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On the Shape Gradient and Shape Hessian of a Shape Functional Subject to Dirichlet and Robin Conditions

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Abstract

This paper focuses on minimizing a shape functional through the solution of a Pure Dirichlet boundary value problem, and a Dirichlet-Robin boundary value problem. This shape optimization problem is a variant of the Kohn-Vogelius shape optimization formulation of a Bernoulli free boundary problem. The first- and second-order shape derivatives of the cost functional under consideration are explicitly derived. Interestingly, the present findings coincide with the existing results regarding solutions to the Bernoulli problem.

Keywords: shape gradient, shape Hessian, Kohn-Vogelius objective functional, Dirichlet boundary value problem, Robin boundary value problem

1 Introduction

The present paper derives the shape gradient and shape Hessian of the functional J in the minimization problem

$$\min_{\Omega} J(\Omega) \equiv \min_{\Omega} \int_{\Omega} |\nabla(u_D - u_N)|^2 \, \mathrm{d}x \tag{1}$$

where the state functions u_D and u_N satisfy the following Dirichlet and Robin boundary value problems, respectively:

$$\begin{cases} -\Delta u_D = 0 & \text{in } \Omega, \\ u_D = 1 & \text{on } \Gamma, \\ u_D = 0 & \text{on } \Sigma. \end{cases} \tag{2}$$

$$\begin{cases} -\Delta u_N = 0 & \text{in } \Omega, \\ u_N = 1 & \text{on } \Gamma, \\ \alpha u_N + \dfrac{\partial u_N}{\partial n} = \lambda & \text{on } \Sigma. \end{cases} \tag{3}$$

where $\alpha \geq 0$ is fixed, and $\lambda < 0$.

The shape optimization formulation (1) subject to (2) and (3) is derived from the two-dimensional exterior Bernoulli free boundary problem, a problem wherein we are given a constant $\lambda < 0$ and a bounded and connected domain, say $A \subset \mathbb{R}^2$ with a fixed boundary $\Gamma := \partial A$, and our task is to find a bounded connected domain $B \subset \mathbb{R}^2$ with a free boundary Σ and containing the closure of A, as well as a state function $u : \Omega \to \mathbb{R}$, where $\Omega = B \backslash \bar{A}$, that satisfies the following boundary value problem

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega, \\ u = 1 & \text{on } \Gamma, \\ u = 0, \dfrac{\partial u}{\partial \mathbf{n}} = \lambda & \text{on } \Sigma, \end{cases} \tag{4}$$

where $\mathbf{n}$ is the outward unit normal vector to Σ.

The present study is motivated by the work of Tiihonen [9] where he computed the shape gradient and shape Hessian of a different functional formulation of (4). In [9], Tiihonen considered the following shape optimization formulation:

$$\min_{\Sigma} J_(\Sigma) \equiv \min_{\Sigma} \int_{\Sigma} u_N^2 \, \mathrm{d}s \tag{5}$$

where u_N satisfies the conditions (3).

2 Preliminaries

The paper requires the following results and tools from shape calculus. These are found in [1, 3]:

Theorem 2.1. *Let Ω and U be nonempty bounded open connected subsets of $\mathbb{R}^2$ with Lipschitz continuous boundaries, such that $\bar{\Omega} \subseteq U$, and $\partial\Omega$ is the union of two disjoint boundaries Γ and Σ. Let T_t be defined as*

$$T_t : \bar{U} \to \mathbb{R}^2, \qquad T_t(x) = x + t\mathbf{V}(x), \quad x \in \bar{U}, \tag{6}$$

where $\mathbf{V}$ *belongs to* Θ*, defined as*

$$\Theta = \left\{ \mathbf{V} \in C^{1,1}(\bar{U}, \mathbb{R}^2) : \mathbf{V}|_{\Gamma \cup \partial U} = 0 \right\}. \tag{7}$$

Then for sufficiently small t*,*

(1.) $T_t : \bar{U} \to \bar{U}$ *is a homeomorphism,* (4.) $\Gamma_t = T_t(\Gamma) = \Gamma$*,*
(2.) $T_t : U \to U$ *is a* $C^{1,1}$ *diffeomorphism,* (5.) $\Sigma_t = T_t(\Sigma)$*, and*
(3.) $T_t : \Omega \to \Omega_t$ *is a* $C^{1,1}$ *diffeomorphism,* (6.) $\partial\Omega_t = \Gamma \cup \Sigma_t$*.*

For the following functions

$$\begin{cases} I_t(x) &= \det DT_t(x),\ x \in \bar{U}, \\ M_t(x) &= (DT_t(x))^{-T},\ x \in \bar{U}, \\ A_t(x) &= I_t M_t^T M_t(x),\ x \in \bar{U}, \\ w_t(x) &= I_t(x) |(DT_t(x))^{-T} \mathbf{n}(x)|,\ x \in \Sigma \end{cases} \tag{8}$$

we have the following lemma:

Lemma 2.2. *[7, 8] Consider the transformation* T_t*, where the fixed vector field* $\mathbf{V}$ *belongs to* Θ*, defined in* (7)*. Then there exists* $t_V > 0$ *such that* T_t *and the functions in* (8) *restricted to the interval* $I_V = (-t_V, t_V)$ *have the following regularity and properties:*

(1.) $t \mapsto T_t \in C^1(I_V, C^{1,1}(\bar{U}, \mathbb{R}^2))$. (8.) $\frac{d}{dt} T_t^{-1}|_{t=0} = -\mathbf{V}$.
(2.) $t \mapsto I_t \in C^1(I_V, C^{0,1}(\bar{U}))$. (9.) $\frac{d}{dt} DT_t|_{t=0} = D\mathbf{V}$.
(3.) $t \mapsto T_t^{-1} \in C(I_V, C^1(\bar{U}, \mathbb{R}^2))$. (10.) $\frac{d}{dt} (DT_t)^{-1}|_{t=0} = -D\mathbf{V}$.
(4.) $t \mapsto w_t \in C^1(I_V, C(\Sigma))$. (11.) $\frac{d}{dt} I_t|_{t=0} = \operatorname{div} \mathbf{V}$.
(5.) $t \mapsto A_t \in C(I_V, C(\bar{U}, \mathbb{R}^{2\times 2}))$. (12.) $\frac{d}{dt} A_t|_{t=0} = A$, *where* $A = (\operatorname{div} \mathbf{V})I - (D\mathbf{V} + (D\mathbf{V})^T$
(6.) *There is* $\beta > 0$ *such that* $A_t(x) \geq \beta I$ *for* $x \in U$. (13.) $\lim_{t \to 0} w_t = 1$.
(7.) $\frac{d}{dt} T_t|_{t=0} = \mathbf{V}$. (14.) $\frac{d}{dt} w_t|_{t=0} = \operatorname{div}_\Sigma \mathbf{V}$ *where* $\operatorname{div}_\Sigma \mathbf{V} = \operatorname{div} \mathbf{V}|_\Sigma - (D\mathbf{V}\mathbf{n}) \cdot \mathbf{n}$.

Material and shape derivatives of states

Definition 2.3. *Let* u *be defined in* $[0, t_V] \times U$*. The* material derivative $\dot{u} \in H^k(\Omega)$ *of* u *is defined as*

$$\dot{u}(x) := \dot{u}(0, x) := \lim_{t \to 0^+} \frac{u(t, T_t(x)) - u(0, x)}{t} = \frac{d}{dt} u(t, x + t\mathbf{V}(x)) \Big|_{t=0}$$

if the limit exists in $H^k(\Omega)$*.*

It can also be written as

$$\dot{u}(x) = \lim_{t\to 0^+} \frac{u_t \circ T_t(x) - u(x)}{t} = \frac{d}{dt}(u_t \circ T_t(x))\bigg|_{t=0}. \tag{9}$$

Definition 2.4. *Let u be defined in $[0, t_V] \times U$. The* shape derivative $u' \in H^k(\Omega)$ *of u is defined as :*

$$u'(x) := u'(0,x) := \lim_{t\to 0^+} \frac{u(t,x) - u(0,x)}{t}. \tag{10}$$

if the limit exists in $H^k(\Omega)$.

It can also be written as

$$u'(x) = \dot{u}(x) - (\nabla u \cdot \mathbf{V})(x). \tag{11}$$

Domain and boundary transformations

Lemma 2.5. *[10]*

1. *Let $\varphi_t \in L^1(\Omega_t)$. Then $\varphi_t \circ T_t \in L^1(\Omega)$ and $\int_{\Omega_t} \varphi_t \, dx_t = \int_\Omega \varphi_t \circ T_t I_t \, dx$.*
2. *Let $\varphi_t \in L^1(\partial\Omega_t)$. Then $\varphi_t \circ T_t \in L^1(\partial\Omega)$ and $\int_{\partial\Omega_t} \varphi_t \, ds_t = \int_{\partial\Omega} \varphi_t \circ T_t w_t \, ds$.*

where I_t and w_t are defined in (8)*.*

Some tangential Calculus

Here are some properties of tangential differential operators which are used in this work (cf. [4, 10]). Let Γ be a boundary of a bounded domain $\Omega \subset \mathbb{R}^n$.

Definition 2.6. *The* tangential gradient *of $f \in C^1(\Gamma)$ is given by*

$$\nabla_\Gamma f := \nabla F|_\Gamma - \frac{\partial F}{\partial \mathbf{n}} \mathbf{n} \in C(\Gamma, \mathbb{R}^n), \tag{12}$$

where F is any C^1 the extension of f into a neighborhood of Γ.

Definition 2.7. *The* tangential Jacobian matrix *of a vector function $\mathbf{v} \in C^1(\Gamma, \mathbb{R}^n)$ is given by*

$$D_\Gamma \mathbf{v} = D\mathbf{V}|_\Gamma - (D\mathbf{V}\mathbf{n})\mathbf{n}^T \in C(\Gamma, \mathbb{R}^{n\times n}), \tag{13}$$

where $\mathbf{V}$ is any C^1 the extension of $\mathbf{v}$ into a neighborhood of Γ.

Definition 2.8. *For a vector function $\mathbf{v} \in C^1(\Gamma, \mathbb{R}^n)$, its* tangential divergence *on Γ is given by*

$$\operatorname{div}_\Gamma \mathbf{v} = \operatorname{div} \mathbf{V}|_\Gamma - D\mathbf{V}\mathbf{n} \cdot \mathbf{n} \quad \in C(\Gamma), \tag{14}$$

where $\mathbf{V}$ is any C^1 the extension of $\mathbf{v}$ into a neighborhood of Γ.

Shape Differentiation of Integrals

Let $u \in L^1(\Omega)$. Suppose there exist $\dot{u} \in L^1(\Omega)$ and $u' \in L^1(\Omega)$. Then for sufficiently smooth Ω and $\mathbf{V}$,

$$\frac{d}{dt}\int_{\Omega_t} u(t,x)\ \mathrm{d}x\bigg|_{t=0} = \int_{\Omega} u'(0,x)\,\mathrm{d}x + \int_{\partial\Omega} u(0,s)\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s \tag{15}$$

Similarly, if $u \in L^1(\Gamma)$ and there exist $\dot{u} \in L^1(\Gamma)$ and $u' \in L^1(\Gamma)$, then

$$\frac{d}{dt}\int_{\Gamma_t} u(t,s)\ \mathrm{d}s\bigg|_{t=0} = \int_{\Gamma} u'(0,s)\,\mathrm{d}s + \int_{\Gamma}(\frac{\partial u}{\partial \mathbf{n}} + u(0,s)\kappa)\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s \tag{16}$$

where κ is the mean curvature of the boundary $\Gamma := \partial\Omega$.

The Eulerian derivatives

The Eulerian derivatives of a shape functional are defined as follows (cf. [9, 7, 4]):

Definition 2.9. *The* first-order Eulerian derivative *or the* shape gradient *of a shape functional $J : \Omega \to \mathbb{R}$ at the domain Ω in the direction of the deformation field $\mathbf{V}$ is given by*

$$dJ(\Omega;\mathbf{V}) := \lim_{t\to 0^+}\frac{J(\Omega_t) - J(\Omega)}{t}, \tag{17}$$

if the limit exists.

Definition 2.10. *The* second-order Eulerian derivative *or the* shape Hessian *of J at the domain Ω in the direction of the deformation fields $\mathbf{V}$ and $\mathbf{W}$ is given by*

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \lim_{s\to 0^+}\frac{dJ(\Omega_s(\mathbf{W});\mathbf{V}) - dJ(\Omega;\mathbf{V})}{s} \tag{18}$$

if the limit exists. Here $\Omega_s(\mathbf{W})$ is the perturbed domain Ω in the direction $\mathbf{W}$.

J is said to be shape differentiable at Ω if $dJ(\Omega;\mathbf{V})$ exists for all $\mathbf{V}$ and is linear and continuous with respect to $\mathbf{V}$. It is twice shape differentiable if for all $\mathbf{V}$ and $\mathbf{W}$, $d^2J(\Omega;\mathbf{V},\mathbf{W})$ exists and if $d^2J(\Omega;\mathbf{V},\mathbf{W})$ is bilinear and continuous with respect to $\mathbf{V}$ and $\mathbf{W}$.

3 Main Results

Here are the main results of this paper.

Theorem 3.1. *The shape gradient of the cost functional*

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

in the direction of the perturbation field $\mathbf{V} \in \Theta$*, where the state functions* u_D *and* u_N *satisfy* (2)*, and* (3)*, respectively, is given by*

$$\begin{aligned} dJ(\Omega;\mathbf{V}) &= \frac{1}{2}\int_\Sigma (\lambda^2 - (\nabla u_D \cdot \mathbf{n})^2 + 2\lambda\kappa u_N - (\nabla u_N \cdot \tau)^2)\mathbf{V}\cdot\mathbf{n}\, ds \\ &\quad + \frac{1}{2}\int_\Sigma (3\alpha^2 u_N^2 - 4\alpha\lambda u_N)\mathbf{V}\cdot\mathbf{n}\, ds + \frac{1}{2}\int_\Sigma -2\alpha u_N u_N'\, ds. \end{aligned} \quad (19)$$

i. If $\alpha = 0$*, then the shape gradient of the cost functional reduces to*

$$dJ(\Omega;\mathbf{V}) = \frac{1}{2}\int_\Sigma (\lambda^2 - (\nabla u_D \cdot \mathbf{n})^2 + 2\lambda\kappa u_N - (\nabla u_N \cdot \tau)^2)\mathbf{V}\cdot\mathbf{n}\, ds. \quad (20)$$

ii. If $\alpha = \kappa$*, the mean curvature of* Σ*, then the shape derivative becomes:*

$$dJ(\Omega;\mathbf{V}) = \frac{1}{2}\int_\Sigma (\lambda^2 - (\nabla u_D \cdot \mathbf{n})^2 - (\nabla u_N \cdot \tau)^2)\mathbf{V}\cdot\mathbf{n}\, ds + \frac{1}{2}\int_\Sigma 3\kappa^2 u_N^2 \mathbf{V}\cdot\mathbf{n}\, ds. \quad (21)$$

Proof. Using the differentiation formula (15), we get the Eulerian derivative of $J(\Omega)$ in the direction $\mathbf{V}$:

$$dJ(\Omega;\mathbf{V}) = \int_\Omega \nabla(u_D' - u_N')\cdot\nabla(u_D - u_N)\,\mathrm{d}x + \frac{1}{2}\int_\Sigma |\nabla(u_D - u_N)|^2 \mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s$$

where the shape derivatives u_D' and u_N' (at Ω in the direction $\mathbf{V}$) satisfy the following boundary problems:

$$\begin{cases} -\Delta u_D' = 0 & \text{in } \Omega, \\ u_D' = 0 & \text{on } \Gamma, \\ u_D' = -\mathbf{V}\cdot\mathbf{n}\dfrac{\partial u_D}{\partial \mathbf{n}} & \text{on } \Sigma. \end{cases} \quad (22)$$

$$\begin{cases} -\Delta u_N' = 0 & \text{in } \Omega, \\ u_N' = 0 & \text{on } \Gamma, \\ \alpha u_N' + \dfrac{\partial u_N'}{\partial \mathbf{n}} = \mathrm{div}_\Sigma(\mathbf{V}\cdot\mathbf{n}\nabla_\Sigma u_N) - \alpha(\dfrac{\partial u_N}{\partial \mathbf{n}} + u_N\kappa)\mathbf{V}\cdot\mathbf{n} + \kappa\lambda\mathbf{V}\cdot\mathbf{n} & \text{on } \Sigma. \end{cases} \quad (23)$$

Derivations for the boundary value problems (22) and (23) can be seen in [2, 9]. Now using Green's identity, and the BVPs (22) and (23), we write dJ as $I_1 + I_2$

and manipulate each integral.

$$\begin{aligned}
I_1 &= \int_\Omega \nabla(u_D' - u_N') \cdot \nabla(u_D - u_N)\,\mathrm{d}x = \int_\Omega \nabla u_D' \cdot \nabla(u_D - u_N)\,\mathrm{d}x - \int_\Omega \nabla u_N' \cdot \nabla(u_D - u_N)\,\mathrm{d}x \\
&= \int_\Sigma u_D' \frac{\partial}{\partial \mathbf{n}}(u_D - u_N)\,\mathrm{d}s - \int_\Sigma \frac{\partial u_N'}{\partial \mathbf{n}}(u_D - u_N)\,\mathrm{d}s \\
&= -\int_\Sigma \left(\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 - \frac{\partial u_D}{\partial \mathbf{n}}\frac{\partial u_N}{\partial \mathbf{n}} \right) \mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s + \int_\Sigma u_N \frac{\partial u_N'}{\partial \mathbf{n}}\,\mathrm{d}s \\
&= -\int_\Sigma \left(\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 - \frac{\partial u_D}{\partial \mathbf{n}}(\lambda - \alpha u_N) \right) \mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s + \int_\Sigma \mathrm{div}_\Sigma(\mathbf{V}\cdot\mathbf{n}\nabla_\Sigma u_N) u_N\,\mathrm{d}s \\
&\quad - \int_\Sigma [\alpha u_N(\lambda - \alpha u_N + u_N\kappa) - \lambda u_N \kappa]\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s - \int_\Sigma \alpha u_N' u_N\,\mathrm{d}s
\end{aligned}$$

$$\begin{aligned}
I_2 &= \frac{1}{2}\int_\Sigma |\nabla(u_D - u_N)|^2 \mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s = \frac{1}{2}\int_\Sigma (|\nabla u_D|^2 - 2\nabla u_D \nabla u_N + |\nabla u_N|^2)\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s \\
&= \frac{1}{2}\int_\Sigma \left(\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 - 2\frac{\partial u_D}{\partial \mathbf{n}}\frac{\partial u_N}{\partial \mathbf{n}} + (\lambda^2 - 2\alpha\lambda u_N + \alpha^2 u_N^2) + (\nabla u_N \cdot \tau)^2 \right) \mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s \\
&= \frac{1}{2}\int_\Sigma \left(\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 - 2\frac{\partial u_D}{\partial \mathbf{n}}(\lambda - \alpha u_N) + (\lambda^2 - 2\alpha\lambda u_N + \alpha^2 u_N^2) + (\nabla u_N \cdot \tau)^2 \right) \mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s
\end{aligned}$$

Combining I_1 and I_2 and using the fact that

$$\int_\Sigma \mathrm{div}_\Sigma(\mathbf{V}\cdot\mathbf{n}\nabla_\Sigma u_N) u_N\,\mathrm{d}s = -\int_\Sigma (\nabla u_N \cdot \tau)^2 \mathbf{V}\cdot\mathbf{n},$$

we get (19).

If $\alpha = 0$, then we obtain (20).

If $\alpha = \kappa$, then $u_N' = 0$ by using Lemma 1 in [9]. Consequently, the shape derivative becomes (21). □

Remark 3.2. *For $\alpha = 0$ our results coincide with our results given in [3]. In [3], however, we did not utilize the shape derivatives of states in obtaining the shape gradient of the functional.*

Corollary 3.3. *At a shape Ω^* wherein the state function u solves the Bernoulli free boundary problem (that is, $u = u_D = u_N$ on $\bar{\Omega}^*$), the first derivative $dJ(\Omega; \mathbf{V})$ vanishes.*

Proof. At the solution of the Bernoulli problem, $u_D = u_N = 0$, $\dfrac{\partial u_D}{\partial \tau} = 0$, $\dfrac{\partial u_N}{\partial \mathbf{n}} = \lambda$ on Σ. Hence, we have

$$dJ(\Omega; \mathbf{V}) = \frac{1}{2}\int_\Sigma (\lambda^2 - \lambda^2 + 0 - 0)\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s + 0 - 0 = 0.$$

□

We also give a result on the second order shape derivative of the functional at the solution of the Bernoulli problem.

Theorem 3.4. *If $u_D = u_N$ where u_D and u_N satisfy the Dirichlet problem* (2), *and the Robin boundary problem* (3), *respectively, then the second order shape derivative $d^2J(\Omega;\mathbf{V};\mathbf{W})$ of the cost functional defined by*

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

at Ω in the directions of the perturbation fields $\mathbf{V}$ and $\mathbf{W}$ is given by

$$\begin{aligned} d^2J(\Omega;\mathbf{V},\mathbf{W}) &= \int_\Sigma (\lambda^2\mathbf{V}\cdot\mathbf{n}S(\mathbf{W}\cdot\mathbf{n}) + \lambda^2\kappa\mathbf{V}\cdot\mathbf{n}\mathbf{W}\cdot\mathbf{n})\, ds + \int_\Sigma (\lambda\kappa u'_{N,W}\mathbf{V}\cdot\mathbf{n} + \lambda^2\kappa\mathbf{V}\cdot\mathbf{n}\mathbf{W}\cdot\mathbf{n})\, ds \\ &- \int_\Sigma (2\alpha\lambda u'_{N,W}\mathbf{V}\cdot\mathbf{n} + 2\alpha\lambda^2\mathbf{V}\cdot\mathbf{n}\mathbf{W}\cdot\mathbf{n})\, ds - \int_\Sigma (\alpha u'_N u'_{N,W} + \alpha\lambda u'_N\mathbf{W}\cdot\mathbf{n})\, ds. \quad (24)\end{aligned}$$

Here S is an operator that relates u'_D and u'_N as $Su'_D = \frac{\partial u'_D}{\partial \mathbf{n}}$, where u'_D satisfies (22), *u'_N is the shape derivative of u_N at Ω in the direction $\mathbf{V}$ and $u'_{N,W}$ is the shape derivative of u_N at Ω in the direction $\mathbf{W}$.*

i. If $\alpha = 0$, then the second order shape derivative is given by

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \int_\Sigma 2\lambda^2\kappa\mathbf{V}\cdot\mathbf{n}\mathbf{W}\cdot\mathbf{n}\, ds + \int_\Sigma (S(\mathbf{W}\cdot\mathbf{n}) + \kappa S^{-1}(\kappa\mathbf{W}\cdot\mathbf{n}))\lambda^2\mathbf{V}\cdot\mathbf{n}.$$

ii. If $\alpha = \kappa$, then the second order shape derivative of the cost functional is given by

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \int_\Sigma \lambda^2\mathbf{V}\cdot\mathbf{n}S(\mathbf{W}\cdot\mathbf{n})\, ds.$$

Proof. Let us decompose $dJ(\Omega;\mathbf{V})$ in Theorem 3.1 as $dJ(\Omega;\mathbf{V}) = L + M + N$. As what we did previously, we write L as $L = L_1 + L_2 + L_3$, where

$$\begin{aligned} L_1 &= \frac{1}{2}\int_\Sigma \left(\lambda^2 - \left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2\right)\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s, \qquad L_2 = \int_\Sigma \lambda\kappa u_N\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s, \\ L_3 &= -\frac{1}{2}\int_\Sigma (\nabla u_N\cdot\tau)^2\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s\end{aligned}$$

Consider another deformation field $\mathbf{W}$. Analogous to the previous computation, we obtain the following at the solution of the Bernoulli problem.

$$\begin{aligned} dL_1(\Omega;\mathbf{W}) &= \int_\Sigma \lambda^2(\mathbf{V}\cdot\mathbf{n}, (S+\kappa I)\mathbf{W}\cdot\mathbf{n})\,\mathrm{d}s, \\ dL_2(\Omega;\mathbf{W}) &= \int_\Sigma (u'_{N,W} + \lambda\mathbf{W}\cdot\mathbf{n})\lambda\kappa\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s, \qquad dL_3(\Omega;\mathbf{W}) = 0,\end{aligned}$$

where $Su'_D = \frac{\partial u'_D}{\partial \mathbf{n}}$, and u'_D satisfies (22). Therefore at the solution,

$$dL(\Omega;\mathbf{W}) = \int_\Sigma \lambda^2(\mathbf{V}\cdot\mathbf{n}, (S+\kappa I)\mathbf{W}\cdot\mathbf{n})\,\mathrm{d}s + \int_\Sigma (u'_{N,W} + \lambda\mathbf{W}\cdot\mathbf{n})\lambda\kappa\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s.$$

Next we consider M and derive its shape gradient at Ω in the direction $\mathbf{W}$.

$$\begin{aligned} M &= \frac{1}{2}\int_{\Sigma}(3\alpha^2 u_N^2 - 4\alpha\lambda u_N)\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s. \\ dM(\Omega;\mathbf{W}) &= \frac{1}{2}\int_{\Sigma}[6\alpha^2 u_N\cdot u'_{N,W} - 4\alpha\lambda u'_{N,W}]\mathbf{V}\cdot\mathbf{n} \\ &\quad + \frac{1}{2}\int_{\Sigma}\left\{\frac{\partial}{\partial\mathbf{n}}[(3\alpha^2 u_N^2 - 4\alpha\lambda u_N)\mathbf{V}\cdot\mathbf{n}] + (3\alpha^2 u_N^2 - 4\alpha\lambda u_N)\mathbf{V}\cdot\mathbf{n}\kappa\right\}\mathbf{W}\cdot\mathbf{n}. \end{aligned}$$

At the solution of the Bernoulli problem,

$$\begin{aligned} dM(\Omega;\mathbf{W}) &= -\int_{\Sigma}2\alpha\lambda u'_{N,W}\mathbf{V}\cdot\mathbf{n} - \int_{\Sigma}2\alpha\lambda\frac{\partial u_N}{\partial\mathbf{n}}\mathbf{V}\cdot\mathbf{n}\mathbf{W}\cdot\mathbf{n} \\ &= -2\int_{\Sigma}\alpha\lambda(u'_{N,W}\mathbf{V}\cdot\mathbf{n} + \lambda\mathbf{W}\cdot\mathbf{n}\mathbf{V}\cdot\mathbf{n})\,\mathrm{d}s. \end{aligned}$$

Last but not least, we consider N and derive also its shape gradient in the direction $\mathbf{W}$.

$$\begin{aligned} N &= \frac{1}{2}\int_{\Sigma} -2\alpha u_N u'_N\,\mathrm{d}s. \\ dN(\Omega;\mathbf{W}) &= -\int_{\Sigma}\left[(\alpha u_N u'_N)'_W + (\frac{\partial}{\partial\mathbf{n}}(\alpha u_N u'_N) + \alpha u_N u'_N\kappa)\right]\mathbf{W}\cdot\mathbf{n} \\ &= -\int_{\Sigma}\left[\alpha u'_{N,W}u'_N + \alpha u_N(u'_N)'_W + \left(\alpha\frac{\partial u_N}{\partial\mathbf{n}}u'_N + \alpha u_N\frac{\partial u'_N}{\partial\mathbf{n}} + \alpha u_N u'_N\kappa\right)\right]\mathbf{W}\cdot\mathbf{n}. \end{aligned}$$

where $(u'_N)'_W$ is the second order shape derivative of the solution u_N, first in the direction of the perturbation field $\mathbf{V}$, then in the direction of the perturbation field $\mathbf{W}$.

At the solution of the Bernoulli problem,

$$dN(\Omega;\mathbf{W}) = -\int_{\Sigma}[\alpha u'_{N,W}u'_N + \alpha\lambda u'_N\mathbf{W}\cdot\mathbf{n}]\,\mathrm{d}s.$$

Combining $dL(\Omega;\mathbf{W}), dM(\Omega;\mathbf{W})$, and $dN(\Omega;\mathbf{W})$, we get (24).

Now, we consider the case $\alpha = 0$. Generally, u'_N satisfies the variational equation:

$$\int_{\Sigma}(\frac{\partial u'_N}{\partial\mathbf{n}} + \alpha u'_N)\varphi = \int_{\Sigma} -\nabla_{\Sigma}u_N\nabla_{\Sigma}\varphi\mathbf{V}\cdot\mathbf{n} - \alpha(\frac{\partial u_N}{\partial\mathbf{n}} + u_N\kappa)\varphi\mathbf{V}\cdot\mathbf{n} + \lambda\kappa\varphi\mathbf{V}\cdot\mathbf{n}.$$

where $\varphi \in H^1(\Omega;\Gamma)$. For this case, at the solution of the Bernoulli problem, u'_N satisfies the following reduced variational equation:

$$\int_{\Sigma}(\frac{\partial u'_N}{\partial\mathbf{n}} - \lambda\kappa\mathbf{V}\cdot\mathbf{n})\varphi = 0$$

And by the fundamental lemma of calculus of variations, we get

$$\frac{\partial u'_N}{\partial\mathbf{n}} - \lambda\kappa\mathbf{V}\cdot\mathbf{n} = 0$$

or equivalently, $\dfrac{\partial u'_N}{\partial \mathbf{n}} = \lambda\kappa \mathbf{V}\cdot\mathbf{n}$. Using the Steklov-Poincare operator: $Su'_N = \dfrac{\partial u'_N}{\partial \mathbf{n}}$, we obtain

$$u'_N = S^{-1}(\lambda\kappa\mathbf{V}\cdot\mathbf{n}) \tag{25}$$

Consequently,

$$u'_{N,W} = S^{-1}(\lambda\kappa\mathbf{W}\cdot\mathbf{n}). \tag{26}$$

Substituting $\alpha = 0$, (25), and (26) into (24), we get

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \int_\Sigma 2\lambda^2\kappa\mathbf{V}\cdot\mathbf{n}\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}s + \int_\Sigma (S(\mathbf{W}\cdot\mathbf{n}) + \kappa S^{-1}(\kappa\mathbf{W}\cdot\mathbf{n}))\lambda^2\mathbf{V}\cdot\mathbf{n}.$$

For $\alpha = \kappa$, we note that $u'_N = 0$ and $u'_{N,W} = 0$ by applying Lemma 1 of [9]. Hence, we obtain

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \int_\Sigma \lambda^2\mathbf{V}\cdot\mathbf{n}S(\mathbf{W}\cdot\mathbf{n})\,\mathrm{d}s.$$

□

Remark 3.5. *For $\alpha = 0$, our results coincides with the one presented in [1] wherein three strategies were utilized to derive the shape Hessian of the functional.*

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