Lecture 5: Shape differential calculus.

Florian Feppon

Spring 2022 – Seminar for Applied Mathematics

ETH zürich

Outline

1. Hadamard's shape derivatives
2. Shape derivatives of volume and surface integrals
3. Proofs: change of variable formulas and tangential calculus

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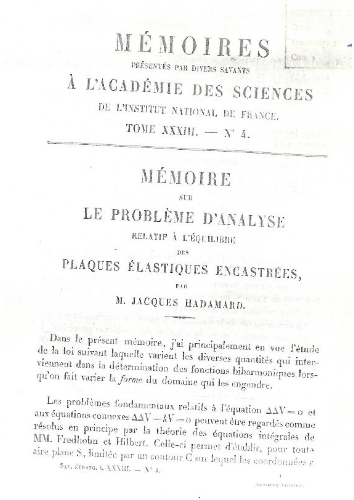
Everything started with a memoir of Hadamard in 1908.



MÉMOIRES

PRÉSENTÉS PAR DIVERS SAVANTS

À L'ACADÉMIE DES SCIENCES

DE L'INSTITUT NATIONAL DE FRANCE.

TOME XXXIII. — N° 4.

MÉMOIRE

SUR

LE PROBLÈME D'ANALYSE

RELATIF À L'ÉQUILIBRE

DES

PLAQUES ÉLASTIQUES ENCASTRÉES,

PAR

M. JACQUES HADAMARD.

Dans le présent mémoire, j'ai principalement en vue l'étude de la loi suivant laquelle varient les diverses quantités qui interviennent dans la détermination des fonctions biharmoniques lorsqu'on fait varier la *forme* du domaine qui les engendre.

Les problèmes fondamentaux relatifs à l'équation $\Delta\Delta V = 0$ et aux équations connexes $\Delta\Delta V - kV = 0$ peuvent être regardés comme résolus en principe par la théorie des équations intégrales de MM. Fredholm et Hilbert. Celle-ci permet d'établir, pour toute aire plane S, limitée par un contour C sur lequel les coordonnées x

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The boundary variation method of Hadamard

Given a Lipschitz domain Ω, we parameterize deformations of Ω by a continuous vector field $\boldsymbol{\theta}$:

$$\Omega_{\boldsymbol{\theta}} := (I + \boldsymbol{\theta})\Omega = \{x + \boldsymbol{\theta}(x) \,|\, x \in \Omega\}$$

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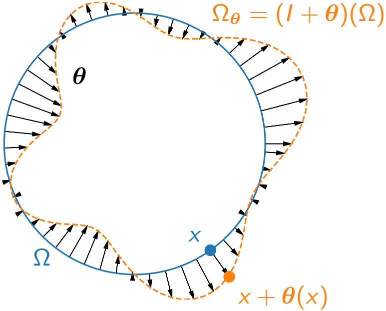

Figure: Deformation of a domain Ω with the method of Hadamard. A small vector field $\boldsymbol{\theta}$ is used to deform Ω into $\Omega_{\boldsymbol{\theta}} = (I + \boldsymbol{\theta})\Omega$.

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We assume that the parameterizing vector field $\boldsymbol{\theta}$ is Lipschitz: $\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ where

$$W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) = \{\boldsymbol{\theta} \in L^\infty(\mathbb{R}^d) \mid \nabla\boldsymbol{\theta} \in L^\infty(\mathbb{R}^d)\}.$$

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Lemma 1

For any $\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ such that $||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)} < 1$, the map $I + \boldsymbol{\theta}$ is a bijection satisfying $(I + \boldsymbol{\theta})^{-1} - I \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.

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Sketch of proof.

Formally, the inverse map is given by

$$(I + \boldsymbol{\theta})^{-1} = \sum_{k=0}^{+\infty} (-1)^k \overbrace{\boldsymbol{\theta} \circ \cdots \circ \boldsymbol{\theta}}^{k \text{ times}},$$

where the above series is convergent in the norm of $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$. . □

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A shape functional $J(\Omega)$ is said shape differentiable if the mapping

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such that the following asymptotics holds true:

$$J(\Omega_{\boldsymbol{\theta}}) = J(\Omega) + \mathrm{D}J(\Omega)(\boldsymbol{\theta}) + o(\boldsymbol{\theta}), \quad \text{where} \quad \frac{|o(\boldsymbol{\theta})|}{||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}} \xrightarrow{\boldsymbol{\theta}\to 0} 0.$$

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The **linear form** $\mathrm{D}J(\Omega)$ is called the shape derivative of J on the domain Ω.

Remark 1

$W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)^*$ is the dual space of $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$. The definition the existence of some constant $C(\Omega)$ independent of $\boldsymbol{\theta}$ such that

$$\forall \boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d),\ |\mathrm{D}J(\Omega)(\boldsymbol{\theta})| \leq C(\Omega)||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}.$$

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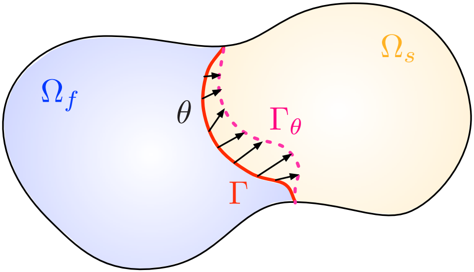
Remark 2

In case where the shape to optimize is an interface Γ, a functional $J(\Gamma)$ is said shape differentiable if $\boldsymbol{\theta} \mapsto J(\Gamma_{\boldsymbol{\theta}})$ is differentiable and the shape derivative $\mathrm{D}J(\Gamma)(\boldsymbol{\theta})$ is defined analogously to theorem 2.



Remark 3

It will be convenient to write shape derivatives with a $\mathrm{d}/\mathrm{d}\boldsymbol{\theta}$ differential notation:

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\bigg|_{\boldsymbol{\theta}=0}[J(\Omega_{\boldsymbol{\theta}})](\boldsymbol{\theta}) := \mathrm{D}J(\Omega)(\boldsymbol{\theta}),$$

where with a little abuse of notations, we have also denoted by $\boldsymbol{\theta}$ the direction in which $\boldsymbol{\theta} \mapsto J(\Omega_{\boldsymbol{\theta}})$ is differentiated.

An important result: Hadamard's structure theorem.

Proposition 1 (Hadamard's structure theorem)

Let Ω a smooth bounded open set of $\mathbb{R}^d$ and $J(\Omega)$ a shape differentiable functional. If $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ are such that $\boldsymbol{\theta}_2 - \boldsymbol{\theta}_1 \in \mathcal{C}^1(\mathbb{R}^d, \mathbb{R}^d)$ and $\boldsymbol{\theta}_1 \cdot \boldsymbol{n} = \boldsymbol{\theta}_2 \cdot \boldsymbol{n}$ on $\partial\Omega$, then it holds

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If we set $\boldsymbol{\theta} = -t v_J(\Omega)\boldsymbol{n}$ for a sufficiently small $t > 0$, then we have

$$J(\Omega_{\boldsymbol{\theta}}) = J(\Omega) - t \int_{\partial\Omega} |v_f(\Omega)|^2 \mathrm{d}\sigma + O(t^2)$$

and $\Omega_{\boldsymbol{\theta}}$ is a "better" candidate than Ω.

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1. Hadamard's shape derivatives
2. Shape derivatives of volume and surface integrals
3. Proofs: change of variable formulas and tangential calculus

Proposition 2

Let Ω be a bounded open set of $\mathbb{R}^d$. For any $f \in W^{1,1}(\mathbb{R}^d)$, the functional $J(\Omega)$ defined by

$$J(\Omega) := \int_\Omega f(x)\mathrm{d}x$$

is shape differentiable, and it holds

$$\mathrm{D}J(\Omega)(\boldsymbol{\theta}) = \int_\Omega \mathrm{div}(f\boldsymbol{\theta})\mathrm{d}x = \int_\Omega (\nabla f \cdot \boldsymbol{\theta} + f\,\mathrm{div}(\boldsymbol{\theta}))\mathrm{d}x, \qquad \boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d).$$

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where $\boldsymbol{n}$ denotes the outward normal to Ω.

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Surface form of the shape derivative.

Shape derivatives of volume and surface integrals

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The volume increases if $\boldsymbol{\theta}$ is positively proportional to $\boldsymbol{n}$ on $\partial\Omega$.

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κ is the mean curvature field of Γ.

Proposition 4 (Principal curvatures)

Let Γ be a $\mathcal{C}^2$ manifold and let $\boldsymbol{n}$ be any differentiable unit vector field normal to Γ. The gradient of the normal $\nabla \boldsymbol{n}$ satisfies:

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2. Let $\boldsymbol{\tau}_1$ and $\boldsymbol{\tau}_2$ be two tangent vector fields on Γ. Recall that the Lie derivative $\mathrm{D}_{\boldsymbol{\tau}_1}\boldsymbol{\tau}_2 - \mathrm{D}_{\boldsymbol{\tau}_2}\boldsymbol{\tau}_1$ is also a tangent vector on Γ (this is a consequence of Schwartz theorem), therefore
$$\boldsymbol{n}\cdot\mathrm{D}_{\boldsymbol{\tau}_1}\boldsymbol{\tau}_2 = \boldsymbol{n}\cdot\mathrm{D}_{\boldsymbol{\tau}_2}\boldsymbol{\tau}_1. \tag{1}$$

Proposition 4 (Principal curvatures)

Let Γ be a $\mathcal{C}^2$ manifold and let $\boldsymbol{n}$ be any differentiable unit vector field normal to Γ. The gradient of the normal $\nabla \boldsymbol{n}$ satisfies:

1. $\forall y \in \Gamma,\ \nabla \boldsymbol{n}(y) \cdot \boldsymbol{n}(y) = 0,$
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Using (1), we obtain $\boldsymbol{\tau}_1 \cdot \nabla \boldsymbol{n}\, \boldsymbol{\tau}_2 = \boldsymbol{\tau}_2 \cdot \nabla \boldsymbol{n}\, \boldsymbol{\tau}_1$, i.e. $\nabla \boldsymbol{n}(y)^T = \nabla \boldsymbol{n}(y)$.

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Let Γ be a $\mathcal{C}^2$ manifold and let $\boldsymbol{n}$ be any differentiable unit vector field normal outward to Γ. The gradient of the normal $\nabla \boldsymbol{n}$ satisfies:

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$$\forall y \in \Gamma,\ \nabla\boldsymbol{n}(y) = \sum_{i=1}^{d-1} \kappa_i(y)\boldsymbol{\tau}_i(y)\boldsymbol{\tau}_i(y)^T.$$

The real numbers $(\kappa_i(y))_{1\leq i\leq d-1}$ and the **tangent** *eigenvectors $(\boldsymbol{\tau}_i(y))_{1\leq i\leq d-1}$ are called* **principal curvatures** *and* **principal directions** *of Γ at y.*

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The **mean curvature** *of Γ is the real number $\kappa(y)$ defined by*

$$\kappa(y) := \sum_{i=1}^{d-1} \kappa_i(y) = \mathrm{Tr}(\nabla \boldsymbol{n}(y)) = \mathrm{div}(\boldsymbol{n}(y)).$$

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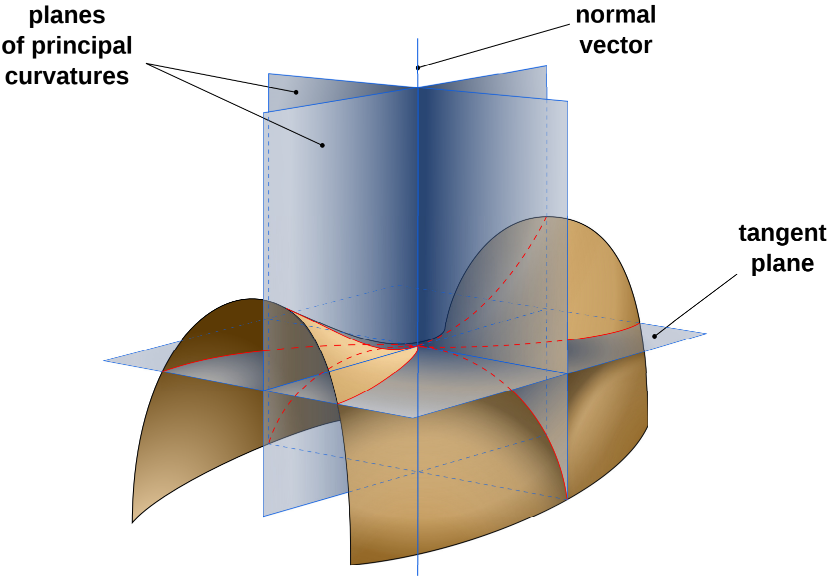
$\nabla \boldsymbol{n}$ is also called the Weingarten map of Γ.

Shape derivatives of volume and surface integrals



Proposition 3

Let Γ *a smooth codimension one surface of* $\mathbb{R}^d$ *with boundary* $\partial\Gamma$*. For any* $f \in W^{2,1}(\mathbb{R}^d)$*, the functional* $J(\Gamma)$ *defined by*

$$J(\Gamma) := \int_\Gamma f \mathrm{d}\sigma$$

is shape differentiable and the shape derivative reads

$$\begin{aligned} \mathrm{D}J(\Gamma)(\boldsymbol{\theta}) &= \int_\Gamma (\mathrm{div}(f\boldsymbol{\theta}) - \boldsymbol{n} \cdot \nabla\boldsymbol{\theta} \cdot \boldsymbol{n} f)\mathrm{d}\sigma \\ &= \int_\Gamma \left(\frac{\partial f}{\partial \boldsymbol{n}} + \kappa f \right) (\boldsymbol{\theta} \cdot \boldsymbol{n})\mathrm{d}\sigma + \int_{\partial\Gamma} f\boldsymbol{\theta} \cdot \boldsymbol{\tau} \mathrm{d}l, \end{aligned}$$

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κ is the mean curvature field of Γ.

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The perimeter decreases if $\boldsymbol{\theta}$ is positively proportional to $-\kappa\boldsymbol{n}$ on $\partial\Omega$.

Outline

1. Hadamard's shape derivatives
2. Shape derivatives of volume and surface integrals
3. Proofs: change of variable formulas and tangential calculus

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The proof of these propositions relies on

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Proposition 6

If Φ is a Lipschitz diffeomorphism of $\mathbb{R}^d$ and $\Omega \subset \mathbb{R}^d$ an open set, then for any $f \in L^1(\Phi(\Omega))$, $f \circ \Phi$ belongs to $L^1(\Omega)$ and it holds

$$\int_{\Phi(\Omega)} f \,\mathrm{d}x = \int_{\Omega} f \circ \Phi \, |\det(\nabla \Phi)| \mathrm{d}x.$$

Proposition 2

Let Ω be a bounded open set of $\mathbb{R}^d$. For any $f \in W^{1,1}(\mathbb{R}^d)$, the functional $J(\Omega)$ defined by

$$J(\Omega) := \int_{\Omega} f(x) \mathrm{d}x$$

is shape differentiable, and it holds

$$\mathrm{D}J(\Omega)(\boldsymbol{\theta}) = \int_{\Omega} \mathrm{div}(f\boldsymbol{\theta}) \mathrm{d}x = \int_{\Omega} (\nabla f \cdot \boldsymbol{\theta} + f \mathrm{div}(\boldsymbol{\theta})) \mathrm{d}x, \qquad \boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d).$$

If in addition Ω is smooth then the above formula can be rewritten as

$$\mathrm{D}J(\Omega)(\boldsymbol{\theta}) = \int_{\partial\Omega} f\, \boldsymbol{\theta} \cdot \boldsymbol{n} \mathrm{d}\sigma, \qquad \boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d).$$

where $\boldsymbol{n}$ denotes the outward normal to Ω.

Shape derivatives of volume and surface integrals

Proof of Proposition 2.

The application of the change of variable formula yields

$$J(\Omega_{\boldsymbol{\theta}}) = \int_{(I+\boldsymbol{\theta})\Omega} f \,\mathrm{d}x = \int_{\Omega} f \circ (I + \boldsymbol{\theta}) \det(I + \nabla\boldsymbol{\theta})\mathrm{d}x$$

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The application of the change of variable formula yields

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The results follow by using

$$\mathrm{div}(f\boldsymbol{\theta}) = \nabla f \cdot \boldsymbol{\theta} + f \mathrm{div}(\boldsymbol{\theta})$$

and an integration by parts. □

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Shape derivatives of volume and surface integrals

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Proposition 7

Let Γ be a $\mathcal{C}^1$ codimension one surface and Φ a $\mathcal{C}^1$ diffeomorphism of $\mathbb{R}^d$. Then for any function $f \in L^1(\Phi(\Gamma))$, it holds $f \circ \Phi \in L^1(\Gamma)$ and

$$\int_{\Phi(\Gamma)} f \, \mathrm{d}\sigma = \int_{\Gamma} f \circ \Phi \, |\det(\nabla\Phi)| \, ||(\nabla\Phi)^{-T} \boldsymbol{n}|| \mathrm{d}\sigma,$$

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where $\boldsymbol{n}$ is any normal vector field to Γ.

The proof use the following result:

Proposition 8

Given a smooth normal vector field $\boldsymbol{n}$ to Γ, a smooth normal vector field to $\Phi(\Gamma)$ is given by

$$\boldsymbol{n}_{\Phi(\Gamma)}(\Phi(y)) = \frac{\nabla \Phi^{-T}(y) \boldsymbol{n}(y)}{||\nabla \Phi^{-T}(y) \boldsymbol{n}(y)||}, \qquad y \in \Gamma.$$

Proposition 3

Let Γ a smooth codimension one surface of $\mathbb{R}^d$ with boundary $\partial\Gamma$. For any $f \in W^{2,1}(\mathbb{R}^d)$, the functional $J(\Gamma)$ defined by

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$$\begin{aligned} \mathrm{D}J(\Gamma)(\boldsymbol{\theta}) &= \int_\Gamma (\mathrm{div}(f\boldsymbol{\theta}) - \boldsymbol{n} \cdot \nabla\boldsymbol{\theta} \cdot \boldsymbol{n} f)\mathrm{d}\sigma \\ &= \int_\Gamma \left(\frac{\partial f}{\partial \boldsymbol{n}} + \kappa f \right) (\boldsymbol{\theta} \cdot \boldsymbol{n})\mathrm{d}\sigma + \int_{\partial\Gamma} f\boldsymbol{\theta} \cdot \boldsymbol{\tau} \mathrm{d}l, \end{aligned}$$

where $\boldsymbol{\tau}$ denotes the outward normal to $\partial\Gamma$ tangent to Γ.

Proof of Proposition 3.

Using the change of variable formula, we find

$$\int_{\Gamma_{\boldsymbol{\theta}}} f \, \mathrm{d}\sigma = \int_{\Gamma} f \circ (I + \boldsymbol{\theta}) \, |\det(\mathrm{I} + \nabla\boldsymbol{\theta})| \, ||(\mathrm{I} + \nabla\boldsymbol{\theta})^{-T} \boldsymbol{n}|| \mathrm{d}\sigma$$

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Finally, the divergence theorem on surfaces reads

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whence the result. □

Shape derivatives of volume and surface integrals

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where $\boldsymbol{\tau}$ *denotes the outward normal to* $\partial\Gamma$ *tangent to* Γ.

Analogous to the surface form of the shape derivative.

Exercise.

Let Γ be a smooth codimension one surface of $\mathbb{R}^d$ with boundary $\partial\Gamma$ and differentiable normal vector field $\boldsymbol{n}$. Let $\boldsymbol{f} \in W^{2,1}(\mathbb{R}^d, \mathbb{R}^d)$.

Exercise.

Let Γ be a smooth codimension one surface of $\mathbb{R}^d$ with boundary $\partial\Gamma$ and differentiable normal vector field $\boldsymbol{n}$. Let $\boldsymbol{f} \in W^{2,1}(\mathbb{R}^d, \mathbb{R}^d)$.

What is the shape derivative of $J(\Gamma) := \displaystyle\int_\Gamma \boldsymbol{f} \cdot \boldsymbol{n} \mathrm{d}\sigma$?