OPTIMAL DESIGN OF STRUCTURES (MAP 562)

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CHAPTER III

A REVIEW OF OPTIMIZATION

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Optimal design of structures

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

 $u \in K$ and $\exists \delta > 0$, $\forall v \in K$, $\|v - u\| < \delta \Longrightarrow J(v) \ge J(u)$.

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

$$u \in K$$
 and $J(v) \ge J(u) \quad \forall v \in K$

(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 continuous function from K to \mathbb{R} satisfying the so-called "infinite at infinity" property, i.e.,

$$\forall (u^n)_{n\geq 0}$$
 sequence in K , $\lim_{n\to+\infty} ||u^n|| = +\infty \Longrightarrow \lim_{n\to+\infty} J(u^n) = +\infty$.

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.

(Main idea: the closed bounded sets are compact in finite dimension.)

Optimization in infinite dimension

Difficulty: a continuous function on a closed bounded set does not necessarily attained 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

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

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. (Difficulty independent on the choice of the functional space.)

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 useful in material sciences !

The Ball-James theory (1987).

Shape memory materials = alloys with phase transition.

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



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





Optimal design of structures



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Optimal design of structures

J. Ball and R. James proposed the following mechanism: to sustain the applied forces, the alloy has a tendency to coexist under different phases, suitably aligned, which minimize the energy \Rightarrow minimizing sequence !



Convex analysis

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

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

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.,

 $\forall (u^n)_{n \ge 0}$ 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 $\Leftrightarrow (V')' = V (V' \text{ is the dual of } V)$
- 2. The theorem is still true if V is just the dual of a separable Banach space.
- 3. In practice, this assumption is satisfied for all the functional spaces which we shall use: for example, $L^p(\Omega)$ with 1 .

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 is not the only tool to prove existence of minimizers. Another method is, for example, compactness.

Differentiability)

Definition. Let V be a Banach 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 form on $V, L \in V'$, such that

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

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

- For V is a Hilbert space, its dual V' can be identified with V itself thanks to the Riesz representation theorem. Thus, there exists a unique $p \in V$ such that $\langle p, w \rangle = L(w)$. We also write p = J'(u).
- \sim We use this identification V = V' if $V = \mathbb{R}^n$ or $V = L^2(\Omega)$.
- The practice, it is often easier to compute the directional derivative $j'(0) = \langle J'(u), w \rangle_{V',V}$ with j(t) = J(u + tw).

A basic example to remember

Consider the variational formulation

find
$$u \in V$$
 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 form.

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 check that the 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 !)

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

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 $\langle J'(u), w \rangle$.

Examples: (we use the "usual" scalar product in L^2)

1.
$$J(v) = \int_{\Omega} \left(\frac{1}{2}v^2 - fv\right) dx$$
 with $v \in L^2(\Omega)$
 $\langle J'(u), w \rangle = \int_{\Omega} (uw - fw) dx.$

Thus

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

2.
$$J(v) = \int_{\Omega} \left(\frac{1}{2}|\nabla v|^2 - fv\right) dx$$
 with $v \in H_0^1(\Omega)$
 $\langle J'(u), w \rangle = \int_{\Omega} \left(\nabla u \cdot \nabla w - fw\right) dx.$

Therefore, after integrating by parts,

$$J'(u) = -\Delta u - f \in H^{-1}(\Omega) = (H^1_0(\Omega))'$$
 (not identified with its dual)

Remark (delicate). If instead of the "usual" scalar product in L^2 we rather use the H^1 scalar product, then we identify J'(u) with a different function.

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

From the directional derivative

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

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

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

Here we identify $H_0^1(\Omega)$ with its dual.

Optimality conditions

Theorem (Euler inequality). Let $u \in K$ with K convex. We assume that J is differentiable at u. If u is a local minimizer of J in K, then

$$\langle J'(u), v - u \rangle \ge 0 \quad \forall v \in K .$$

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

Remarks.

- $rac{}$ 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

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

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 $(F'_i(u))_{1 \leq i \leq M}$ 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

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

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 into \mathbb{R} .

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

$$I(u) = \{i \in \{1, \dots, M\}, F_i(u) = 0\}$$

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

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

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, there exist Lagrange multipliers $\lambda_1, \ldots, \lambda_M \geq 0$ such that

$$J'(u) + \sum_{i=1}^{M} \lambda_i F'_i(u) = 0, \quad \lambda_i \ge 0, \quad \lambda_i = 0 \text{ if } F_i(u) < 0 \quad \forall i \in \{1, \dots, M\}$$

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 $(\mathbb{R}^+)^M$

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

Interpreting the Lagrange multipliers

Define the Lagrangian for the minimization of J(v) under the constraint F(v) = c

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

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

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

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

$$\inf_{v \in U} \mathcal{J}(v) \; ,$$

and dual problem

 $\sup_{q\in P} \mathcal{G}(q) \; .$

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 the simple one, $q \in P$).

Lemma (weak duality). It always holds true that

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

Proof: inf sup $\mathcal{L} \geq \sup \inf \mathcal{L}$.

Theorem (strong duality). The couple (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 obtained through an unconstrained minimization.

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

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

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 p.d.e. Defining $\sigma = \nabla u$ we have

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

and σ is the unique maximizer of G.

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

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

By integrating by parts

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

v is the Lagrange multiplier for the constraint $-\operatorname{div}\tau = f$. We check that the dual of the dual is the primal !

au

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

End of the proof)

By definition, if τ satisfies the constraint $-\operatorname{div}\tau = f$, we have

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

On the other hand,

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

Besides, integrating by parts yields $\int_{\Omega} |\nabla u|^2 dx = \int_{\Omega} f u \, dx$, thus

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

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

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

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

Numerical algorithms for minimization problems

A simplified classification:

- Stochastic algorithms: global minimization. Examples: Monte-Carlo, simulated annealing, genetic. See the last chapter and the last course.
 Inconvenient: high CPU cost.
- Deterministic algorithms: local minimization. Examples: gradient methods, Newton.

Inconvenient: they require the gradient of the objective function.

Gradient descent with an optimal step

The goal is to solve

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

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

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

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

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

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 $\alpha > 0$,

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

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

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

Then the gradient algorithm with an 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,
- \Leftrightarrow 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 $n \ge 0$

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

Theorem. Assume that J is differentiable, strongly convex, and J' is Lipschitzian 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. An intermediate variant is: increase the step, $\mu_{n+1} = 1.1 \times \mu_n$, if J decreases, and reduce the step, $\mu_{n+1} = 0.5 \times \mu_n$, if J increases.

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 $n \ge 0$

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

where P_K is the projection on K.

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

Remark. Another possibility is to **penalize** the constraints, i.e., for small $\epsilon > 0$ we replace

$$\inf_{v \in V, F(v) \le 0} J(v) \quad \text{by} \quad \inf_{v \in V} \left(J(v) + \frac{1}{\epsilon} \sum_{i=1}^{M} \left[\max\left(F_i(v), 0\right) \right]^2 \right).$$

Examples of projection operators P_K

 $K = \{ \phi \in V \mid \int_{\Omega} \phi \, dx = c_0 \}.$

For more general closed convex sets K, 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 $J'' \ge 0$

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

the minimizer of which is $w = v - (J''(v))^{-1} J'(v)$. Algorithm: $u^{n+1} = u^n - (J''(u^n))^{-1} J'(u^n)$.

 \Im It converges faster if u^0 is close to the minimizer u

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

 \Im It requires solving a linear system with the matrix $J''(u^n)$.

The can be generalized in a quasi-Newton method (without computing J'') or to the constrained case.