Topological Gradient

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The standard geometrical shape optimization method proceed by the application of successive diffeomorphisms close to the identity starting from an initial guessed shape. Consequently, it does not allow for the optimization of the topology which is kept unchanged from one iteration to the other. The topological gradient enables to determine if the inclusion of a small hole of given shape is cost efficient. Such holes can be included at any time during the geometrical shape optimization process. Moreover, as seen thereafter, the topological gradient can be explicitly computed from the primal and adjoint states of the optimization problem that are already computed during standard geometrical shape optimization. Finally let us mention that level set methods can also handle topological changes during the optimization process [2], possibly coupled with the use of topological gradient [1].

1 Definition

Let J be a cost function from an admissible set $\mathcal{U}_{ad}$ of the open subsets of $\mathbb{R}^N$ with value in $\mathbb{R}$. Let ω be a bounded open subset of $\mathbb{R}^N$. The cost function J is said to admit a topological gradient at $\Omega \in \mathcal{U}_{ad}$ with respect to holes of shapes ω if there exists a function $s : \mathbb{R}^+ \to \mathbb{R}^+$ and a function g_ω from Ω into $\mathbb{R}$ such that for all $x_0 \in \Omega$,

$$J(\Omega_\rho) = J(\Omega) + s(\rho) g_\omega(x_0) + o(s(\rho)),$$

with $s(\rho) = 0$ if and only if $\rho = 0$ and Ω_ρ is the open set obtained after the creation at x_0 of a hole of shape ω rescaled by a factor ρ,

$$\Omega_\rho := \Omega \setminus \overline{\omega}_\rho,$$

$$\omega_\rho := \left\{ x \in \mathbb{R}^N \;:\; \frac{x - x_0}{\rho} \in \omega \right\}.$$

Note that the dependence of Ω_ρ with respect to ω and x_0 is implicitly understood. The function g_ω is called the topological gradient of J (or the topological sensitivity). If $g_\omega(x_0)$ is negative, for a given element $x_0 \in \Omega$, the creation of a small enough hole will end up with a decrease of the cost function, and thus lead to a more optimal shape.

A trivial example. Let f be a continuous map from $\mathbb{R}^N$ into $\mathbb{R}$ and let

$$J(\Omega) = \int_\Omega f(x)\,dx.$$

Then J admits a topological gradient and we have

$$J(\Omega_\rho) = J(\Omega) + \rho^N |\omega| f(x_0) + o(\rho^N).$$

In most applications though, we are interested in cases where the cost function depends on the solution of a PDE. In the following, we are going to study the case of the Poisson equation. The complete computation of the cost function will be given in the case of circular holes in dimension two. The present analysis can be extended to other state equations (like the elasticity) or to the creation of inclusions (rather than holes).

2 The case of the Poisson equation in $\mathbb{R}^N$

In the following, we are going to consider a cost function J of the following form

$$J(\Omega) = \int_\Omega F(u_\Omega)\,dx + \int_{\Gamma_N} G(u_\Omega)\,dx, \tag{1}$$

where F and G are regular functions from $\mathbb{R}$ into $\mathbb{R}$, and u_Ω is the solution of the Poisson equation

$$\begin{cases} -\Delta u_\Omega = f & \text{in } \Omega, \\ u_\Omega = u_D & \text{on } \Gamma_D, \\ \frac{\partial u_\Omega}{\partial n} = g & \text{on } \Gamma_N, \\ \frac{\partial u_\Omega}{\partial n} = 0 & \text{on } \Gamma, \end{cases} \tag{2}$$

where $f \in L^2(\mathbb{R}^N)$, $g \in L^2(\Gamma_N)$, $u_D \in H^1(\mathbb{R}^N)$ and $\Gamma = \partial\Omega \setminus (\Gamma_D \cup \Gamma_N)$, assuming that $\Gamma_N \cup \Gamma_D \subset \partial\Omega$ for every admissible shapes Ω of $\mathcal{U}_{ad}$.

Let Ω be a given admissible set. We denote by $j(\rho) = J(\Omega_\rho)$ and in order to simplify the notations, we set $u_\rho = u_{\Omega_\rho}$. Computing the topological gradient of J consists to determine the asymptotic development of j at $\rho = 0$. To this end, we are first going to compute the gradient of j using the classical fast derivative method of Céa. In a second step we are going to compute an approximation of $j'(\rho)$ for ρ small. Finally, an integration with respect to ρ will lead us to the desired result.

Remark 1 *Cost functions depending on the gradient of u_Ω can also be considered, but require a more subtle analysis [5].*

2.1 Geometrical derivative

We introduce the Lagrangian

$$\mathcal{L}(\rho, u, p) = \int_{\Omega_\rho} F(u)\,dx + \int_{\Gamma_N} G(u)\,ds + \int_{\Omega_\rho} \nabla u \cdot \nabla p\,dx - \int_{\Omega_\rho} fp\,dx - \int_{\Gamma_N} gp\,ds.$$

Moreover, we introduce the adjoint state

$$p_\rho \in H^1_{\Gamma_D}(\Omega_\rho) := \left\{ p \in H^1(\Omega_\rho) \text{ such that } p = 0 \text{ on } \Gamma_D \right\},$$

such that for all $q \in H^1_{\Gamma_D}(\Omega_\rho)$ we have

$$\left\langle \frac{\partial \mathcal{L}}{\partial u}(\rho, u_\rho, p_\rho), q \right\rangle = 0,$$

that is

$$\int_{\Omega_\rho} F'(u) q \, dx + \int_{\Gamma_N} G'(u) q \, ds + \int_{\Omega_\rho} \nabla p_\rho \cdot \nabla q \, dx = 0. \tag{3}$$

As for every $p \in H^1_{\Gamma_D}(\mathbb{R}^N)$, we have $j(\rho) = \mathcal{L}(\rho, u_\rho, p)$, it follows that

$$j'(\rho) = \frac{\partial \mathcal{L}}{\partial \rho}(\rho, u_\rho, p) + \left\langle \frac{\partial \mathcal{L}}{\partial u}(\rho, u_\rho, p), u'_\rho \right\rangle,$$

where u'_ρ is the Eulerian derivative of u_ρ with respect to ρ. Using that $\partial\mathcal{L}/\partial u(\rho, u_\rho, p_\rho) = 0$, we get

$$j'(\rho) = \frac{\partial \mathcal{L}}{\partial \rho}(\rho, u_\rho, p_\rho).$$

Let $X(\rho, y) = \rho y + x_0$, we have

$$\omega_\rho = X(\rho, \omega).$$

Derivating X with respect to ρ, we obtain the velocity of the interface $\partial\omega$, we have for every $y \in \partial\omega$,

$$\dot{X}(\rho, y) = y.$$

For all $x \in \partial\omega_\rho$, the velocity of the interface is equal to $\dot{X}(\rho, y)$, with $x = X(\rho, y)$ that is $y = (x - x_0)/\rho$. It follows that

$$j'(\rho) = -\int_{\partial\omega_\rho} \left(F(u_\rho) + \nabla u_\rho \cdot \nabla p_\rho - f p_\rho\right) \frac{(x - x_0)}{\rho} \cdot n \, ds, \tag{4}$$

n being the outward normal to ω_ρ.

2.2 Approximation of u_ρ and p_ρ

Let us introduce the map $v(\rho)$ from $\mathbb{R}^N \setminus \omega$ into $\mathbb{R}$ defined by

$$v(\rho)(y) = \left(\frac{u_\rho - u_0}{\rho} \right) (\rho y + x_0).$$

Note that $v(\rho)$ is not strictly speaking defined for all y in the set $\mathbb{R}^N \setminus \omega$. Nevertheless for such a given y, it is correctly defined for ρ small enough. It is easily seen that

$$\nabla v(\rho)(y) = \nabla (u_\rho - u_0)(\rho y + x_0),$$

and that

$$\begin{cases} -\Delta v(\rho) = 0 & \text{in } \mathbb{R}^N \setminus \omega, \\ \frac{\partial v(\rho)}{\partial n}(y) = -\nabla u_0(\rho y + x_0) \cdot n & \text{on } \partial\omega, \end{cases}$$

Passing formally to the limit in those equations we obtain that

$$v(\rho) \to v_0,$$

where

$$\begin{cases} -\Delta v_0 = 0 & \text{in } \mathbb{R}^N \setminus \omega, \\ \frac{\partial v_0}{\partial n}(y) = \nabla u_0(x_0) \cdot n & \text{on } \partial\omega, \end{cases}$$

Finally, as the perturbations generated by the inclusion of a hole at x_0 are small far from the hole, we should have

$$v_0(y) \to 0 \text{ as } y \to \infty.$$

We do not give the rigorous proof of this convergence result, which is too technical to be developed here (we do not even precise in which sense the convergence do hold).

Note that the function v depends linearly on $\nabla u_0(x_0)$. More precisely, denoting by w_i the solutions of the problems

$$\begin{cases} -\Delta w_i = 0 & \text{in } \mathbb{R}^N \setminus \omega \\ \frac{\partial w_i}{\partial n} = -n_i & \text{on } \partial\omega \\ w_i(y) \to 0 & \text{as } y \to +\infty, \end{cases} \tag{5}$$

We have $v_0 = W\nabla u_0(x_0)$, where $W = (w_1, \cdots, w_N)$. A similar analysis can be carried out for the adjoint state and we get that

$$q(\rho)(y) = \left(\frac{p_\rho - p_0}{\rho}\right)(\rho y + x_0)$$

converges toward $q_0 = W\nabla p_0(x_0)$.

2.3 Approximation of the shape gradient

We recall that from formula (4),

$$j'(\rho) = -\int_{\partial\omega_\rho} \left(F(u_\rho)\frac{(x-x_0)}{\rho} \cdot n + \nabla u_\rho \cdot \nabla p_\rho \frac{(x-x_0)}{\rho} \cdot n - f p_\rho\right) \frac{(x-x_0)}{\rho} \cdot n \, ds.$$

Performing the change of variable $y = (x - x_0)/\rho$, we get

$$j'(\rho) = -\rho^{N-1} \int_{\partial\omega} \Big(F(u_\rho(\rho y + x_0))$$
$$+(\nabla v(\rho)(y)+\nabla u_0(\rho y+x_0))\cdot(\nabla q(\rho)(y)+\nabla p_0(\rho y+x_0))-f(\rho y+x_0)p_\rho(\rho y+x_0)\Big)(y\cdot n)\, ds$$

As u_ρ converges toward u_0, the first term of this expression can be approximated by

$$\begin{aligned}\int_{\partial\omega} F(u_\rho(\rho y + x_0)(y\cdot n)\,ds &= F(u_0)\int_{\partial\omega}(y\cdot n)\,ds + r_1(\rho)\\ &= F(u_0)\int_{\omega}(\nabla\cdot y)\,dy + r_1(\rho)\\ &= N|\omega|F(u_0) + r_1(\rho),\end{aligned}$$

where $r_1(\rho)$ is a *small* correction. The same analysis can be performed for the third term of the expression of $j'(\rho)$ and we get

$$\int_{\partial\omega} f(\rho y + x_0)p_\rho(\rho y + x_0)(y\cdot n)\,ds = N|\omega|f(x_0)p_0(x_0) + r_3(\rho).$$

Moreover, as $v(\rho)$ is close to $v_0 = W\nabla u_0$ for ρ small, $\nabla v(\rho)$ is close to $\nabla W\nabla u_0$, where ∇W stands for the matrix $(\nabla w_1, \cdots, \nabla w_N)$. It follows that

$$\begin{aligned}\int_{\partial\omega}(\nabla v(\rho)(y) + \nabla u_0(\rho y + x_0))\cdot(\nabla q(\rho)(y) + \nabla p_0(\rho y + x_0))(y\cdot n)\,ds =\\ \int_{\partial\omega}((\nabla W + \mathrm{Id})\nabla u_0)\cdot((\nabla W + \mathrm{Id})\nabla p_0)(y\cdot n)\,ds + r_2(\rho),\end{aligned}$$

where $r_2(\rho)$ is a small correction. Setting

$$M = N^{-1}|\omega|^{-1}\int_{\partial\omega}(\nabla W + \mathrm{Id})^T(\nabla W + \mathrm{Id})(y\cdot n)\,ds, \tag{6}$$

we get

$$\int_{\partial\omega}(\nabla v(\rho)(y)+\nabla u_0(\rho y+x_0))\cdot(\nabla q(\rho)(y)+\nabla p_0(\rho y+x_0))(y\cdot n)\,ds = N|\omega|\nabla u_0^T M\nabla p_0 + r_2(\rho).$$

Note that M is a positive symmetric positive matrix that does only depend on the shape ω of the hole. Finally, we obtain that

$$j'(\rho) = N\rho^{N-1}|\omega|(f(x_0)p_0(x_0) - M\nabla u_0(x_0)\cdot\nabla p_0(x_0) - F(u_0(x_0))) + o(\rho^{N-1}). \tag{7}$$

2.4 Expression of the topological sensitivity

By integration of (7) with respect to ρ, we get

$$j(\rho) = j(0) + \rho^N|\omega|\left(fp_0 - M\nabla u_0\cdot\nabla p_0 - F(u_0)\right)(x_0) + o(\rho^N). \tag{8}$$

3 Explicit expression of the shape gradient

If ω is the unit ball in $\mathbb{R}^N$ ($N = 2, 3$), the solutions of the elementary problems (5) – and thus the matrix M – can be computed explicitly. We propose to perform the computations in the two dimensional case and give the result in the three dimensional case (without proof).

3.1 The two dimensional case

In order to compute the solutions $(w_i)_{i=1,2}$ of (5) in the case $N = 2$, it is convenient to use polar coordinates. It can be easily seen that $w_2(\theta, r) = w_1(\theta - \pi/2, r)$. Consequently, we only have to determine w_1, which we will denote w in the following. For all $r \geq 1$, the function $\theta \to w(\theta, r)$ is periodic and thus admits a Fourier decomposition of coefficients $a_k(r)$ depending on r,

$$w(\theta, r) = \sum_{k \in \mathbb{Z}} a_k(r) e^{ik\theta}.$$

In order to determine the coefficients $a_k(r)$ of this decomposition, we first have to express the Laplacian in polar coordinates. For all regular map φ of $\mathbb{R}^2$, we have

$$\nabla\varphi = \frac{\partial\varphi}{\partial r} e_r + \frac{1}{r}\frac{\partial\varphi}{\partial\theta} e_\theta,$$

where $e_r = x/|x|$ and (e_r, e_θ) is a local orthonormal base.

$$\Delta\varphi = \nabla\left(\frac{\partial\varphi}{\partial r}\right) \cdot e_r + \frac{\partial\varphi}{\partial r}\nabla \cdot e_r + \nabla\left(\frac{1}{r}\frac{\partial\varphi}{\partial\theta}\right) \cdot e_\theta + \frac{1}{r}\frac{\partial\varphi}{\partial\theta}\nabla \cdot e_\theta.$$

We have

$$\nabla\cdot e_r = \nabla\cdot(x/|x|) = |x|^{-1}(\nabla\cdot x) + x\cdot\nabla((|x|^2)^{-1/2}) = 2|x|^{-1} - (|x|^2)^{-3/2} x\cdot x = 1/r.$$

and $\nabla \cdot e_\theta = 0$, leading us to

$$\Delta\varphi = \frac{\partial^2\varphi}{\partial r^2} + \frac{1}{r}\frac{\partial\varphi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\varphi}{\partial\theta^2}.$$

From $\Delta w = 0$, we deduce that

$$\sum_k (a_k'' + r^{-1}a_k' - r^{-2}a_k)e^{ik\theta} = 0,$$

and that for every $k \in \mathbb{Z}$,

$$a_k'' + r^{-1}a_k' - r^{-2}a_k = 0.$$

We seek for elementary solutions of the form r^α. We get $\alpha(\alpha-1) + \alpha - 1 = 0$, that is $\alpha = \pm 1$. Due the to limit condition $w(r,\theta) \to 0$ as $r \to 0$, we obtain that $a_k(r,\theta) = b_k r^{-1}$, where $b_k \in \mathbb{R}$. From the limit condition on $\partial\omega$, we get

$$\sum_{k\in\mathbb{Z}} a_k' e^{i\theta} = -x_1 = -\cos(\theta) = -(e^{i\theta} + e^{-i\theta})/2.$$

It follows that $b_k = 0$ for every $k \in \mathbb{Z}$ such that $|k| \neq 1$ and $b_k = 1/2$ for $k = \pm 1$, hence

$$w(r,\theta) = r^{-1}\cos(\theta) = r^{-2}x_1.$$

Finally, for $i = 1, 2$, $w_i = |x|^{-2} x_i$, and

$$\nabla w_i = |x|^{-2} e_i - 2|x|^{-4} x_i x.$$

In particular, for any $x \in \partial\omega$, we have

$$\nabla w_i = e_i - 2x_i x.$$

It follows, from the definition of M, that

$$\begin{aligned} M_{ij} &= (2\pi)^{-1} \int_{\partial\omega} (e_i + \nabla w_i) \cdot (e_j + \nabla w_j)\, ds \\ &= 2\pi^{-1} \int_{\partial\omega} (e_i - x_i x) \cdot (e_j - x_j x)\, ds \\ &= 2\pi^{-1} \int_{\partial\omega} (e_i \cdot e_j - x_i x_j)\, ds. \end{aligned}$$

If $i \neq j$, we have $M_{ij} = 0$. And for $i = j$,

$$M_{ij} = 2\pi^{-1} \int_0^{2\pi} (1 - \cos(\theta)^2)\, d\theta = 2.$$

From (8), we get the expression of the topological gradient

$$j(\rho) = j(0) + \rho^2 \pi \left(f(x_0) p_0(x_0) - 2\nabla u_0(x_0) \cdot \nabla p_0(x_0) - F(u_0(x_0)) \right) + o(\rho^2).$$

3.2 The three dimensional case

In the three dimensional case, the topological gradient where ω is the unit ball can still be computed explicitly. Once again, M is proportional to the identity matrix and we have $M = 3/2\,\mathrm{Id}$. We referee the reader to [3].

4 Applications

We consider two applications. We begin by considering the minimization of the compliance. In a second step, we study the problem consisting into reaching a target state.

4.1 Compliance

The compliance, defined by

$$J(\Omega) = \int_\Omega f u_\Omega\, dx + \int_{\Gamma_N} g u_\Omega\, ds,$$

corresponds to the case $F(u) = fu$ and $G(u) = gu$ in (1). From (3), $p_0 \in H^1_{\Gamma_D}(\Omega)$ is such that for all $q \in H^1_{\Gamma_D}(\Omega)$

$$\int_{\Omega_\rho} \nabla p_0 \cdot \nabla q\, dx = -\int_\Omega f q\, dx - \int_\Gamma g q\, ds,$$

and the expression of the topological gradient (8) is given by

$$J(\Omega_\rho) = J(\Omega) + \rho^2|\omega| \left(fp_0 - M\nabla u_0 \cdot \nabla p_0 - fu_0\right)(x_0) + o(\rho^2).$$

In particular, for homogeneous boundary Dirichlet conditions, that is $u_D = 0$, we have $p_0 = -u_0$ and

$$J(\Omega_\rho) = J(\Omega) + \rho^2|\omega| \left(M\nabla u_0 \cdot \nabla u_0 - 2fu_0\right)(x_0) + o(\rho^2).$$

Note that if $f = 0$, then the topological gradient is always negative, and the creation of holes will always lead to an increase of the cost function. Moreover, if ω is the unit disk, we recall that $M = 2$ and $|\omega| = \pi$.

4.2 Target state

We consider in this section the cost function

$$J(\Omega) = \frac{1}{2}\int_\Omega |u_\Omega - u_t|^2 \, dx,$$

where u_t is the target state. The adjoint state is the element $p_0 \in H^1_{\Gamma_D}(\Omega)$ such that for all $q \in H^1_{\Gamma_D}(\Omega)$,

$$\int_{\Omega_\rho} \nabla p_0 \cdot \nabla q \, dx = -\int_\Omega (u - u_t) q \, ds.$$

The topological gradient is then given by

$$J(\Omega_\rho) = J(\Omega) + \rho^2|\omega| \left(fp_0 - M\nabla u_0 \cdot \nabla p_0 - fu_0\right)(x_0) + o(\rho^2).$$

Once again, if ω is the unit ball, we have $M = 2$ and $|\omega| = \pi$.

5 The elasticity case

The same analysis can be carried out when the state equation is the solution of linear elasticity. The state u_Ω in this section is assumed to be the displacement of a homogeneous elastic body of Hooke law A. In other words $u_\Omega \in H^1(\Omega)^N$ is thus that for all test functions $v \in H^1_{\Gamma_D}(\Omega)^N$, we have

$$\int_\Omega Ae(u_\Omega) : e(v) \, dx = \int_\Omega f \cdot v \, dx + \int_{\Gamma_N} g \cdot v \, ds$$

with $u = u_D$ on Γ_D. In this case, f and g are prescribed volume and surface loads applied to the body and u_D a given displacement on part of the boundary. We consider a similar cost function that for the Laplacian case, that is

$$J(\Omega) = \int_\Omega F(u_\Omega) \, dx + \int_{\Gamma_N} G(u_\Omega) \, ds.$$

5.1 Topological Gradient

We introduce also the adjoint state $p_\Omega \in H^1_{\Gamma_D}(\Omega)^N$ such that for all $q \in H^1_{\Gamma_D}(\Omega)^N$,

$$\int_\Omega Ae(p_\Omega) : e(q)\,dx = -\int_\Omega \nabla F(u)\cdot q\,dx - \int_\Gamma \nabla G(u)\cdot q\,ds. \tag{9}$$

Then J admits a topological gradient of the form

$$J(\Omega_\rho) = J(\Omega) + \rho^N|\omega|\Big(f\cdot p_\Omega - Me(u_\Omega) : e(p_\Omega) - F(u_\Omega)\Big)(x_0) + o(\rho^N).$$

The operator M is defined as follows. Let w^{ij} we the solution of the PDE

$$\begin{cases} -\nabla\cdot e(w^{ij}) = 0 & \text{in } \mathbb{R}^N\setminus\omega \\ e(w^{ij})\cdot n = E^{ij}\cdot n & \text{on } \partial\omega \\ w^{ij}(y)\to 0 \text{ as } y\to 0. \end{cases}$$

where E^{ij} is the symmetric matrix defined by $E^{ij}_{kl} = \delta^i_k\delta^j_l$. We then have

$$v = \lim_{\rho\to 0}\frac{u_\rho - u_0}{\rho}(\rho\cdot - x_0) = We(u_0)(x_0),$$

where W is the operator that maps any symmetric matrix ξ_{ij} to the element of $H^1(\Omega\setminus\omega)^N$ defined by

$$W\xi = \sum_{i,j} w^{ij}\xi_{ij}.$$

The symmetric bilinear for M on the space of $N\times N$ symmetric matrices is defined by

$$M\xi : \xi = N^{-1}|\omega|^{-1}\int_{\partial\omega} A(\xi + e(W\xi)) : (\xi + e(W\xi))\,ds.$$

5.2 Case of spherical holes

As in the Laplacian case, the operator M can be explicitly compute when ω is the unit ball (see [4, 1]) in the case of linear isotropic elasticity, that is

$$A\xi : \xi = 2\mu\xi : \xi + \lambda\,\mathrm{Tr}(\xi)^2.$$

We have in the case $N = 2$,

$$M\xi : \xi = \frac{2\mu(\lambda+2\mu)}{\lambda+\mu}\xi : \xi + \frac{\lambda+2\mu}{2}\left(\frac{(\lambda+\mu)^2 - 2\mu^2}{\mu(\lambda+\mu)}\right)\mathrm{Tr}(\xi)^2.$$

and in the case $N = 3$,

$$M\xi : \xi = |\omega|^{-1}\frac{5\pi(2\mu+\lambda)}{14\mu+9\lambda}\left(4\mu\xi : \xi - \frac{(2\mu+7\lambda-5\nu(2\mu+\lambda))}{(2+5\nu)}\,\mathrm{Tr}(\xi)^2\right)$$

with

$$\nu = \frac{\lambda}{2(\lambda+\mu)}.$$

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