Second order directional shape derivatives

Anton Schiela & Julian Ortiz

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Abstract

We propose a variant in the definition of a second order shape derivative. The result is a quadratic form in terms of one perturbation vector field that yields a second order quadratic model of the perturbed functional. We discuss the structure of this derivative, derive domain expressions and Hadamard forms in a general geometric framework, and give a detailed geometric interpretation of the arising terms.

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1 Introduction

In this work we consider shape sensitivity analysis of functionals of the form

$$\int_S f(x)\, dx$$

with respect to perturbations of the smooth k-dimensional sub-manifold $S \subset \mathbb{R}^d$ by one-parameter families $\phi(t, \cdot) : \mathbb{R}^d \to \mathbb{R}^d$ of (orientation preserving) diffeomorphisms.

Since we are concerned here with issues of calculus, rather than questions of differentiability, we assume that all quantities have sufficient smoothness. In particular, ϕ, S, and its boundary ∂S are assumed to be smooth enough to guarantee that all used quantities are well defined.

This question is classical in a couple of areas in mathematics. It is, for example, the theoretical basis of shape optimization, but also plays a role - with slightly different perspective – in differential geometry, in particular in the study of geodesics and minimal surfaces (cf. e.g. [7, Chapter XI] or [13, Chapter 9]).

In shape optimization we find several different approaches to shape sensitivity analysis. They differ in the way, $\phi(t, \cdot)$ is constructed from a given vector field v. The oldest approach seems to be the so called perturbation of identity method [8, 12, 4], where one defines $\phi(t, x) = x + tv(x)$. More recently the velocity method was proposed (cf. e.g. [2] and for a similar approach [16]) in which ϕ is given as a flow of v. Even more recently, in [10] it was proposed to construct ϕ from v by geometrical considerations in an infinite dimensional manifold of shapes, establishing also a framework for Newton methods in shape spaces.

While the first shape derivatives coincide in all approaches, the second shape derivatives differ among the approaches. The reason is that for given vector fields v the corresponding transformations $\phi(t, \cdot)$ differ up to second order. Moreover, in order to obtain a bilinear form, definitions of shape hessians employ two vector fields v_i and two temporal parameters

t_i, the combination of which defines ϕ. For example in the perturbation of identity method the definition $\phi(t_1, t_2, x) = x + t_1 v_1 + t_2 v_2$ has been considered, for example, in [11, 9, 4].

For the velocity method $\phi(t_1, t_2, x)$ has been defined as the composition of two mappings [2, Sect. 9.6]. Consequently ϕ depends on v_1 and v_2 in a non-commutative way, which leads to a non-symmetric shape hessian. A connection to the second Lie derivative has been drawn in [6], applications in image segmentation can be found in [5]. Relations between these variants and application of Newton's method have been discussed in [15].

In the approach, proposed in this paper we start with a *single* family of transformations $\phi(t, \cdot)$, use only a single vector field $v = \phi_t(0, \cdot)$ and look for a quadratic approximation of the perturbed integral. We end up with a quadratic form $q(v)$ in terms of a single vector field, which contrasts with the approaches mentioned above which all yield bilinear forms in two vector fields. In addition, we observe that a linear term arises that depends on an acceleration field $v_t = \phi_{tt}(0, \cdot)$ which depends on the chosen approach. This term vanishes at critical points. A symmetric bilinear form can be derived by differentiating q with respect to v. Our approach yields a unifying perspective on the shape hessian and a convenient basis for a couple of applications, such as stability analysis (cf. e.g. [1]) and SQP-methods.

Concerning the geometric setting we choose a rather general setting, using the k-dimensional measure tensor on $S \subset \mathbb{R}^d$ in a general way. This includes the well known cases $S = \Omega$, where Ω is an open domain in $\mathbb{R}^d$ and $S = \partial\Omega$ but also a couple of others, such as hypersurfaces with boundaries and lines. Also any other combinations of k and d are covered. Of course, S and its boundary ∂S have to be sufficiently smooth to obtain a well defined tangent space at each point, and also (for the discussion of the Hadamard form) to define the second fundamental form and notions of curvature, derived from it.

Much care is taken to the derivation and geometrical interpretation of the Hadamard form of the second derivative. Here it is helpful to deal only with a quadratic form for a single perturbation instead of a bilinear form for two perturbations. Finally, we sketch, how our results can be applied and extended to settings with partial differential equations.

1.1 A general embedding

Consider a one-parameter family of orientation preserving diffeomorphisms

$$\begin{aligned} \phi : I \times \mathbb{R}^d &\to \mathbb{R}^d \\ (t, x) &\to \phi(t, x), \end{aligned}$$

where $I \subset \mathbb{R}$ is an open interval, containing 0 and $\phi(0, \cdot) = Id$. We define for $t \in I$ the vector fields

$$v(t), v_t(t) : \mathbb{R}^d \to \mathbb{R}^d$$

via $v(t, x) := \phi_t(t, x)$, $v_t(t, x) = \phi_{tt}(t, x)$. For brevity, we will write $v = v(0)$ and $v_t = v_t(0)$. Thus, local Taylor expansion around $t = 0$ yields:

$$\phi(t, x) = x + vt + \frac{1}{2} v_t t^2 + o(t^2).$$

For kinematic interpretation of this approach, we may think about t as (pseudo-)time, so that v can be interpreted as a velocity field and v_t as an acceleration.

Consider also two smooth functions $f : I \times \mathbb{R}^d \to \mathbb{R}$ and $F : I \times \mathbb{R}^d \to \mathbb{R}$, such that

$$F(t, \phi(t, x)) = f(t, x) \quad \forall (t, x) \in I \times \mathbb{R}^d$$

and thus consequently

$$F(0, x) = f(0, x) \quad \forall x \in \mathbb{R}^d.$$

We observe that $F(t, \cdot)$ is defined on the codomain of ϕ, while $f(t, \cdot)$ is defined on the domain of ϕ.

By the relation of $F(t, \phi(t, x)) = f(t, x)$ and by the chain rule we easily derive relations between the derivatives of F and f at $t = 0$:

$$F_x = f_x, \qquad F_t + F_x \phi_t = f_t \quad \text{i.e.} \quad F_t = f_t - f_x v. \tag{1}$$

The expression F_t is commonly called *shape derivative* of f (with respect to ϕ), while f_t is called the *material derivative* of f. This naming suggests a tacit identification of the two different functions f and F. In fact, often they are identified, and one writes $F_t = f'$ for the shape derivative and $f_t = \dot{f}$ for the material derivative of f. In our paper, we will, however, distinguish both functions, by using capital and lower case letters.

Denoting $X := \phi(t, x)$ we are interested in the time dependent integral:

$$I(t) := \int_{\phi(t,S)} F(t, X)\, dX, \tag{2}$$

and in particular in its first and second derivatives with respect to t. Since

$$I(0) = \int_S f(0, x)\, dx$$

we will denote these derivatives as first and second order shape derivatives or shape sensitivities of $\int_S f(x)\, dx$ with respect to the embedding $\phi(t, x)$ and $f(t, x)$. In classical shape-optimization one chooses $F(t, X)$ constant in time. In view of (2) this corresponds to the geometrical intuition that the integrand is chosen fixed in the back-ground, while the domain of integration evolves.

The basis of our considerations is the following integral transformation rule:

$$I(t) = \int_{\phi(t,S)} F(t, X)\, dX = \int_S F(t, \phi(t, x)) J(t, x)\, dx = \int_S f(t, x) J(t, x)\, dx \tag{3}$$

where we observe the occurrence of the well known measure tensor:

$$J(t, x) := \sqrt{\det(B(x)^T \phi_x(t, x)^T \phi_x(t, x) B(x))}$$

with $B(x) \in \mathbb{R}^{d \times k}$ being a matrix that consists of k orthonormal tangent vectors to S.

Our task is now to compute the first and second derivative $I_t(0)$ and $I_{tt}(0)$ of $I(t)$ with respect to time. This can be done via the right-most expression in (3), because it is defined on a fixed domain.

Theorem 1.1. *The first and second order shape sensitivities satisfy:*

$$I_t(0) = \int_S f_t + f J_t\, dx \tag{4}$$

$$I_{tt}(0) = \int_S f_{tt} + 2 f_t J_t + f J_{tt}\, dx. \tag{5}$$

Proof. Straightforward application of the product rule to

$$I(t) = \int_S f(t, x) J(t, x)\, dx,$$

taking into account that $J(0, x) = Id$. □

The most difficult part of this paper will be the analysis of J_{tt}. We note that the case $k = d$, where $J = \det \phi_x$ is well understood. For the case $k = d - 1$ one also finds results in the literature, where, however, a different representation of J, via a unit normal field is employed. Our approach treats these cases in a unified way.

In addition to the computation of the terms involved it is common to rearrange and analyse them further, in order to get some geometric understanding of the situation. For example, we expect that $I(t) = const$, if F is constant in time and ϕ leaves S invariant. As a consequence, only certain parts of the vector field v contribute to $I_t(0)$ and $I_{tt}(0)$. Such formulas are known as Hadamard forms of I_t and I_{tt}. It is known that the derivation of the Hadamard form requires higher regularity of the employed data, but yields useful geometrical understanding.

1.2 General structure

Before we carry out our program in detail, we discuss the general structure that we expect, in particular, concerning second derivatives.

In Section 2.3 we will see that J_t depends linearly on v and J_{tt} is quadratic in v and linear in v_t. Similarly, in the case $F(t) = const$, f_t depends linearly on v and f_{tt} contains quadratic terms in v and linear terms in v_t.

This yields that $I_t(0)$ is a linear form in $v = \phi_t(0)$:

$$I_t(0) = l(v)$$

while $I_{tt}(0)$ is the sum of a quadratic form $q(v)$, and a linear form $l(v_t)$:

$$I_{tt}(0) = l(v_t) + q(v).$$

Very often v_t is given as a function of v so that $l(v_t(v))$ is quadratic in v, so that we can define the following quadratic form in v:

$$\hat{q}(v) := l(v_t(v)) + q(v)$$

Remark 1.2. Terms of the form $l(v_t)$ always occur when the composition of a function $g : X \to \mathbb{R}$ with a family of non-linear mappings $\phi : I \times X \to X$ is differentiated at $t = 0$:

$$\frac{d}{dt} g \circ \phi|_{t=0} = g_x \phi_t = g_x v$$
$$\frac{d^2}{dt^2} g \circ \phi|_{t=0} = g_{xx}(\phi_t, \phi_t) + g_x \phi_{tt} = g_{xx}(v, v) + g_x v_t$$

In that case, we would have $q(v) = g_{xx}(v, v)$, $l(v_t) = g_x v_t$. We also observe that the second term vanishes if $g_x = 0$, i.e., at critical points of $g \circ \phi$.

For a given family $\phi(t, \cdot)$ of transformations we can now predict the value of $I(t)$ by

$$\begin{aligned} I(t) &= I(0) + I_t(0)t + \frac{1}{2} I_{tt}(0)t^2 + o(t^2) \\ &= I(0) + l(v)t + \frac{1}{2}(q(v) + l(v_t))t^2 + o(t^2). \end{aligned}$$

up to second order, as long as v and v_t are available.

If $I_t(0) = 0$, i.e., at a critical point of the above shape-functional, we can derive second order optimality conditions, depending only on v (because then $I_t = l = 0$):

$$I(t) - I(0) = \frac{1}{2}(q(v) + l(v_t))t^2 + o(t^2) = \frac{1}{2}q(v)t^2 + o(t^2).$$

Once, the quadratic form $\hat{q}$ has been computed, it is easy to construct a corresponding bilinear form $b(\cdot, \cdot)$, such that

$$b(v, v) = \hat{q}(v) \quad \forall v.$$

Since q is quadratic, its second derivative $\hat{q}''$ is independent of the point of differentiation and symmetric as a bilinear form by the Schwarz theorem. We thus set

$$b(v, w) := \frac{1}{2}\hat{q}''(0)(v, w) = \frac{1}{2}\hat{q}''(0)(w, v) = b(w, v).$$

This may be useful in the context of SQP-methods for shape optimization. However, we will not elaborate on this topic.

Special cases

Concerning the construction of $\phi(t, x)$ there are two approaches which are commonly used and an additional, more recent approach. All of them construct $\phi(t, x)$ from a given velocity field $v_0(x)$:

i) The *perturbation of identity method* [12, 4] chooses $\phi(t, x) := x + tv_0(x)$. This means that $\phi(t, x)$ satisfies the initial value problem:

$$\begin{aligned} \phi_t(t, x) &= v_0(x) \\ \phi(0, x) &= x. \end{aligned} \tag{6}$$

Hence, $\phi(t, x)$ may be interpreted as the flow of a moving vector field. Each point $\phi(t, x)$ evolves with constant velocity $v_0(x)$.

We see that $v(t, x) = \phi_t(t, x) = v_0(x)$ and

$$\begin{aligned} v_t &= \phi_{tt}(0, \cdot) = 0, \\ \tilde{q}(v) &= q(v), \\ b(v, w) &= \frac{1}{2}q''(0)(v, w). \end{aligned}$$

ii) The *velocity method* [2] defines $\phi(t, x)$ via the following modified initial value problem:

$$\begin{aligned} \phi_t(t, x) &= v_0(\phi(t, x)) \\ \phi(0, x) &= x. \end{aligned} \tag{7}$$

In this construction we may view w as a time-independent velocity field in the background and $\phi(t, x)$ as the trajectory of a particle that moves in this field.

It follows $v(0, x) = v_0(x)$ and

$$\begin{aligned} v_t &= v_0(\phi(t, \cdot))_t|_{t=0} = v_{0,x}\phi_t = v_{0,x}v_0 = v_x v, \\ \tilde{q}(v) &= q(v) + l(v_x v), \\ b(v, w) &= \frac{1}{2}q''(0)(v, w) + \frac{1}{2}l(v_x w + w_x v). \end{aligned}$$

The non-symmetric shape hessian discussed in [2] is given by

$$\tilde{b}(v,w) := \frac{1}{2}q''(0)(v,w) + l(v_x w).$$

iii) Alternatively, an approach via *Riemannian shape manifolds* can be chosen [10]. We only sketch this approach. A second order initial value problem of the following form is used to define $\phi(t,x)$:

$$\begin{aligned} v_t(t,x) &= B_{\phi(t,S)}(x, v(t,x), v(t,x)) \\ \phi_t(t,x) &= v(t,x) \\ v(0,x) &= v_0(x) \\ \phi(0,x) &= x. \end{aligned} \tag{8}$$

Here B is the spray (cf. e.g. [7, IV.§3]) associated with the given Riemannian metric of the infinite dimensional shape manifold. $B_{\phi(t,S)}$ is for each ϕ a bilinear mapping in v, which is assumed to have appropriate transformation properties with changes of charts. We remark that this spray is the infinite dimensional analogue to the well known Christoffel symbols and depends on the metric of the shape manifold. The above initial value problem is used to define geodesics on an infinite dimensional manifold of diffeomorphisms. We note

$$\begin{aligned} v_t = \phi_{tt}(0,\cdot) &= B_S(v,v), \\ \tilde{q}(v) &= q(v) + l(B_S(v,v)), \\ b(v,w) &= \frac{1}{2}q''(0)(v,w) + \frac{1}{2}l(B_S(v,w)). \end{aligned}$$

2 Domain expressions of shape derivatives

In the following, we consider $\mathbb{R}^d$ equipped with the standard scalar product

$$a \cdot b := \sum_{i=1}^{d} a_i b_i$$

and a smooth submanifold of $S \subset \mathbb{R}^d$. We denote by T_xS the tangent space of S at $x \in S$ and by N_xS its orthogonal complement, the normal space of S at x.

2.1 Projection onto the tangent space

A central quantity in the differential geometry of submanifolds is the *orthogonal projection* to the tangent space at a given point $x \in S$. We associate to each $s \in S$ an orthonormal basis $\{b_1, \dots, b_k\}$ of T_xS, whose members form the columns of a matrix $B = B(x)$. Then we define the orthogonal projection onto T_xS as follows:

$$\begin{aligned} P(x) : \mathbb{R}^d &\to \mathbb{R}^d \\ w &\mapsto P(x)w = B(x)B^T(x)w. \end{aligned}$$

We see that $P(x)$ is independent of the choice of orthonormal basis B of T_xS: if B is replaced by BQ and $Q \in \mathbb{R}^{k\times k}$ is an orthogonal matrix, then $BQ(BQ)^T = BB^T$. Recall that $P(x)P(x) = P(x)$, $\operatorname{ran} P(x) = T_xS$ is the tangent space, and $\ker P(x) = N_xS$ is the normal space. By $I - P(x)$ we obtain the projection onto N_xS. Most of the time we will drop the argument x and just write P instead of $P(x)$.

Splittings. Let $v : S \to \mathbb{R}^d$ be a vector field on S. By Pv we denote the vector-field, defined by $(Pv)(x) = P(x)v(x)$ for all $x \in S$. In this way we can be *split* v *orthogonally* into a tangential field s and a normal field n:

$$v = Pv + (I - P)v = s + n.$$

Similarly, we can *split the derivative* f_x of a function $f : \mathbb{R}^d \to \mathbb{R}$ as follows into a normal and a tangential part:

$$f_x = f_x P + f_x(I - P) = f_s + f_n,$$

so that $f_s v = f_x P v = f_x s$ and $f_n v = f_x(I - P)v = f_x n$.

Further, just as the gradient $\nabla f(x) \in \mathbb{R}^d$ is defined as the unique vector, such that $\nabla f(x) \cdot w = f_x(x)w$ for all $w \in \mathbb{R}^d$, we define the *tangential gradient* $\nabla_s f(x) \in T_x S$ via $\nabla_s f(x) \cdot w = f_s(x)w$.

Tangential trace. Consider the classical trace of a matrix $A \in \mathbb{R}^{d \times d}$:

$$\operatorname{tr} A := \sum_{i=1}^{d} e_i \cdot A e_i \qquad (e_i = i^{th} \text{ unit vector in } \mathbb{R}^d).$$

The *tangential trace* of A can be defined as:

$$\operatorname{tr}_S A := \operatorname{tr} AP = \operatorname{tr} B^T A B = \sum_{i=1}^{k} b_i \cdot A b_i.$$

Obviously tr_S only depends on P and not on the particular choice of B and $\operatorname{tr}_S A = \operatorname{tr}_S A^T$. With its help we define corresponding (in general only positive semi-definite) *matrix scalar products* for linear mappings:

$$\langle A_1, A_2 \rangle_{S \to S} := \operatorname{tr}_S(A_1^T P A_2) = \sum_{i=1}^{k} P A_1 b_i \cdot P A_2 b_i,$$

$$\langle A_1, A_2 \rangle_{S \to N} := \operatorname{tr}_S(A_1^T (I - P) A_2) = \sum_{i=1}^{k} (I - P) A_1 b_i \cdot (I - P) A_2 b_i.$$

From the expressions on the right we immediately see symmetry and positive semi-definiteness. For $\langle \cdot, \cdot \rangle_{S \to S}$ we observe additional symmetries:

$$\langle A_1^T, A_2 \rangle_{S \to S} = \operatorname{tr}(A_1 P A_2 P) = \operatorname{tr}(A_2 P A_1 P) = \langle A_2^T, A_1 \rangle_{S \to S} = \langle A_1, A_2^T \rangle_{S \to S}. \tag{9}$$

Tangential divergence. Application of the tangential trace to the derivative v_x of a vector field v yields the *tangential divergence*:

$$\operatorname{div}_S v := \operatorname{tr}_S v_x.$$

By a straightforward computation we obtain the following well known product rule with a scalar function f:

$$\operatorname{div}_S(fv) = f_s v + f \operatorname{div}_S v. \tag{10}$$

2.2 Derivatives of the measure tensor

In view of Theorem 1.1 we need expressions for the derivatives J_t and J_{tt} of the measure tensor

$$J(t,x) = \sqrt{\det(B(x)^T \phi_x(t,x)^T \phi_x(t,x) B(x))}.$$

Lemma 2.1. *The first and second order sensitivities of the measure tensor are given by:*

$$J_t := J_t(0,\cdot) = \operatorname{div}_S v \tag{11}$$

$$J_{tt} := J_{tt}(0,\cdot) = (\operatorname{div}_S v)^2 - \langle v_x^T, v_x \rangle_{S\to S} + \langle v_x, v_x \rangle_{S\to N} + \operatorname{div}_S v_t. \tag{12}$$

Proof. We abbreviate $C(t,x) := \phi_x(t,x)^T \phi_x(t,x)$ (known as the right Cauchy-Green tensor in elasticity) and $A(t,x) = B^T(x) C(t,x) B(x)$ so that $J(t,x) = \sqrt{\det A(t,x)}$.

$$\begin{aligned}(\det A)_t &= \operatorname{tr}((\det A) A^{-1} A_t) = \det A \operatorname{tr}(A^{-1} A_t)\\ \operatorname{tr}(A^{-1} A_t)_t &= \operatorname{tr}(-A^{-1} A_t A^{-1} A_t + A^{-1} A_{tt}),\end{aligned}$$

so at $t = 0$, where $A = I_k$ and $\phi_x = I_d$ we have, inserting

$$A_t = B^T C_t B = B^T (\phi_x^T \phi_{xt} + \phi_{xt}^T \phi_x) B = B^T (v_x + v_x^T) B$$

and

$$A_{tt} = B^T C_{tt} B = B^T (\phi_x^T \phi_{xtt} + \phi_{xtt}^T \phi_x + 2\phi_{xt}^T \phi_{xt}) B = B^T (v_{xt} + v_{xt}^T + 2 v_x^T v_x) B$$

we get

$$\begin{aligned}J_t &= ((\det A)^{1/2})_t = \frac{1}{2} (\det A)^{-1/2} \det A \operatorname{tr}(A^{-1} A_t)\\ &= \frac{1}{2} (\det A)^{1/2} \operatorname{tr}(A^{-1} A_t) \overset{A=I}{=} \frac{1}{2} \operatorname{tr}(A_t) = \frac{1}{2} \operatorname{tr}(B^T (v_x + v_x^T) B) = \operatorname{div}_S v,\end{aligned}$$

$$\begin{aligned}J_{tt} &= ((\det A)^{1/2})_{tt} = \frac{1}{2} ((\det A)^{1/2})_t \operatorname{tr}(A^{-1} A_t) + \frac{1}{2} (\det A)^{1/2} \operatorname{tr}(A^{-1} A_t)_t\\ &= \frac{1}{4} \det A \operatorname{tr}(A^{-1} A_t)^2 + \frac{1}{2} (\det A)^{1/2} \operatorname{tr}(-A^{-1} A_t A^{-1} A_t + A^{-1} A_{tt})\\ &\overset{A=I}{=} \frac{1}{4} \operatorname{tr}(A_t)^2 - \frac{1}{2} \operatorname{tr}(A_t A_t) + \frac{1}{2} \operatorname{tr}(A_{tt})\\ &= (\operatorname{div}_S v)^2 - \frac{1}{2} \operatorname{tr} B^T C_t B B^T C_t B + \frac{1}{2} \operatorname{tr}_S (v_{xt} + v_{xt}^T + 2 v_x^T v_x)\\ &= (\operatorname{div}_S v)^2 - \frac{1}{2} \langle C_t, C_t^T \rangle_{S\to S} + \operatorname{div}_S v_t + \operatorname{tr}_S v_x^T v_x.\end{aligned}$$

We continue

$$\langle C_t, C_t^T \rangle_{S\to S} = \langle v_x + v_x^T, v_x + v_x^T \rangle_{S\to S} \overset{(9)}{=} \langle v_x + v_x^T, v_x + v_x \rangle_{S\to S} = 2 \operatorname{tr}_S (v_x + v_x^T) P v_x.$$

Hence,

$$\begin{aligned}-\frac{1}{2} \langle C_t, C_t^T \rangle_{S\to S} + \operatorname{tr}_S v_x^T v_x &= -\operatorname{tr}_S (v_x + v_x^T) P v_x + \operatorname{tr}_S v_x^T v_x\\ &= -\operatorname{tr}_S v_x P v_x + \operatorname{tr}_S v_x^T (I - P) v_x = -\langle v_x^T, v_x \rangle_{S\to S} + \langle v_x, v_x \rangle_{S\to N}.\end{aligned}$$

Summing up, this yields the claimed representation of J_{tt}. □

As a short hand notation we introduce the bilinear form:

$$Q(v,w) = \operatorname{div}_S v \operatorname{div}_S w - \langle v_x^T, w_x \rangle_{S\to S} + \langle v_x, w_x \rangle_{S\to N}, \tag{13}$$

which is symmetric by (9) and by symmetry of $\langle \cdot, \cdot \rangle_{S\to N}$ and write:

$$J_{tt} = Q(v,v) + \operatorname{div}_S v_t.$$

2.3 First and second shape derivative

Inserting the results from Lemma 2.1 into the formulas of Theorem 1.1 yields:

$$I_t(0) = \int_S f_t + f \operatorname{div}_S v \, dx$$
$$I_{tt}(0) = \int_S f_{tt} + 2 f_t \operatorname{div}_S v + f\big(Q(v,v) + \operatorname{div}_S v_t\big)\, dx.$$

Next we formulate the second derivative in terms of F and its temporal derivatives. Since $f_t = F_t + f_x v$ we obtain

$$I_t(0) = \int_S F_t + f_x v + f \operatorname{div}_S v \, dx.$$

If we define

$$l(f,v) := \int_S f_x v + f \operatorname{div}_S v \, dx \tag{14}$$

we can write

$$I_t(0) = \int_S F_t \, dx + l(f,v). \tag{15}$$

Differentiating $F_t + F_x v = f_t$ once more with respect to t we obtain at $t = 0$:

$$F_{tt} + 2F_{tx} v + F_{xx} v^2 + F_x v_t = f_{tt}. \tag{16}$$

where again $F_x = f_x$ and $F_{xx} = f_{xx}$. This yields a volume formulation of the second derivative:

$$I_{tt}(0) = \int_S F_{tt} + 2(F_{tx} v + F_t \operatorname{div}_S v) + (f_x v_t + f \operatorname{div}_S v_t)\, dx$$
$$+ \int_S f_{xx}(v,v) + 2 f_x v \operatorname{div}_S v + f Q(v,v)\, dx.$$

If we define $q(f,v)$ as the integral in the second line of this equation:

$$q(f,v) := \int_S f_{xx}(v,v) + 2 f_x v \operatorname{div}_S v + f\big((\operatorname{div}_S v)^2 - \langle v_x^T, v_x \rangle_{S\to S} + \langle v_x, v_x \rangle_{S\to N}\big)\, dx \tag{17}$$

and l is given by (14) we obtain:

$$I_{tt}(0) = \int_S F_{tt} \, dx + 2l(F_t, v) + l(f, v_t) + q(f,v). \tag{18}$$

The representation of (15) is sometimes called *domain expression* of the shape derivative.

3 Concepts from differential geometry

Our next aim is to analyse (14) and (17) further by deriving the Hadamard form of these expressions. This will yield a deeper geometrical understanding of I_t and I_{tt}. It will turn out that only certain parts of v enter into the shape derivatives. Further the curvature of S and its boundary ∂S will play an important role.

To carry out our program we need some concepts from differential geometry of submanifolds. For convenience of the reader (the notation varies in the literature) we will give a rather self contained exposition, based on the projection $P : \mathbb{R}^d \to T_x S$ at a point x onto the tangent space and its derivative $T_x P$. Readers familiar with these concepts may want to browse quickly over this section.

We assume that the mapping:

$$\begin{aligned} P : S &\to L(\mathbb{R}^d, \mathbb{R}^d) \\ x &\mapsto P(x) \end{aligned}$$

is differentiable. The derivative of P at x is a linear mapping

$$T_x P : T_x S \to L(\mathbb{R}^d, \mathbb{R}^d).$$

Thus, for $b \in T_x S$ we obtain a linear mapping $T_x P(b) \in L(\mathbb{R}^d, \mathbb{R}^d)$. We write $T_x P(b) v \in \mathbb{R}^d$ to denote the derivative of P at $x \in S$ in direction $b \in T_x S$, applied to $v \in \mathbb{R}^d$. From the product rule, we obtain for any vector field $v : S \to \mathbb{R}^d$ at $x \in S$ and $b \in T_x S$:

$$(Pv)_x b = T_x P(b) v + P v_x b. \tag{19}$$

Lemma 3.1. *Let $b \in T_x S$ be arbitrary. Let s be a tangential and n a normal vector field on S. Then the following relations hold:*

$$T_x P(b) s = (I - P) s_x b \in N_x S, \tag{20}$$

$$T_x P(b) n = -P n_x b \in T_x S. \tag{21}$$

The following symmetries are valid:

$$s_1, s_2 \in T_x S \quad \Rightarrow \quad T_x P(s_1) s_2 = T_x P(s_2) s_1 \tag{22}$$

$$v_1, v_2 \in \mathbb{R}^d \quad \Rightarrow \quad v_1 \cdot (T_x P(b) v_2) = v_2 \cdot (T_x P(b) v_1) \tag{23}$$

$$i.e. \quad T_x P(b) = (T_x P(b))^T$$

$$s_1, s_2 \in T_x S \quad \Rightarrow \quad s_1 \cdot n_x s_2 = s_2 \cdot n_x s_1. \tag{24}$$

Proof. Since $Ps = s$, (19) yields $s_x b = T_x P(b) s + P s_x b$ and thus (20). Similarly, we use $Pn = 0$ to deduce (21). For (22) we compute for two tangent vector fields:

$$T_x P(s_1) s_2 - T_x P(s_2) s_1 = (I - P)(s_{1,x} s_2 - s_{2,x} s_1) = (I - P)[s_1, s_2] = 0,$$

since the Lie-Bracket $[s_1, s_2]$ of two tangent vector fields lies again in the tangent space $T_x S$. Next, (23) follows from differentiating the following identity w.r.t. x in direction b:

$$0 = v_1 \cdot P(x) v_2 - v_2 \cdot P(x) v_1,$$

which expresses the symmetry of the orthogonal projection $P(x)$. Finally, we show (24):

$$\begin{aligned} s_1 \cdot n_x s_2 = s_1 \cdot P n_x s_2 &\overset{(21)}{=} -s_1 \cdot T_x P(s_2) n \overset{(23)}{=} -n \cdot T_x P(s_2) s_1 \\ &\overset{(22)}{=} -n \cdot T_x P(s_1) s_2 \overset{(23)}{=} -s_2 \cdot T_x P(s_1) n \overset{(21)}{=} s_2 \cdot n_x s_1. \end{aligned}$$

□

For any vector field $\hat{v}$ of constant norm, we have the identity:

$$0 = \frac{1}{2}(\hat{v} \cdot \hat{v})_x w = \hat{v}_x w \cdot \hat{v} \quad \Rightarrow \hat{v}_x w \perp \hat{v} \quad \forall w \in \mathbb{R}^d. \tag{25}$$

In particular, if $\dim S = k - 1$ and $\hat{n}$ is a unit normal field, we obtain

$$\hat{n}_x s \perp \hat{n} \quad \Rightarrow \quad \hat{n}_x s \in T_x S \quad \forall s \in T_x S \quad \Rightarrow \quad \operatorname{ran} \hat{n}_x \subset T_x S.$$

3.1 Second fundamental form

By (22) we see that the *second fundamental form*:

$$\begin{aligned} h : T_x S \times T_x S &\to N_x S \\ (s_1, s_2) &\mapsto h(s_1, s_2) := -T_x P(s_1) s_2 \end{aligned} \tag{26}$$

is well defined as a symmetric bilinear vector valued mapping (cf. e.g. [7, XIV §1]). We have chosen the sign of $h(\cdot, \cdot)$, such that the corresponding curvature vector points outward, if S is a sphere.

If $\{b_i\}_{i=1\ldots k}$ is an orthonormal basis of $T_x S$, we define a *curvature vector* κ on S:

$$\kappa := \sum_{i=1}^{k} h(b_i, b_i) = -\sum_{i=1}^{k} T_x P(b_i) b_i \in N_x S. \tag{27}$$

We will see that $\kappa \cdot n$ locally approximates the change of k-volume of S, if S is moved in normal direction n.

Proposition 3.2. *For any normal vector field n we have the formula:*

$$n \cdot \kappa = \operatorname{div}_S n. \tag{28}$$

For any scalar function $\alpha : S \to \mathbb{R}$ it holds $\operatorname{div}_S \alpha n = \alpha \operatorname{div}_S n$.

Proof. We compute:

$$\begin{aligned} \operatorname{div}_S n &= \operatorname{tr}_S n_x = \operatorname{tr}_S P n_x = -\operatorname{tr}_S T_x P(\cdot) n \\ &= -\sum_{i=1}^{k} b_i \cdot T_x P(b_i) n = -\sum_{i=1}^{k} n \cdot T_x P(b_i) b_i = \sum_{i=1}^{k} n \cdot h(b_i, b_i) = n \cdot \kappa. \end{aligned}$$

With this we get $\alpha \operatorname{div}_S n = \alpha(n \cdot \kappa) = (\alpha n) \cdot \kappa = \operatorname{div}_S \alpha n$. □

Hypersurfaces and principal curvatures

If S is an orientable $k = d - 1$ dimensional manifold (a hypersurface), then $N_x S$ has dimension 1. Thus we can define (up to sign) a unit normal field $\hat{n}$ on S with $\hat{n} \cdot \hat{n} = 1$. Moreover, $h(s_1, s_2)$ is collinear with $\hat{n}$. In this case, the second fundamental form can also be defined as a scalar function:

$$\hat{h}(s_1, s_2) := \hat{n} \cdot h(s_1, s_2).$$

Since this is a symmetric bilinear form, we get an orthonormal basis of eigenvectors with eigenvalues $\kappa_1 \ldots \kappa_k$, the *principal curvatures*. These are the eigenvectors and eigenvalues of the mapping $-T_x P(\cdot)\hat{n} : T_x S \to T_x S$ (which is known as the shape operator).

Further, we can define the (scalar valued) additive curvature,

$$\hat{\kappa} := \hat{n} \cdot \kappa = \operatorname{div}_S \hat{n} = \operatorname{tr}_S \hat{h}(\cdot,\cdot) = \sum_{i=1}^{k} \kappa_i \in \mathbb{R}$$

and the mean curvature $H := \hat{\kappa}/k$.

3.2 Gaussian curvature and Laplace-Beltrami operator

In this section we indicate the geometrical meaning of some expressions that arise in the Hadamard form, derived below.

Concerning (12) we observe that for purely normal fields $v = n$ and $v_t = 0$:

$$J_{tt} = Q(n,n) = \big((\operatorname{div}_S n)^2 - \langle n_x^T, n_x\rangle_{S\to S}\big) + \langle n_x, n_x\rangle_{S\to N}.$$

We will see that the sum of the first two terms

$$K(n,n) := (\operatorname{div}_S n)^2 - \langle n_x^T, n_x\rangle_{S\to S} \tag{29}$$

and also the last term $\langle n_x, n_x\rangle_{S\to N}$ have a clear interpretation.

Gaussian curvature. The first part of J_{tt} can be seen as a generalization of the *Gaussian curvature.* Taking into account that $T_x(b)n \in T_xS$ for all $b \in T_xS$ we observe:

$$\langle n_x^T, n_x\rangle_{S\to S} \overset{(24)}{=} \langle n_x, n_x\rangle_{S\to S} \overset{(21)}{=} \langle T_xP(\cdot)n, T_xP(\cdot)n\rangle_{S\to S} = \sum_{i=1}^{k} T_xP(b_i)n \cdot T_xP(b_i)n$$

we observe

$$K(n,n) = (\kappa\cdot n)^2 - \langle T_xP(\cdot)n, T_xP(\cdot)n\rangle_{S\to S}.$$

Thus, $K(n,n)$ does not depend on the derivatives of the normal field n.

The following proposition gives $K(n,n)$ a geometric interpretation:

Proposition 3.3. *For the term $K(n,n)$ we distinguish the following special cases:*

i) for $k \in \{0,1,d\}$ we have $K(n,n) = 0$.

ii) for $k = d-1$ let $n = \eta\hat{n}$, where $\hat{n}$ is a unit normal field. Then with the principal curvatures $\kappa_1 \dots \kappa_k$ and

$$\hat{K} := \sum_{1\le i<j\le k} \kappa_i\kappa_j$$

we have

$$K(n,n) = \eta^2 K(\hat{n},\hat{n}) = \eta^2\, 2\hat{K}.$$

In particular, $\hat{K} = \kappa_1\kappa_2$ is the Gaussian-curvature for $k = 2$ and $\hat{K} = 0$ for $k = 1$.

Proof. If $k = 0$, then $T_xS = \{0\}$ and all terms vanish, if $k = 3$, then $n = 0$ and all terms vanish.

For the remaining terms we recall that $T_xP(\cdot)n : T_xS \to T_xS$ is symmetric, and thus there is an orthonormal basis $\{b_i\}_{i=1\ldots k}$ of T_xS, consisting of eigenvectors of $T_xP(\cdot)n$ with eigenvalues $\lambda_1, \ldots, \lambda_k$. Further, we compute

$$-n \cdot \kappa = \sum_{i=1}^{k} n \cdot T_xP(b_i)b_i = \sum_{i=1}^{k} b_i \cdot T_xP(b_i)n = \sum_{i=1}^{k} b_i \cdot \lambda_i b_i = \sum_{i=1}^{k} \lambda_i,$$

$$\langle T_xP(\cdot)n, T_xP(\cdot)n\rangle_{S\to S} = \sum_{i=1}^{k} T_xP(b_i)n \cdot T_xP(b_i)n = \sum_{i=1}^{k} \lambda_i b_i \cdot \lambda_i b_i = \sum_{i=1}^{k} \lambda_i^2.$$

Thus we obtain:

$$K(n,n) = \Big(\sum_{i=1}^{k} \lambda_i\Big)^2 - \sum_{i=1}^{k} \lambda_i^2 = \sum_{1\le i<j\le k} 2\lambda_i\lambda_j.$$

For $k = 1$ this sum is empty, for $k = d-1$ and $n = \eta\hat{n}$ we have $T_xP(\cdot)n = \eta T_xP(\cdot)\hat{n}$ and thus $\lambda_i = \eta\kappa_i$, with the principal curvatures κ_i. Hence in this case

$$K(n,n) = (n\cdot\kappa)^2 - \langle T_xP(\cdot)n, T_xP(\cdot)n\rangle_{S\to S} = \sum_{1\le i<j\le k} 2\lambda_i\lambda_j = 2\eta^2 \sum_{1\le i<j\le k} \kappa_i\kappa_j = 2\eta^2\hat{K}.$$

□

The scalar quantity $\hat{K}$ that is defined for hypersurfaces thus adds up products of pairs of principal curvatures. In other words, $\hat{K}$ is the sum of second order minors of $\hat{h}(\cdot,\cdot)$. For $k = 2$ there is only one such minor, namely $\det \hat{h}(\cdot,\cdot) = \hat{K}$. Later $\hat{K}$ helps to approximate to second order how much S is stretched, if moved in direction $\hat{n}$.

Laplace-Beltrami Operator. Next, we relate the term $\langle n_x, n_x\rangle_{S\to N}$ to the Laplace-Beltrami operator on S in weak form.

Proposition 3.4. *For the term $\langle n_x, n_x\rangle_{S\to N}$ we distinguish the following special cases:*

i) for $k \in \{0, d\}$ it holds $\langle n_x, n_x\rangle_{S\to N} = 0$.

ii) for $k = 1$ we have $\langle n_x, n_x\rangle_{S\to N} = (I-P)n_s \cdot (I-P)n_s$.

iii) for $k = d-1$ let $n = \eta\hat{n}$, where $\hat{n}$ is a unit normal field. Then:

$$\langle n_x, n_x\rangle_{S\to N} = \nabla_s\eta \cdot \nabla_s\eta \qquad \textit{(Laplace-Beltrami Operator)}\ .$$

Proof. If $k = 0$ or $k = 3$, $\langle n_x, n_x\rangle_{S\to N}$ is an empty expression. The case $k = 1$ follows simply from the definition of $\langle\cdot,\cdot\rangle_{S\to N}$ and the relation $n_s = n_x b_1$, where b_1 is the only basis vector of T_xS.

Consider the case $k = d-1$. Let $b \in T_xS$. Then we compute:

$$\hat{n}\cdot n_x b = (\eta\hat{n})_x b = \hat{n}\cdot\eta_x b\hat{n} + \eta\hat{n}\cdot\hat{n}_x b \overset{(25)}{=} \eta_x b.$$

With this we get for an orthonormal basis $\{b_i\}_{i=1\ldots k}$:

$$\langle n_x, n_x\rangle_{S\to N} = \sum_{k=1}^{n} (I-P)n_x b_i \cdot (I-P)n_x b_i = \sum_{k=1}^{n} (\hat{n}\cdot n_x b_i)\hat{n} \cdot (\hat{n}\cdot n_x b_i)\hat{n}$$
$$= \sum_{k=1}^{n} (\eta_x b_i)^2 = \nabla_s\eta\cdot\nabla_s\eta.$$

□

3.3 The boundary ∂S of S

Since we need the Gauss-theorem we will also consider the boundary ∂S of S. We will assume that ∂S is either empty or a $k-1$ dimensional submanifold of $\mathbb{R}^d$. In the latter case there exists a unique field of outer unit-normals $\hat{\nu}$, where $\hat{\nu}(x) \in N_x\partial S \cap T_xS$. This yields orthogonal splittings:

$$T_xS = \operatorname{span}\{\hat{\nu}\} \oplus T_x\partial S, \quad N_x\partial S = \operatorname{span}\{\hat{\nu}\} \oplus N_xS, \quad \mathbb{R}^d = N_xS \oplus \operatorname{span}\{\hat{\nu}\} \oplus T_x\partial S.$$

Of course, also ∂S has, as any smooth $k-1$-dimensional submanifold of $\mathbb{R}^d$, a projection $P_{\partial S} : \mathbb{R}^d \to \mathbb{R}^d$ with range $T_x\partial S$ and kernel $N_x\partial s$, a tangential trace $\operatorname{tr}_{\partial S} A = \operatorname{tr} AP_{\partial S}$, a divergence $\operatorname{div}_{\partial S} v = \operatorname{tr}_{\partial S} v_x$, a second fundamental form:

$$\begin{aligned} h_{\partial S} : T_x\partial S \times T_x\partial S &\to N_x\partial S \\ h_{\partial S}(\sigma_1, \sigma_2) &= -T_xP_{\partial S}(\sigma_1)\sigma_2, \end{aligned}$$

and a curvature vector (here $\{\beta_i\}_{i=1\ldots k-1}$ is an orthonormal basis of $T_x\partial S$):

$$\kappa_{\partial S} := \sum_{i=1}^{k-1} h_{\partial S}(\beta_i, \beta_i) \in N_x\partial S.$$

Since ∂S has a unique outer normal field $\hat{\nu} \in N_x\partial S \cap T_xS$ it is reasonable to define an additive curvature of ∂S relative to S as above by:

$$\hat{\kappa}_{\partial S} := \hat{\nu} \cdot \kappa_{\partial S} \in \mathbb{R}.$$

Lemma 3.5. *For any $n \in N_xS$ and $x \in \partial S$ we have the relations:*

$$\kappa \cdot n = (\kappa_{\partial S} + h(\hat{\nu}, \hat{\nu})) \cdot n \tag{30}$$

$$\operatorname{div}_S v = \operatorname{div}_{\partial S} v + \hat{\nu} \cdot v_x\hat{\nu}. \tag{31}$$

Proof. If $n \in N_xS$ is a normal vector and $\sigma_1, \sigma_2 \in T_x\partial S$, then

$$\begin{aligned} n \cdot h(\sigma_1, \sigma_2) &= -n \cdot (I-P)\sigma_{1,x}\sigma_2 = -(I-P)n \cdot \sigma_{1,x}\sigma_2 = -(I-P_{\partial S})n \cdot \sigma_{1,x}\sigma_2 \\ &= -n \cdot (I-P_{\partial S})\sigma_{1,x}\sigma_2 = n \cdot h_{\partial S}(\sigma_1, \sigma_2). \end{aligned} \tag{32}$$

The third step is possible, because $n \in N_xS \subset N_x\partial S$ and so $n = (I-P)n = (I-P_{\partial S})n$.

With the orthonormal basis $\{\beta_1, \ldots, \beta_{k-1}, \hat{\nu}\}$ of $T_xS = T_x\partial S \oplus \operatorname{span}\{\hat{\nu}\}$ we compute:

$$\begin{aligned} \kappa \cdot n &= \sum_{i=1}^{k-1} h(\beta_i, \beta_i) \cdot n + h(\hat{\nu}, \hat{\nu}) \cdot n \\ &\overset{(32)}{=} \sum_{i=1}^{k-1} h_{\partial S}(\beta_i, \beta_i) \cdot n + h(\hat{\nu}, \hat{\nu}) \cdot n = \kappa_{\partial S} \cdot n + h(\hat{\nu}, \hat{\nu}) \cdot n. \end{aligned}$$

Similarly we obtain

$$\operatorname{div}_S v = \sum_{i=1}^{k-1} \beta_i \cdot v_x\beta_i + \hat{\nu} \cdot v_x\hat{\nu} = \operatorname{div}_{\partial S} v + \hat{\nu} \cdot v_x\hat{\nu}.$$

□

If s is a tangential vector field, $\operatorname{div}_S s$ is the intrinsic divergence on the manifold S and we have the Gauss integral theorem

$$\int_S \operatorname{div}_S s\, dx = \int_{\partial S} \hat{\nu} \cdot s\, d\xi, \tag{33}$$

where $\hat{\nu}$ is the outer unit-normal field of ∂S.

Proposition 3.6. *For any vector field $v = s+n = Pv+(I-P)v$ on S we have the formula:*

$$\int_S \operatorname{div}_S v\, dx = \int_S \kappa \cdot n\, dx + \int_{\partial S} \hat{\nu} \cdot s\, d\xi = \int_S \kappa \cdot v\, dx + \int_{\partial S} \hat{\nu} \cdot v\, d\xi. \tag{34}$$

If f is a scalar function on S then we have

$$\int_S f \operatorname{div}_S v\, dx = \int_S f\kappa \cdot v - f_s v\, dx + \int_{\partial S} f\hat{\nu} \cdot v\, d\xi. \tag{35}$$

Proof. (34) follows from (28) by linearity of div_S and (33). For the second identity in (34) we note that $\kappa \in N_x T$, so $v \cdot \kappa = n \cdot \kappa$ and $\hat{\nu} \in T_x P$, so that $v \cdot \hat{\nu} = s \cdot \hat{\nu}$. Finally, (33) follows from (34) and the product rule (10). □

The theorem of Gauss can be used to connect the weak and the classical form of the Laplace-Beltrami operator of a scalar function $\eta : S \to \mathbb{R}$:

$$\begin{aligned}\int_S \nabla_s\varphi \cdot \nabla_s\eta\, dx &= \int_S \varphi_s(\nabla_s\eta)\, dx = \int_S \operatorname{div}_S(\varphi\nabla_s\eta) - \varphi(\operatorname{div}_S \nabla_s\eta)\, dx \\ &= \int_S \varphi(-\operatorname{div}_S \nabla_s\eta)\, dx + \int_{\partial S} \varphi\nabla_s\eta \cdot \hat{\nu}\, d\xi \quad \forall\varphi \in C^\infty(S,\mathbb{R}).\end{aligned}$$

3.4 A lemma on nested divergence

In the derivation of the Hadamard form we will observe the occurrence of nested divergence. The following lemma yields a useful formula:

Lemma 3.7. *For a vector field v and a tangential vector field s we have:*

$$Q(v,s) = \operatorname{div}_S v \operatorname{div}_S s - \langle v_x^T, s_x\rangle_{S\to S} + \langle v_x, s_x\rangle_{S\to N} = \operatorname{div}_S((\operatorname{div}_S v)s - v_x s).$$

Proof. By the product rule (10) we obtain:

$$\operatorname{div}_S(\operatorname{div}_S vs - v_x s) = \operatorname{div}_S v \operatorname{div}_S s + (\operatorname{div}_S v)_x s - \operatorname{div}_S v_x s.$$

Now we analyse $(\operatorname{div}_S v)_x s - \operatorname{div}_S v_x s$ further:

$$\begin{aligned}(\operatorname{div}_S v)_x s &= (\operatorname{tr} Pv_x)_x s = \operatorname{tr}(T_x P(s)v_x + Pv_{xx}(s,\cdot)) = \operatorname{tr}(v_x T_x P(s)) + \operatorname{tr}_S v_{xx}(s,\cdot)), \\ \operatorname{div}_S v_x s &= \operatorname{tr}_S(v_x s)_x = \operatorname{tr}_S v_{xx}(s,\cdot) + \operatorname{tr}_S(v_x s_x).\end{aligned}$$

We observe that v_{xx} cancels out:

$$\begin{aligned}(\operatorname{div}_S v)_x s - \operatorname{div}_S(v_x s) &= \operatorname{tr}(v_x T_x P(s)) - \operatorname{tr}_S(v_x s_x) \\ &= \operatorname{tr}(v_x T_x P(s)(I-P)) + \operatorname{tr}_S(v_x(T_x P(s) - s_x)).\end{aligned}$$

For the first term of the right hand side we compute:

$$\begin{aligned}\operatorname{tr}(v_x T_x P(s)(I-P)) &\overset{(21)}{=} \operatorname{tr}(v_x P T_x P(s)(I-P)) = \operatorname{tr}(T_x P(s)(I-P) v_x P) \\ &= \langle T_x P(s)^T, v_x\rangle_{S\to N} \overset{(23)}{=} \langle T_x P(s), v_x\rangle_{S\to N} = \langle (I-P)s_x, v_x\rangle_{S\to N} = \langle s_x, v_x\rangle_{S\to N}.\end{aligned}$$

For the second term we obtain:

$$\operatorname{tr}_S(v_x((I-P)s_x - s_x)) = -\operatorname{tr}_S(v_x P s_x) = \langle v_x^T, s_x\rangle_{S\to S}.$$

Adding everything up yields the desired result. □

4 Hadamard forms of shape derivatives

To derive Hadamard forms we split our perturbation field v on S into a tangential part s and a normal part n, i.e.,

$$v = s + n = Pv + (I-P)v.$$

We stress that this is only possible on the manifold S and not on all of $\mathbb{R}^d$. Consequently, while expressions like $s_x s$, $n_x s$, or $v_x n$ are well defined, expressions like $s_x n$ would require an extension of s beyond S, which is not available in a canonical way.

Further, let s tangential vector field s on S. Then on ∂S we split s as follows:

$$s = \sigma + \nu = P_{\partial S} s + (I - P_{\partial S})s$$

into a normal part ν and tangential part σ with respect to the boundary ∂S. Thus on ∂S we can write $v = \sigma + \nu + n$.

4.1 First shape derivative

Application of the Gauss theorem (34) immediately yields the well known Hadamard form of the first shape derivative. Recall the definition of the curvature vector κ in (27) and the outer unit vector $\hat{\nu}$ of ∂S.

Theorem 4.1. *The first shape derivative is given by the following formulas:*

$$I_t(0) = \int_S F_t \, dx + l(f, v) \tag{36}$$

where

$$l(f, v) = \int_S (f_n + f\kappa\cdot) v \, dx + \int_{\partial S} f\hat{\nu} \cdot v \, d\xi. \tag{37}$$

Proof. We compute straightforwardly, using the product rule for div_S and the Gauss theorem:

$$\begin{aligned}I_t(0) &= \int_S f_t + f J_t \, dx = \int_S F_t + f_x v + f \operatorname{div}_S v \, dx \\ &\overset{(10)}{=} \int_S F_t + f_x v + \operatorname{div}_S fv - f_s v \, dx = \int_S F_t + f_n v + \operatorname{div}_S fv \, dx \\ &\overset{(34)}{=} \int_S F_t + f_n v + f\kappa \cdot v \, dx + \int_{\partial S} f\hat{\nu} \cdot v \, d\xi.\end{aligned}$$

□

Taking into account that $f_n v = f_x n$, $\kappa \cdot v = \kappa \cdot n$, and $v \cdot \hat{\nu} = \nu \cdot \hat{\nu}$ we can write alternatively:

$$I_t(0) = \int_S F_t + (f_x + f\kappa\cdot)n \, dx + \int_{\partial S} f\hat{\nu} \cdot \nu \, d\xi. \tag{38}$$

4.2 Second shape derivative

We recall that the second shape derivative in volume form reads:

$$I_{tt}(0) = \int_S F_{tt} \, dx + 2l(F_t, v) + l(f, v_t) + q(f, v).$$

Since the Hadamard form of the linear term l is already known, it remains to analyse the quadratic part:

$$q(f, v) = \int_S f_{xx}(v, v) + 2f_x v \operatorname{div}_S v + fQ(v, v) \, dx.$$

Our strategy is the same as for the first shape derivative. First, we use the product rule to write as many terms as possible as tangential divergence of some vector fields. Second we apply the Gauss theorem on S to interpret them as boundary terms. Finally, an additional application of the Gauss theorem on ∂S yields further information.

Recall the definition of the symmetric bilinear form $Q(\cdot, \cdot)$ in (13) and the discussion of

$$Q(n, n) = K(n, n) + \langle n_x, n_x \rangle_{S \to N}, \tag{39}$$

in Section 3.2. We have seen that $K(n, n)$ generalizes the Gauss curvature, and $\langle n_x, n_x \rangle_{S \to N}$ is a generalization of the Laplace-Beltrami Operator.

Now we derive a form of $q(f, v)$ that is amenable to the application of the Gauss theorem.

Lemma 4.2. *The following formula holds:*

$$\begin{aligned} fQ(v, v) + 2f_x v \operatorname{div}_S v + f_{xx}(v, v) &= fQ(n, n) + 2f_x n(\kappa\cdot n) + f_{xx}(n, n) \\ &+ \operatorname{div}_S \big(f(\operatorname{div}_S(s + 2n) - (s + 2n)_x)s + f_x(s + 2n)s\big) - f_n(s + 2n)_x s. \end{aligned} \tag{40}$$

Proof. By Lemma 3.7 we compute (taking into account the symmetry of Q):

$$\operatorname{div}_S(\operatorname{div}_S(s + 2n)s - (s + 2n)_x s) = Q(s + 2n, s) = Q(v + n, v - n) = Q(v, v) - Q(n, n).$$

and thus

$$fQ(v, v) = f \operatorname{div}_S \big(\operatorname{div}_S(s + 2n)s - (s + 2n)_x s\big) + fQ(n, n).$$

To pull f into the divergence term we compute by the product rule:

$$\begin{aligned} &f \operatorname{div}_S(\operatorname{div}_S(s + 2n)s - (s + 2n)_x s) - \operatorname{div}_S \big(f(\operatorname{div}_S(s + 2n) - (s + 2n)_x)s - f_x s s\big) \\ &\overset{(10)}{=} -f_s(\operatorname{div}_S(s + 2n)s - (s + 2n)_x s) + f_x s \operatorname{div}_S s + (f_x s)_s s \\ &= f_s(s + 2n)_x s + f_{xx}(s, s) + f_x s_x s - \operatorname{div}_S(2n) f_x s \\ &= (f_s + f_x)s_x s + 2f_s(n_x s) + f_{xx}(s, s) - \operatorname{div}_S(f_x s \, 2n) \end{aligned}$$

and conclude

$$\begin{aligned} fQ(v, v) = &\operatorname{div}_S(f(\operatorname{div}_S(s + 2n) - (s + 2n)_x)s) + fQ(n, n) \\ &- \operatorname{div}_S(f_x s(s + 2n)) + (f_s + f_x)s_x s + 2f_s(n_x s) + f_{xx}(s, s). \end{aligned} \tag{41}$$

The terms in the first line of (41) can already be found in (40). Next, we compute:

$$2 f_x v \operatorname{div}_S v = 2 \operatorname{div}_S(f_x v v) - 2(f_x v)_s v = 2 \operatorname{div}_S(f_x v v) - 2 f_x v_x s - 2 f_{xx}(v, s). \tag{42}$$

To show (40) we have to add (41), (42), and $f_{xx}(v, v)$, and then simplify the expression. In particular, we observe:

$$\begin{aligned}
&- \operatorname{div}_S(f_x s(s + 2n)) + 2 \operatorname{div}_S(f_x v v) = \operatorname{div}_S(-f_x s(s + 2n) + 2 f_x s v + 2 f_x n v)\\
&= \operatorname{div}_S(f_x s s) + 2 \operatorname{div}_S(f_x n s) + 2 \operatorname{div}_S(f_x n n) = \operatorname{div}_S(f_x(s + 2n)s) + 2 f_x n(\kappa \cdot n),\\
&(f_s + f_x)s_x s + 2 f_s(n_x s) - 2 f_x v_x s = (-f_n + 2 f_x)s_x s - 2 f_x v_x s + 2 f_s(n_x s)\\
&\quad = -f_n s_x s - 2 f_x(n_x s) + 2 f_s(n_x s) = -f_n s_x s - 2 f_n n_x s = -f_n(s + 2n)_x s,\\
&f_{xx}(s, s) - 2 f_{xx}(v, s) + f_{xx}(v, v) = f_{xx}(v, n) - f_{xx}(n, s) = f_{xx}(n, n).
\end{aligned}$$

Taking all this into account finally yields (40). □

We will now apply the Gauss theorem on S to the first line of (40) and then, in Lemma 4.4, a second time to some terms on ∂S. This yields the main result of this paper:

Theorem 4.3. *The second shape derivative is given by the formula*

$$I_{tt}(0) = \int_S F_{tt}\, dx + 2l(F_t, v) + l(f, v_t) + q(f, v) \tag{43}$$

where

$$l(f, v) = \int_S (f_n + f\kappa\cdot)v\, dx + \int_{\partial S} f\hat{\nu} \cdot v\, d\xi$$

and

$$\begin{aligned}
q(f, v) = &\int_{\partial S} f\hat{\nu}\cdot\big(h_{\partial S}(\sigma, \sigma) - 2(n + \nu)_x\sigma\big) + (f_x + f\kappa_{\partial S}\cdot)(\nu + 2n)(\nu\cdot\hat{\nu})\, d\xi\\
+ &\int_S (f_n + f\kappa\cdot)(h(s, s) - 2n_x s) + f\big(K(n, n) + \langle n_x, n_x\rangle_{S\to N}\big) + 2 f_x n(n\cdot\kappa) + f_{xx}(n,n)\, dx.
\end{aligned} \tag{44}$$

Proof. We apply the Gauss theorem to the divergence term in the second line of (40) and obtain:

$$\begin{aligned}
&\int_S \operatorname{div}_S\big(f(\operatorname{div}_S(s + 2n) - (s + 2n)_x)s + f_x(s + 2n)s\big)\, dx\\
&\quad = \int_S -f((s + 2n)_x s) \cdot \kappa\, dx + I_{\partial S}
\end{aligned} \tag{45}$$

with the boundary term

$$I_{\partial S} = \int_{\partial S} f\big(\operatorname{div}_S(s + 2n)(s\cdot\hat{\nu}) - ((s + 2n)_x s)\cdot\hat{\nu}\big) + f_x(s + 2n)(s\cdot\hat{\nu})\, d\xi.$$

Adding the second line of (40) to the first integral in the second line of (45) we can also define a full term:

$$I_S = \int_S -(f_n + f\kappa\cdot)((s + 2n)_x s) + fQ(n, n) + 2 f_x n(\kappa\cdot n) + f_{xx}(n, n)\, dx \tag{46}$$

and thus split (40) as follows:

$$q(f, v) = I_{\partial S} + I_S.$$

We will prove that $I_{\partial S}$ and I_S are equal to the first and the second line in (44), respectively. We begin with I_S. Taking into account (39) the last three terms of the integrand in (46) can easily be identified in the second line of (44). Concerning the first term, we note that for any vector field w

$$(f_n + f\kappa\cdot)w = (f_n + f\kappa\cdot)(I - P)w$$

and thus may compute

$$(f_n + f\kappa\cdot)s_x s = (f_n + f\kappa\cdot)(I - P)s_x s = (f_n + f\kappa\cdot)T_x P(s)s = -(f_n + f\kappa\cdot)h(s, s),$$

and conclude

$$\int_S -(f_n + f\kappa\cdot)((s + 2n)_x s)\, dx = \int_S (f_n + f\kappa\cdot)(h(s, s) - 2n_x s)\, dx.$$

Summing up yields the integral terms over S as stated in (44).

Let us turn to $I_{\partial S}$. First, we regroup terms as follows:

$$\begin{aligned} I_{\partial S} &= \int_{\partial S} f\Big(\operatorname{div}_S(s + 2n)(s\cdot\hat\nu) - ((s + 2n)_x s)\cdot\hat\nu\Big) + f_x(s + 2n)(s\cdot\hat\nu)\, d\xi \\ &= \int_{\partial S} f\big(\operatorname{div}_S(s) - s_x s\cdot\hat\nu\big)\, d\xi + \int_{\partial S} 2f\big((\kappa\cdot n)(\nu\cdot\hat\nu) - (n_x s)\cdot\hat\nu\big) + f_x(s + 2n)(\nu\cdot\hat\nu)\, d\xi. \end{aligned}$$

Now we apply the Gauss theorem is to the first integral of the second line, which is performed in Lemma 4.4, below. In the second integral we split $\kappa\cdot n = (\kappa_{\partial S} + h(\hat\nu, \hat\nu))\cdot n$ by Lemma 3.5. By these two operations and subsequent reordering of terms we get:

$$\begin{aligned} I_{\partial S} &= \int_{\partial S} (f\kappa_{\partial S}\cdot\nu)(\nu\cdot\hat\nu) + f\hat\nu\cdot\big(h_{\partial S}(\sigma, \sigma) - 2\nu_x\sigma\big) - (f_x\sigma)(\nu\cdot\hat\nu)\, d\xi \\ &+ \int_{\partial S} 2f\Big(\big((\kappa_{\partial S} + h(\hat\nu, \hat\nu))\cdot n\big)(\nu\cdot\hat\nu) - (n_x(\nu + \sigma))\cdot\hat\nu\Big) + f_x(\sigma + \nu + 2n)(\nu\cdot\hat\nu)\, d\xi \\ &= \int_{\partial S} f\hat\nu\cdot\big(h_{\partial S}(\sigma, \sigma) - 2(n + \nu)_x\sigma\big) + (f_x + f\kappa_{\partial S}\cdot)(\nu + 2n)(\nu\cdot\hat\nu)\, d\xi \\ &+ \int_{\partial S} 2f\big((h(\hat\nu, \hat\nu)\cdot n)(\nu\cdot\hat\nu) - (n_x\nu)\cdot\hat\nu\big)\, d\xi. \end{aligned}$$

We observe that the third line of this computation coincides with the first line of (44). To show that the fourth line vanishes, we compute, taking into account that $\hat\nu \in T_x S$:

$$n_x\nu\cdot\hat\nu = Pn_x\nu\cdot\hat\nu \overset{(21)}{=} -T_x P(\nu)n\cdot\hat\nu \overset{(23)}{=} -T_x P(\nu)\hat\nu\cdot n = h(\nu, \hat\nu)\cdot n = (\nu\cdot\hat\nu)h(\hat\nu, \hat\nu)\cdot n.$$

Thus, also $I_{\partial S}$ is equal to the boundary integral that appears in (44), as claimed. □

Lemma 4.4.

$$\begin{aligned} &\int_{\partial S} f\big(\operatorname{div}_S(s)(\nu\cdot\hat\nu) - (s_x s)\cdot\hat\nu\big)\, d\xi \\ &\quad= \int_{\partial S} f(\kappa_{\partial S}\cdot\nu)(\nu\cdot\hat\nu) + f\hat\nu\cdot\big(h_{\partial S}(\sigma, \sigma) - 2\nu_x\sigma\big) - (f_x\sigma)(\nu\cdot\hat\nu)\, d\xi. \end{aligned} \tag{47}$$

Proof. Application of (31) and the Gauss-theorem (35) on ∂S, using $\partial(\partial S) = \emptyset$ yields:

$$\begin{aligned}\int_{\partial S} f(\nu\cdot\hat\nu)\,\mathrm{div}_S\, s\, d\xi &= \int_{\partial S} f(\nu\cdot\hat\nu)\,(\mathrm{div}_{\partial S}\, s + (\hat\nu\cdot s_x\hat\nu))\; d\xi \\ &= \int_{\partial S} f(\nu\cdot\hat\nu)(\nu\cdot\kappa_{\partial S} + \hat\nu\cdot s_x\hat\nu) - (f(\nu\cdot\hat\nu))_\sigma s\, d\xi.\end{aligned} \tag{48}$$

Here $\kappa_{\partial S}\in N_x\partial S$ is the curvature vector of ∂S and $(f(\nu\cdot\hat\nu))_\sigma$ is the tangential derivative of $f(\nu\cdot\hat\nu)$ in ∂S. Now

$$(f(\nu\cdot\hat\nu))_\sigma s = (f(\nu\cdot\hat\nu))_x\sigma = f\big((\nu_x\sigma)\cdot\hat\nu + \nu\cdot\hat\nu_x\sigma\big) + f_x\sigma(\nu\cdot\hat\nu).$$

Since ν and $\hat\nu$ are collinear we have $\nu\cdot\hat\nu_x\sigma = 0$ by (25) and also $\nu = (\nu\cdot\hat\nu)\hat\nu$, implying $(\nu\cdot\hat\nu)\hat\nu\cdot s_x\hat\nu = \hat\nu s_x\nu$. So we obtain

$$\int_{\partial S} f\,\mathrm{div}_S\, s(\nu\cdot\hat\nu)\, d\xi = \int_{\partial S} f\big((\nu\cdot\hat\nu)(\nu\cdot\kappa_{\partial S}) + \hat\nu\cdot(s_x\nu - \nu_x\sigma)\big) - f_x\sigma(\nu\cdot\hat\nu)\, d\xi.$$

Taking into account the term $-s_x s\cdot\hat\nu$ in the left hand side of (47) we compute:

$$\hat\nu\cdot(s_x\nu - \nu_x\sigma - s_x s) = -\hat\nu\cdot(s_x\sigma + \nu_x\sigma) = -\hat\nu\cdot(\sigma_x\sigma + 2\nu_x\sigma) = \hat\nu\cdot(h_{\partial S}(\sigma,\sigma) - 2\nu_x\sigma).$$

Inserting this into our previous computation yields the desired result. □

Extension to piecewise smooth boundaries

In applications one sometimes encounters domains S with non-smooth boundaries, such as polygons. Let us discuss briefly changes of our formula in the case that ∂S is only piecewise smooth. It is well known that the Gauss theorem on a smooth manifold S can still be applied, under relatively weak assumptions on the smoothness of ∂S. By and large, ∂S is allowed to be non-smooth on a set of ∂S-measure zero. Under this assumption, our first application of the Gauss-theorem in the proof of Theorem 4.3 is still feasible.

However, the second application of the Gauss theorem in the proof of Lemma 4.4 has to be done with care. Assume that ∂S is the finite union of smooth manifolds ∂S_i with unit outer normal fields $\hat\nu_i$. Assume further that each ∂S_i has a boundary $\partial\partial S_i = \partial(\partial S_i)$ with unit outer normal field $\hat{\mathfrak{n}}_i$. Then the left hand side in (48) can be replaced by:

$$\int_{\partial S} f\big(\mathrm{div}_S(s)(\nu\cdot\hat\nu) - (s_x s)\cdot\hat\nu\big)\, d\xi = \sum_i \int_{\partial S_i} f\big(\mathrm{div}_S(s)(\nu\cdot\hat\nu) - (s_x s)\cdot\hat\nu\big)\, d\xi$$

Separate application of the Gauss theorem to each of the summands yields the following sum of boundary terms in addition to (48):

$$\sum_i \int_{\partial\partial S_i} f(s\cdot\hat\nu_i)(s\cdot\hat{\mathfrak{n}}_i)\, d\mathfrak{x}.$$

This sum then has to be added to (44). If two parts ∂S_i and ∂S_j share part of their boundary, then one can summarize the contribution of this part to $q(f,v)$ as follows:

$$\int_{\partial\partial S_i\cap\partial\partial S_j} f\big((s\cdot\hat\nu_i)(s\cdot\hat{\mathfrak{n}}_i) + (s\cdot\hat\nu_j)(s\cdot\hat{\mathfrak{n}}_j)\big)\, d\mathfrak{x}.$$

If the transition between ∂S_i and ∂S_j is smooth, then this contribution vanishes, because then $\hat\nu_i = \hat\nu_j$ and $\hat{\mathfrak{n}}_i = -\hat{\mathfrak{n}}_j$.

Similarly, if S itself is non-smooth, but can be decomposed into finitely many smooth parts S_i, then the results of Theorem 4.1 and Theorem 4.3 still apply to each S_i and can be summed up.

5 Geometric Interpretation and Applications

This section is devoted to the geometrical interpretation of our formulas for I_t and I_{tt}. It turns out that each term of the Hadamard form models a distinct effect that occurs during deformation of S.

5.1 Sensitivity of k-volumes

Of special interest is the case $F = f \equiv 1 = const$, which captures changes in the pure k-dimensional volume of S. First of all we note that all terms with derivatives of f and F drop out in (44) and we obtain the shorter formulas:

$$I_t(0) = \int_S \kappa \cdot n \, dx + \int_{\partial S} \hat{\nu} \cdot \nu \, dx, \tag{49}$$

$$\begin{aligned} I_{tt}(0) = &\int_S \kappa \cdot (h(s,s) + v_t - 2n_x s) + K(n,n) + \langle n_x, n_x \rangle_{S \to N} \, dx \\ &+ \int_{\partial S} \hat{\nu} \cdot (h_{\partial S}(\sigma,\sigma) + v_t - 2(n+\nu)_x \sigma) + \kappa_{\partial S} \cdot (\nu + 2n)(\nu \cdot \hat{\nu}) \, d\xi. \end{aligned} \tag{50}$$

The *first shape derivative* is rather straightforward to interpret. The first part of $I_t(0)$ reveals that S expands or shrinks in the presence of curvature $\kappa \neq 0$ by moving in normal direction, because normals spread or converge due to curvature. This is also reflected by the identity $\kappa \cdot n = \operatorname{div}_S n$. Second, S expands or shrinks by moving across ∂S in direction of the outer unit normal $\hat{\nu}$ of ∂S. This change is approximated by the second part of $I_t(0)$. While ∂S is moving, it sweeps over a certain k-dimensional submanifold of $\mathbb{R}^d$, a “boundary strip”. The integrand $\hat{\nu} \cdot \nu$ can be interpreted the rate of change of the local width of this boundary strip, thus the corresponding integral approximates the rate of change of its k-volume.

Also the *second shape derivative* consists of a full part that covers stretching and shrinking of S and a boundary part that describes how the k-volume of S changes if ∂S moves. We observe purely normal, purely tangential and mixed terms that we will discuss in detail in the following.

By Proposition 3.3 we can interpret $K(n,n)$ as a sum of increase of two-dimensional area. Recall that K describes the Gauss curvature for $d = 3$ and $k = 2$. Together with its counterpart $\kappa \cdot n$ the term $K(n,n)$ captures stretching of S due to curvature and movement in normal direction n to second order.

The term $\langle n_x, n_x \rangle_{S \to N}$ is present even for flat S and has been identified in Proposition 3.4 as the Laplace-Beltrami operator on S if $k = d - 1$. It captures stretching of S that occurs due to changes in curvature. A spatially varying normal field may produce “wrinkles“ in S, increasing its k-volume.

The last term in the boundary integral $\kappa_{\partial S} \cdot (\nu + 2n)(\nu \cdot \hat{\nu})$ describes change of k-volume of S that is caused by a combination of moving ∂S in direction $\hat{\nu}$ and at the same time stretching ∂S. The quantities $\kappa_{\partial S} \cdot n$ and $\kappa_{\partial S} \cdot \nu$ describe the change of $k-1$-volume of ∂S to first order when ∂S is moved in direction n and ν, respectively. This is then multiplied by $\nu \cdot \hat{\nu}$, the rate of change of width of the boundary strip. The effect of n on the k-volume of S is twice as large as the effect of ν.

Modified acceleration. Finally, we consider the mixed term $\kappa \cdot (h(s,s) + v_t - 2n_x s)$ (and its counterpart on the boundary $\hat{\nu} \cdot (h_{\partial S}(\sigma,\sigma) + v_t - 2(n+\nu)_x \sigma)$). As we will explain in the following, this term describes a stretching of S that is induced by curvature and simultaneous *acceleration* of the movement of S into normal direction.

This statement is obviously true for $v_t = \phi_{tt}(0,\cdot)$, the acceleration of each point.

In addition, the presence of the term $h(s,s)$ indicates that straight movement along a purely tangential field in total may result in an acceleration of S into normal direction. The resulting change of k-volume is reflected by the term $\kappa \cdot h(s,s)$. Later we will see that in the velocity method tangential fields satisfy $h(s,s) + v_t = 0$.

Let, for example $S \subset \mathbb{R}^2$ be a circle around 0 with radius r_0 and unit tangent field $\hat{s}$. Its second fundamental form is known as $h(\alpha\hat{s}, \beta\hat{s}) = \alpha\beta/r_0$. Consider the tangential field $s(x) = \tau\hat{s}(x)$ of constant velocity τ and the deformation $\phi(t,x) = x + ts(x)$. Since $x \cdot s(x) = 0$ we may compute:

$$r(t,x) := \sqrt{\phi(t,x)\cdot\phi(t,x)} = \sqrt{x\cdot x + ts(x)\cdot ts(x)} = \sqrt{r_0^2 + t^2\tau^2}.$$

Thus, $r(t,x)$ is independent of x and so $\phi(t,S)$ is again a circle that expands as time progresses. Differentiation of this formula with respect to time yields $r_t(0) = 0$ as expected, but also a radial acceleration $r_{tt}(0) = \tau^2/r_0 = h(s,s)$. This is the acceleration in normal direction, predicted by our formulas.

Next we illustrate the occurrence of the third term $-2n_x s$, which describes tangential transport of a non-constant normal velocity, by an example. Consider $S = \mathbb{R}\times\{0\}$ in $\mathbb{R}^2$ so $T_xS = \mathbb{R}\times\{0\}$ and $\hat{n} \equiv e_2$. We introduce cartesian coodinates $x = pe_1 + qe_2$, where e_1, e_2 are the unit vectors. Set $s = s(x) := \tau e_1$, i.e., tangential transport with constant speed, and $n(x) = \eta p e_2$, i.e., a normal velocity that depends linearly on the first coordinate. Setting $\phi(t,x) := x + t(s + n(x))$ we notice that $\phi(t,S)$ is the graph of the linear function $q(t,p) = (p - \tau t)\eta t$. We observe acceleration of the graph in negative normal direction: $q_{tt}(0,p) = -2\tau\eta = -2n_x s$, as predicted.

In the same way we can interpret the summands in the corresponding boundary term $\hat{\nu}\cdot(h_{\partial S}(\sigma,\sigma) + v_t - 2(n+\nu)_x\sigma)$. This term describes the change of k-volume of S due to acceleration effects into direction $\hat{\nu}$ at ∂S. Let us point out the perfect analogy of these two terms:

$$n_x s = ((I-P)v)_x Pv \quad \text{and} \quad (n+\nu)_x\sigma = ((I-P_{\partial S})v)_x P_{\partial S} v$$

and remark the interesting identity:

$$n_x\sigma\cdot\hat{\nu} \overset{(21)}{=} Pn_x\sigma\cdot\hat{\nu} \overset{(23)}{=} -T_xP(\sigma)n\cdot\hat{\nu} = -T_xP(\sigma)\hat{\nu}\cdot n = h(\hat{\nu},\sigma)\cdot n, \tag{51}$$

which shows that no derivatives of v are needed to evaluate this term.

To reflect these considerations in our formulas, we introduce a *modified acceleration field* $\tilde{v}_t$ on $S\times\partial S$ as follows:

$$\tilde{v}_t(x) := \begin{cases} h(s,s) + v_t - 2n_x s & : \quad x \in S\setminus\partial S \\ h_{\partial S}(\sigma,\sigma) + v_t - 2(n+\nu)_x\sigma & : \quad x\in\partial S. \end{cases} \tag{52}$$

With that notation we can write the second shape derivative in the following way:

$$I_{tt}(0) = l(1,\tilde{v}_t) + \int_S K(n,n) + \langle n_x, n_x\rangle_{S\to N}\,dx + \int_{\partial S}\kappa_{\partial S}\cdot(\nu+2n)(\nu\cdot\hat{\nu})\,d\xi.$$

5.2 Sensitivity of general integrals

Also for general integrands, we will give an interpretation of the arising terms. We start with the *first shape derivative* and split it into three parts:

$$I_t(0) = \int_S F_t\,dx + \int_S f_n v\,dx + \Big[\int_S f\kappa\cdot v\,dx + \int_{\partial S} f\hat{\nu}\cdot v\,d\xi\Big].$$

The first integral captures the temporal change of F on S. The second integral models how $I(t)$ changes for spatially non-constant f due to a slight shift of S in space. The two integrals in square brackets are known from Section 5.1. They approximate the change of $I(t)$ that is caused by a change of k-volume of S, scaled by f.

In full detail, the *second shape derivative* looks as follows:

$$\begin{aligned} I_{tt}(0) = &\int_S F_{tt}\,dx + \int_S 2(F_{tn} + F_t\kappa\cdot)v\,dx + \int_{\partial S} 2F_t\hat{\nu}\cdot v\,d\xi \\ &+ \int_S (f_n + f\kappa\cdot)(h(s,s) + v_t - 2n_x s) + f\big(K(n,n) + \langle n_x, n_x\rangle_{S\to N}\big) + 2f_x n(n\cdot\kappa) + f_{xx}(n,n)\,dx \\ &+ \int_{\partial S} f\hat{\nu}\cdot\big(h_{\partial S}(\sigma,\sigma) + v_t - 2(n+\nu)_x\sigma\big) + (f_x + f\kappa_{\partial S}\cdot)(\nu + 2n)(\nu\cdot\hat{\nu})\,d\xi. \end{aligned}$$

In the first line we recognize the second order model F_{tt} for F and the mixed term $2l(F_t, v)$, where l is given by (37). This term combines first order temporal changes of F and the change of $I(t)$ due to deformation of S. Further, the first parts of the second and the third line are modified acceleration terms, discussed in Section 5.1. Using the modified acceleration field $\tilde{v}_t$ from (52) they can be summarized by $l(f, \tilde{v}_t)$. Now our formula looks much more concise:

$$\begin{aligned} I_{tt}(0) = &\int_S F_{tt}\,dx + 2l(F_t, v) + l(f, \tilde{v}_t) \\ &+ \int_S f\big(K(n,n) + \langle n_x, n_x\rangle_{S\to N}\big) + 2f_x n(n\cdot\kappa) + f_{xx}(n,n)\,dx \\ &+ \int_{\partial S} (f_x + f\kappa_{\partial S}\cdot)(\nu + 2n)(\nu\cdot\hat{\nu})\,d\xi. \end{aligned}$$

This form can be related to the structure theorem of the hessian, presented in [9].

Having discussed the first line of this expression, let us consider the integral over S in the second line. It consists of three parts. The first part is a second order model for the k-volume of S, scaled by f. We have already discussed this term in Section 5.1. The second term $2f_x n(n\cdot\kappa)$ is a mixed term that combines first order change of f due to shifts of S in normal direction and first order change of the k-volume of S. Finally, by $f_{xx}(n,n)$ second order changes due to shifts of S in normal direction are captured.

The integrand $(f_x + f\kappa_{\partial S}\cdot)(\nu + 2n)(\nu\cdot\hat{\nu})$ in the third line is the product of two factors. The two summands of the first factor $(f_x + f\kappa_{\partial S}\cdot)\nu$ and $(f_x + f\kappa_{\partial S}\cdot)n$ approximate to first order the change of $\int_{\partial S} f\,d\xi$, when ∂S moved in direction ν and n, respectively. As in Section 5.1 the second factor $(\nu\cdot\hat{\nu})$ can be interpreted as rate of change of local width of the boundary strip. Their product gives us a second order term for the change of $I(t)$ caused by movement of ∂S. At first glance, the factor of 2 in $\nu + 2n$ looks surprising. However, below we will give an example that illustrates its significance.

5.3 Special cases

In the following we consider a couple of special cases to relate our results to existing formulas and to illustrate some effects. Throughout this section we consider the case that F is constant in time (so $F_t = F_{tt} = 0$) for the sake of brevity.

Tangential fields. If $v = s$, i.e, $n = 0$ on S our shape derivatives simplify to:

$$I_t(0) = \int_{\partial S} f\hat{\nu} \cdot \nu \, d\xi$$
$$I_{tt}(0) = \int_S (f_n + f\kappa\cdot)(h(s,s) + v_t)\, dx + \int_{\partial S} f\hat{\nu}\cdot(h_{\partial S}(\sigma,\sigma) + v_t - 2\nu_x\sigma) + (\kappa_{\partial S}\cdot\nu)(\hat{\nu}\cdot\nu)\, d\xi.$$

If additionally $v = \sigma$, i.e., $\nu = 0$ on ∂S, then $I_t(0) = 0$ and

$$I_{tt}(0) = \int_S (f_n + f\kappa\cdot)(h(s,s) + v_t)\, dx + \int_{\partial S} f\hat{\nu} \cdot (h_{\partial S}(\sigma,\sigma) + v_t)\, d\xi$$

For the perturbation of identity method, where $v_t = 0$, we observe a second order change of I that depends on the curvature of S and ∂S. This reflects, as described above, that straight movement along tangential directions induces a normal acceleration.

For the velocity method we have $v_t = s_x s$ on S and thus $(h(s,s) + v_t) \cdot \kappa = 0$. Similarly, on ∂S we have $v_t = \sigma_x\sigma$ and thus $(h_{\partial S}(\sigma,\sigma) + v_t)\cdot\hat{\nu} = 0$. Hence, for the velocity method we obtain in $I_{tt}(0) = 0$ in the fully tangential case. This fits to our expectation: if $\phi(t,\cdot)$ is the flow of a field that is tangential to S and ∂S, then S should not change and thus $I(t)$ should be constant.

Volume integrals. Consider the case that S is a smoothly bounded open subset of $\mathbb{R}^d$. This implies that $T_xS = \mathbb{R}^d$ and thus $v = s$ and $n = 0$. Moreover, $h(\cdot,\cdot) = 0$ and $\kappa = 0$. Consequently, the integral over S in I_t and I_{tt} vanishes. On ∂S we can write $s = \nu + \sigma = \theta\hat{\nu} + \sigma$ with $\theta = \nu \cdot \hat{\nu}$ and compute $(\kappa_{\partial S}\cdot\nu)(\nu\cdot\hat{\nu}) = \theta^2(\kappa_{\partial S}\cdot\hat{\nu}) = \theta^2\hat{\kappa}_{\partial S}$. From (25) we obtain $\hat{\nu}_x\sigma \cdot \hat{\nu} = 0$ and thus:

$$\nu_x\sigma \cdot \hat{\nu} = (\theta\hat{\nu})_x\sigma \cdot \hat{\nu} = ((\theta_x\sigma)\hat{\nu} + \theta\hat{\nu}_x\sigma) \cdot \hat{\nu} = \theta_x\sigma.$$

Abbreviating $f_{\hat{\nu}} := f_x\hat{\nu}$ we thus obtain the formulas:

$$I_t(0) = \int_{\partial S} f\theta \, d\xi, \tag{53}$$
$$I_{tt}(0) = \int_{\partial S} f(\hat{h}_{\partial S}(\sigma,\sigma) + v_t \cdot \hat{\nu} - 2\theta_x\sigma) + \theta^2(f_{\hat{\nu}} + f\hat{\kappa}_{\partial S})\, d\xi. \tag{54}$$

In $I_{tt}(0)$ we observe a modified acceleration term and a purely normal contribution. If $v = \nu$ is purely normal on ∂S, $F = const$, and $v_t = 0$, we retrieve the well-known formula:

$$I_{tt}(0) = \int_{\partial S} \theta^2(f_{\hat{\nu}} + f\hat{\kappa}_{\partial S})\, d\xi.$$

Hypersurface integrals. In the case of closed orientable hypersurfaces, where $\partial S = \emptyset$, we have a distinguished outer unit normal field $\hat{n}$. Then we can write our splitting $v = \eta\hat{n} + s$ on S where $\eta : S \to \mathbb{R}$ is a scalar function. The curvature vector can now be written as $\kappa = \hat{\kappa}\hat{n}$, and thus

$$n_x s \cdot \kappa = \hat{\kappa}(\eta\hat{n})_x s \cdot \hat{n} = \hat{\kappa}(\eta_x s\hat{n} \cdot \hat{n} + \eta\hat{n}_x s \cdot \hat{n}) \overset{(25)}{=} \hat{\kappa}\eta_x s.$$

Moreover, by Proposition 3.4 $\langle n_x, n_x\rangle_{S\to N} = \nabla_s\eta \cdot \nabla_s\eta$ is the Laplace-Beltrami Operator in weak form on S. Using the notations $\hat{h}(\cdot,\cdot) = h(\cdot,\cdot) \cdot \hat{n}$, $f_{\hat{n}} := f_x\hat{n}$ and $f_{\hat{n}\hat{n}} := f_{xx}(\hat{n},\hat{n})$ we obtain the following formulas:

$$I_t(0) = \int_S \eta(f_{\hat{n}} + f\hat{\kappa})\,dx,$$
$$I_{tt}(0) = \int_S (f_{\hat{n}}+f\hat{\kappa})(\hat{h}(s,s) + v_t\cdot\hat{n} - 2\eta_x s) + \eta^2(2\hat{K}f + 2f_{\hat{n}}\hat{\kappa} + f_{\hat{n}\hat{n}}) + f(\nabla_s\eta\cdot\nabla_s\eta)\,dx.$$

The first term in $I_{tt}(0)$ is again a modified acceleration term. In Proposition 3.3 the role of $\hat{K}$ has been discussed. It is the sum of the second order minors of the second fundamental form and thus $2\eta^2\hat{K}$ describes the second order change of local area by normal translation. For $d = 2$ we have $\hat{K} = 0$, while $\hat{K}$ is the Gauss curvature for $d = 3$.

The Laplace-Beltrami term $\nabla_s\eta\cdot\nabla_s\eta$ takes into account changes of curvature due to non-constant normal velocity. It is still present if S is flat and then reduces to the classical Laplace operator.

A similar formula for I_{tt} has been derived in [6]. However, the Laplace-Beltrami term seems to be missing there. For normal fields $v = n$ this formula simplifies to

$$I_{tt}(0) = \int_S \eta^2(f_{\hat{n}\hat{n}} + 2f_{\hat{n}}\hat{\kappa} + 2\hat{K}f) + f(\nabla_s\eta\cdot\nabla_s\eta)\,dx.$$

This formula can also be found in [5] for the special case $d = 2$ (so $\hat{K} = 0$).

If S is not closed, then the boundary term in (44) must be added. However, no significant simplifications arise in this case.

Let us illustrate the role of $\hat{K}$ with an example: let S be the sphere in $\mathbb{R}^3$ around 0 with radius r_0. Define $\phi(t,x) := x + v(x)$ with $v(x) = \eta\hat{n}(x)$ and $\eta = const$ on S. Since $\hat{n}$ points in radial direction, the radius $r(t)$ of the sphere changes linearly in time as $r(t) = r_0 + t\eta$. Further, we have for the surface area $I(t)$:

$$I(t) = \int_S dx = 4\pi r(t)^2 = 4\pi(r_0 + t\eta)^2 = 4\pi r_0 + t\,8\pi\eta r_0 + \frac{t^2}{2}\,8\pi\eta^2,$$

which coincides with its own second order expansion. It is known that the principal curvatures of the sphere satisfy $\kappa_1 = \kappa_2 = 1/r_0$ so $\kappa = \kappa_1 + \kappa_2 = 2/r_0$ and $\hat{K} = 1/r_0^2$. Now we can evaluate our formulas:

$$I_t(0) = \int_S \hat{\kappa}\eta\,dx = \hat{\kappa}\eta\,4\pi r_0^2 = 8\pi\eta r_0,$$
$$I_{tt}(0) = \int_S 2\hat{K}\eta^2\,dx = 2\hat{K}\eta^2\,4\pi r_0^2 = 8\pi\eta^2,$$

and confirm that they coincide with the exact result.

Line Integrals. In this case we have (up to sign) a unit tangent field $\hat{s}$ and we may write $v = n + \tau\hat{s}$, where $\tau = (s\cdot\hat{s})$. Now ∂S consists of just two points, say x_1 and x_0 and it holds $\hat{\nu} = \pm\hat{s}$, depending on the direction of $\hat{s}$. Assuming that $\hat{s}(x_1) = \hat{\nu}(x_1)$ we obtain the opposite at x_0. With this we can compute

$$I_t(0) = \int_S f_x n + f(n\cdot\kappa)\,dx + f\tau\Big|_{x_0}^{x_1}.$$

To write down I_{tt} concisely, we define $n_{\hat{s}} := n_x\hat{s}$, so that $n_x s = \tau n_x\hat{s} = \tau n_{\hat{s}}$ By Proposition 3.3 we get $K(n,n) = 0$ and by Proposition 3.4 we obtain, setting $\tilde{n}_{\hat{s}} := (I-P)n_{\hat{s}}$.

$$\langle n_x, n_x\rangle_{S\to N} = (I-P)n_s\cdot(I-P)n_s = \tilde{n}_s\cdot\tilde{n}_s.$$

Further, we observe $\kappa = h(\hat{s},\hat{s})$ and thus $h(s,s) = \tau^2 h(\hat{s},\hat{s}) = \tau^2\kappa$. We end up with the formula:

$$I_{tt}(0) = \int_S (f_n + f\kappa\cdot)(\tau^2\kappa + v_t - 2\tau n_{\hat{s}}) + \big(f\tilde{n}_s\cdot\tilde{n}_s + 2f_x n(\kappa\cdot n) + f_{xx}(n,n)\big)\,dx \\ + \big(f_x(\nu+2n)\tau + v_t\cdot\hat{s}\big)\big|_{x_0}^{x_1}.$$

As usual we observe the modified acceleration term and the contribution of the normal field in the full integral.

Let us illustrate here the occurrence of the factor 2 in the term $f_x(2n+\nu)$ with an example. Let $S = [0, e_1]$ be a straight line in $\mathbb{R}^2$ with end-points 0 and e_1, so $\hat{s} = e_1$. Let also $F(t,x) = f(x) = f_x x$ be a linear function on $\mathbb{R}^2$. We shift and stretch S by the transformation $\phi(t,x) = x + t(n + s(x))$, where $n = e_2$ and $s(x) = \tau(x)e_1 = (e_1\cdot x)e_1$. We observe that 0 is mapped to tn and e_1 is mapped to $tn + (1+t)e_1$. Further we observe $\nu(0) = -s(0) = 0$ and $\nu(e_1) = s(e_1) = e_1$. Exact computation of $I(t)$ yields:

$$I(t) = \int_{\phi(t,S)} F(t,x)\,dx = \int_{[tn,tn+(1+t)e_1]} f_x x\,dx = \int_0^{1+t} f_x(tn + \lambda e_1)\,d\lambda \\ = f_x\Big((1+t)tn + \frac{(1+t)^2}{2}e_1\Big) = \frac{1}{2}f_x e_1 + t(f_x n + f_x e_1) + \frac{t^2}{2}f_x(2n+e_1) \\ = \frac{1}{2}f_x e_1 + t\Big(\int_S f_x n\,dx + f\tau|_0^{e_1}\Big) + \frac{t^2}{2}f_x(2n+\nu)\tau|_0^{e_1} = I(0) + tI_t(0) + \frac{t^2}{2}I_{tt}(0).$$

So in this case $I(t)$ coincides with its second order expansion, which coincides with our computations.

Point evaluations. For completeness we also consider the trivial case $k = 0$, so $S = \{x_0\}$ is a single point, $\partial S = \emptyset$, $T_x S = \{0\}$, $N_x S = \mathbb{R}^d$ and $v = n$. In this case our formulas read, as expected:

$$I_t(0) = F_t + f_x v, \\ I_{tt}(0) = F_{tt} + 2F_{xt}v + f_{xx}(v,v) + f_x v_t,$$

to be evaluated at x_0.

5.4 Integrands involving derivatives of functions

In this section we extend our study of sensitivity to integrals of the form

$$\int_S f(x)\,dx = \int_S l(x, u(x), u_x(x))\,dx,$$

where $u : \mathbb{R}^d \to \mathbb{R}$ and $l : S \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$. Again, we construct an embedding of that problem, first defining pairs of functions:

$$U(t,\phi(t,x)) = u(t,x) \\ L(t,\phi(t,x),u,g) = l(t,x,u,g)$$

and then consider again the integral

$$I(t) := \int_{\phi(t,S)} F(t,X)\,dX = \int_S f(t,x)J(t,x)\,dx$$

where

$$F(t,X) := L(t,X,U(t,X),U_X(t,X)) \text{ and } f(t,x) = F(t,\phi(t,x)).$$

Since $U(t,\phi(t,x)) = u(t,x)$ we obtain by the chain-rule:

$$u_x(t,x) = (U(t,\phi(t,x)))_x = U_X(t,\phi(t,x))\phi_x(t,x).$$

Thus, we have to define

$$f(t,x) := l(t,x,u(t,x),u_x(t,x)\phi_x^{-1}(t,x))$$

to achieve:

$$F(t,\phi(t,x)) = f(t,x).$$

With these definitions, our previous results are applicable straightforwardly.

Sensitivity of solutions of a semi-linear elliptic equation

As a simple application and illustration we consider the following equation with Dirichlet boundary conditions:

$$0 = \int_\Omega \nabla u(x)\cdot\nabla w(x) - d(x,u(x))w(x)\,dx \quad \forall w \in C_0^\infty(\Omega).$$

The following sensitivity results (at least to first order) are well known (cf. e.g. [12]), the aim of this discussion is rather to demonstrate the ease of derivation of these formulas with the help of our general results. Here it is helpful that F_t and F_{tt} are still present in (36) and (43). Again, questions of differentiability are excluded here (for a discussion cf. e.g. [2, Chapter 10] and [14, 3]). We focus only on the formal derivation of the sensitivity equation.

Here, as usual $\nabla u = u_x^T$, and we can write the above equation as follows:

$$0 = \int_\Omega f(x)\,dx = \int_\Omega l(x,u(x),u_x(x),w(x),w_x(x))\,dx = \int_\Omega u_x(x)w_x^T(x) - d(x,u(x))w(x)\,dx.$$

We establish a sensitivity result for any solution u with respect to small perturbations of $S = \Omega$. Hence, we would like to compute to first and second order the change in $U(t,X)$, if Ω is transformed slightly.

To establish an embedding of this integral for a family of deformations, we have to give ∇u, or better u_x sense in the deformed region. Here the physically meaningful embedding is to use the derivative w.r.t $X = \phi(t,x)$:

$$\nabla_X U(t,X) := U_X^T(t,X) = \phi_x^{-T}(t,x)u_x^T(t,x).$$

This leads us to the embedding:

$$I(t) = \int_{\phi(t,\Omega)} \nabla_X U(t,X)\cdot\nabla_X W(t,X) - D(t,X,U(t,X))W(t,X)\,dX \quad \forall W(t,\cdot) \in C_0^\infty(\phi(t,\Omega))$$

so that our integrand is given by

$$F(t,X) := \nabla_X U(t,X)\cdot\nabla_X W(t,X) - D(t,X,U(t,X))W(t,X).$$

Its first time-derivative at $t = 0$ reads:

$$F_t := \nabla_X U_t \cdot \nabla_X W + \nabla_X U \cdot \nabla_X W_t - (D_t W + D_u U_t W + D W_t).$$

Classically, $D(t,X,u) = D(X,u)$ is constant in time for fixed argument u, so that $D_t W = 0$. Our embedded equation now is $0 = I(t)$ and thus $0 = I_t(0) = I_{tt}(0)$.

Since W has compact support on Ω this yields in general:

$$I_t(0) = \int_\Omega F_t \, dx + \int_{\partial\Omega} f(v \cdot \hat{\nu}) \, d\xi = \int_\Omega F_t \, dx = 0. \tag{55}$$

The boundary term vanishes, because f has compact support in Ω.

To compute the shape derivatives U_t and U_{tt} it is easiest to choose the testfunction $W(t,X) = W(X)$ independent of time, since W has compact support in Ω which is inherited for small t to $\phi(t,\Omega)$. Then $W_t \equiv 0$ and most terms in F_t drop out so that we obtain:

$$F_t = \nabla_X U_t \cdot \nabla_X W + D_u U_t W.$$

From (55) we conclude the first order sensitivity equation:

$$0 = \int_\Omega \nabla U_t \cdot \nabla W + D_u U_t W \, dx \quad \forall W \in C_0^\infty(\Omega). \tag{56}$$

As for the second time derivative of F we compute (taking into account $D_{ut} = D_{tu} = 0$):

$$F_{tt} = \nabla_X U_{tt} \cdot \nabla_X W + (D_{uu} U_t^2 + D_u U_{tt}) W.$$

Similarly, the second order sensitivity equation (54) becomes a quite simple expression, because all boundary terms drop out due to compactness of the support of f:

$$0 = I_{tt}(0) = \int_\Omega F_{tt} \, dx = \int_\Omega \nabla U_{tt} \cdot \nabla W + D_u U_{tt} W + D_{uu} U_t^2 W \, dx \quad \forall W \in C_0^\infty(\Omega).$$

The Dirichlet boundary conditions read $u(t,x) := u_0(x)$ for all $x \in \partial\Omega$, which implies $u_t(x) = u_{tt}(x) = 0$ for all $x \in \partial\Omega$. By the relation between U and u we obtain the following boundary conditions (the second via (16)):

$$\begin{aligned} U_t &= u_t - u_x v = -u_x v = -u_\nu v && \text{on } \partial\Omega, \\ U_{tt} &= u_{tt} - 2U_{xt} v - u_{xx} v^2 - u_x v_t = -2(U_t)_x v - u_{\nu x} v^2 - u_\nu v_t && \text{on } \partial\Omega. \\ &= 2u_{\nu x} v^2 + 2u_\nu v_x v - u_{\nu x} v^2 - u_\nu v_t = u_{\nu x} v^2 + u_\nu (2v_x v - v_t). \end{aligned}$$

For the velocity method $v_t = v_x v$ we compute $U_{tt} = u_{\nu x} v^2 + u_\nu v_x v = (u_\nu v)_x v = -(U_t)_x v$. If $v = \sigma$ is purely tangential on $\partial\Omega$, then $U_t \equiv 0$ on Ω. For $v_t = v_x v$ this implies $U_{tt} = -(U_t)_x \sigma = 0$, for $v_t = 0$ we have in contrast $U_{tt} = -u_{\nu x} \sigma^2 = u_\nu \sigma_x \sigma = -u_\nu h_{\partial\Omega}(\sigma,\sigma) \neq 0$.

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