$\inf_{v \in U} \mathcal{J}(v) \geq \sup_{q \in P} \mathcal{G}(q).$$

Proof:
$\mathcal{L}(u,q) \geq \inf_v \mathcal{L}(v,q) \Rightarrow \sup_q \mathcal{L}(u,q) \geq \sup_q \inf_v \mathcal{L}(v,q), \qquad \forall u$
$\Rightarrow \inf_v \sup_q \mathcal{L}(v,q) \geq \sup_q \inf_v \mathcal{L}(v,q).$

Theorem (strong duality)

The pair (u,p) is a saddle point of $\mathcal{L}$ in $U \times P$ if and only if

$$\mathcal{J}(u) = \min_{v \in U} \mathcal{J}(v) = \max_{q \in P} \mathcal{G}(q) = \mathcal{G}(p) \ .$$

Remark. The dual problem is often simpler than the primal one because it has no constraints. After solving the dual, the primal solution is among the solutions of the unconstrained problem

$$\inf_{v \in U} \mathcal{L}(v,p) \ .$$

Application: dual or complementary energy

Very important for the sequel !

Let $f \in L^2(\Omega)$. We already know that solving

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

is equivalent to minimizing the (primal) energy

$$\min_{v \in H_0^1(\Omega)} \left\{ J(v) = \frac{1}{2} \int_\Omega |\nabla v|^2 dx - \int_\Omega fv \, dx \right\}.$$

We introduce a dual or complementary energy

$$\max_{\substack{\tau \in L^2(\Omega)^N \\ -\operatorname{div}\tau = f \text{ in } \Omega}} \left\{ G(\tau) = -\frac{1}{2} \int_\Omega |\tau|^2 dx \right\}.$$

J is convex and G is concave.

Proposition. Let $u \in H_0^1(\Omega)$ be the unique solution of the BVP. Defining $\sigma = \nabla u$ we have

$$\boxed{J(u) = \min_{v \in H_0^1(\Omega)} J(v) = \max_{\substack{\tau \in L^2(\Omega)^N \\ -\mathrm{div}\tau = f \text{ in } \Omega}} G(\tau) = G(\sigma)}$$

and σ is the unique maximizer of G.

Proof. We define the Lagrangian in $H_0^1(\Omega) \times L^2(\Omega)^N$

$$\mathcal{L}(v, \tau) = J(v) - \frac{1}{2} \int_\Omega |\tau - \nabla v|^2 dx.$$

Clearly

$$J(v) = \max_{\tau \in L^2(\Omega)} \mathcal{L}(v, \tau).$$

By expanding and integrating by parts

$$\mathcal{L}(v, \tau) = -\frac{1}{2} \int_\Omega |\tau|^2 dx - \int_\Omega (f + \mathrm{div}\tau) v \, dx.$$

v is a Lagrange multiplier for the constraint $-\mathrm{div}\tau = f$.

(end of the proof)
By definition, if τ satisfies the constraint $-\mathrm{div}\tau = f$, we have

$$G(\tau) = \mathcal{L}(v, \tau) \quad \forall v.$$

Of course,

$$\mathcal{L}(v, \tau) \leq \max_{\tau} \mathcal{L}(v, \tau) = J(v).$$

The variational formulation yields $\int_\Omega |\nabla u|^2 dx = \int_\Omega fu\, dx$, thus

$$J(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 dx - \int_\Omega fu\, dx = -\frac{1}{2}\int_\Omega |\nabla u|^2 dx = G(\nabla u).$$

In other words, for any τ satisfying $-\mathrm{div}\tau = f$,

$$G(\tau) = \mathcal{L}(u, \tau) \leq J(u) = G(\sigma)$$

which means that $\sigma = \nabla u$ is a maximizer of G among all τ such that $-\mathrm{div}\tau = f$.

Numerical algorithms for minimization problems

A simplified classification:

- Stochastic algorithms: global minimization. Examples: Monte-Carlo, simulated annealing, genetic.
  Inconvenient: high CPU cost.
- Deterministic algorithms: local minimization. Examples: gradient methods, Newton.
  Inconvenient: they require the gradient (or further derivatives) of the objective function.

Gradient descent with optimal step

The goal is to solve in V Hilbert space

$$\inf_{v \in V} J(v) \ .$$

Initialization: choose $u^0 \in V$.
Iterations: for $n \geq 0$

$$u^{n+1} = u^n - \mu^n J'(u^n) \ ,$$

where $\mu^n \in \mathbb{R}$ is chosen at each iteration such that

$$J(u^{n+1}) = \inf_{\mu \in \mathbb{R}_+} J\big(u^n - \mu J'(u^n)\big) \ .$$

Main idea: if $u^{n+1} = u^n + \mu w^n$ with a small $\mu > 0$, then

$$J(u^{n+1}) = J(u^n) + \mu \langle J'(u^n), w^n \rangle + \mathcal{O}(\mu^2),$$

thus, to decrease J, the best "first order" choice is w^n proportional to $-J'(u^n)$.

Convergence

Theorem

Assume that J is differentiable, strongly convex with $\alpha > 0$, i.e.

$$\langle J'(u) - J'(v), u - v\rangle \geq \alpha \|u - v\|^2 \quad \forall\, u, v \in V,$$

and J' is Lipschitz on any bounded set of V, i.e.,

$$\forall\, M > 0\,, \exists\, C_M > 0\,, \|v\| + \|w\| \leq M \;\Rightarrow\; \left\|J'(v) - J'(w)\right\| \leq C_M \|v - w\|.$$

Then the gradient algorithm with optimal step converges: for any u^0, the sequence (u^n) converges to the unique minimizer u.

Remark. If J is not strongly convex:

- the algorithm may not converge because it oscillates between several minimizers,
- the algorithm may converge to a local minimizer,
- the minimizer obtained by the algorithm may vary with the initialization.

Gradient descent with a fixed step

The goal is to solve

$$\inf_{v \in V} J(v) \, .$$

Initialization: choose $u^0 \in V$.
Iterations: for $n \geq 0$

$$u^{n+1} = u^n - \mu \, J'(u^n) \, .$$

Theorem

Assume that J is differentiable, strongly convex, and J' is Lipschitz on any bounded set of V. Then, if $\mu > 0$ is small enough, the gradient algorithm with fixed step converges: for any u^0, the sequence (u^n) converges to the unique minimizer u.

Remark. It is difficult to estimate a priori the maximal acceptable step. In practice we often choose a variable step, not necessarily optimal, by a line search.

Line search

Given a descent direction w^n, searching for $\mu > 0$ such that

$$J(u^n + \mu w^n) < J(u^n)$$

is called line search.

A classical procedure is:

- Start with μ_0.
- Loop until $J(u^n + \mu_k w^n) < J(u^n)$

  $\mu_{k+1} = \mu_k / 2$

  $k \leftarrow k + 1$

Identification of the gradient

Typical iteration of a gradient method:

$$u^{n+1} = u^n - \mu\, J'(u^n)$$

where all terms $u^n, u^{n+1}, J'(u^n)$ belong to the same Hilbert space V.

Example when $V = \mathbb{R}^N$:

$$J(x) = \frac{1}{2} Ax \cdot x - b \cdot x \quad \Rightarrow \quad J'(x) = Ax - b$$

Clearly x and $J'(x)$ belong to $\mathbb{R}^N$.

Example when $V = H_0^1(\Omega)$:

$$J(u) = \frac{1}{2} \int_\Omega |\nabla u|^2 dx - \int_\Omega fu\, dx$$

$$\langle J'(u), w \rangle_{V',V} = \int_\Omega (\nabla u \cdot \nabla w - fw) dx = \int_\Omega (-\Delta u - f) w dx$$

Clearly $u \in H_0^1(\Omega)$ but not $\Delta u + f$.

Identification of the gradient (ctd.)

We must use the H^1 scalar product to identify $J'(u)$!

We did that already:

$$-\Delta J'(u) + J'(u) = -\Delta u - f \quad \text{and } J'(u) \in H_0^1(\Omega).$$

In other words, we identify $H_0^1(\Omega)$ with its dual.

Example when $V = L^2(\Omega)$: $J(v) = \int_\Omega \left(\frac{1}{2}v^2 - fv\right) dx$ with $v \in V = L^2(\Omega)$

We have already obtained

$$J'(u) = u - f \ \in L^2(\Omega) \text{ (identified with its dual)}$$

If instead we use the H^1 scalar product:

$$-\Delta J'(u) + J'(u) = u - f \quad \text{and } \frac{\partial J'(u)}{\partial n} = 0.$$

But strong convexity is lost. Nevertheless it provides a descent direction.

Projected gradient

Let K be a non-empty closed convex subset of V. The goal is to solve

$$\inf_{v \in K} J(v) .$$

Initialization: choose $u^0 \in K$. Iterations: for $n \geq 0$

$$u^{n+1} = P_K\big(u^n - \mu\, J'(u^n)\big) ,$$

where P_K is the projection on K.

Theorem

Assume that J is differentiable, strongly convex, and J' is Lipschitz on any bounded set of V. Then, if $\mu > 0$ is small enough, the projected gradient algorithm with fixed step converges.

Moreover, if μ is small enough then

$$J(P_K\big(u^n - \mu\, J'(u^n)\big)) \leq J(u^n).$$

Remark. The projection is defined through the scalar product of V, the same to define the gradient !

Examples of projection operators P_K

- If $V = \mathbb{R}^M$ with canonical scalar product and $K = \prod_{i=1}^M [a_i, b_i]$, then for $x = (x_1, x_2, \ldots, x_M) \in \mathbb{R}^M$

$$P_K(x) = y \quad \text{with} \quad y_i = \min\left(\max\left(a_i, x_i\right), b_i\right) \quad \text{pour} \quad 1 \leq i \leq M \,.$$

- If $V = \mathbb{R}^M$ and $K = \{x \in \mathbb{R}^M \;\; \sum_{i=1}^M x_i = c_0\}$, then

$$P_K(x) = y \quad \text{with} \quad y_i = x_i - \lambda \quad \text{and} \quad \lambda = \frac{1}{M}\left(-c_0 + \sum_{i=1}^M x_i\right).$$

- Same if $V = L^2(\Omega)$ and $K = \{\phi \in V \mid a(x) \leq \phi(x) \leq b(x)\}$ or $K = \{\phi \in V \mid \int_\Omega \phi \, dx = c_0\}$.

For more general closed convex sets K or other scalar products, P_K can be very hard to determine. In such cases one rather uses the Uzawa algorithm which looks for a saddle point of the Lagrangian.

Newton algorithm (of order 2)

Main idea: if $V = \mathbb{R}^N$ and if $J'' \geq 0$

$$J(w) \approx J(v) + J'(v) \cdot (w - v) + \frac{1}{2} J''(v)(w - v) \cdot (w - v),$$

the minimizer of which is $w = v - \left(J''(v)\right)^{-1} J'(v)$.

Algorithm: $u^{n+1} = u^n - \left(J''(u^n)\right)^{-1} J'(u^n)$.

- It converges very fast if u^0 is close to the minimizer u

$$\|u^{n+1} - u\| \leq C \|u^n - u\|^2 \,.$$

- It requires solving a linear system with the matrix $J''(u^n)$.
- It can be generalized in a quasi-Newton method (without computing J'') or to the constrained case.