Second order directional shape derivatives of integrals on submanifolds

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Abstract

We compute first and second order shape sensitivities of integrals on smooth submanifolds using a variant of shape differentiation. 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 $\phi(t,\cdot) : S \to \mathbb{R}^d$ 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. For example, we need a well defined tangent space at each point, and also (for the discussion of the Hadamard form) a well defined second fundamental form and notions of curvature, derived from it.

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. [8, Chapter XI] or [14, Chapter 9]).

In shape optimization we find several different approaches to shape sensitivity analysis. They usually start with a given vector field v on $\mathbb{R}^d$ and construct a family of perturbations $\phi(t,\cdot)$, such that $\phi_t(0,x) = v(x)$. They differ in the way, $\phi(t,\cdot)$ is constructed from v. The so called perturbation of identity method [9, 13, 5], defines $\phi(t,x) = x + tv(x)$. The velocity method (cf. e.g. [18, 19], the monograph [3], and for a similar approach [17]) defines ϕ as a flow of (possibly time dependent) v. In [11] 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, classical 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 in [12, 10, 5].

For the velocity method $\phi(t_1, t_2, x)$ has been defined as the composition of two mappings [3, 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 [1, 7], applications in image segmentation can be found in [6]. 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 $\phi(t, \cdot)S \to \mathbb{R}^d$, use only a single vector field $v = \phi_t(0, \cdot)$ on S 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. This 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 $v_t = \phi_{tt}(0, \cdot)$. A symmetric bilinear form can be derived by differentiating q with respect to v twice. 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. [2]) and SQP-methods.

Concerning the geometry of S we choose a rather general setting, namely a k-dimensional submanifold $S \subset \mathbb{R}^d$ with (possibly empty) boundary. This includes the well known special cases $S = \overline{\Omega}$, 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 curves. Except for [16], where a structure theorem is derived for first order shape derivatives, little work on shape calculus has been done in this general setting. Apart from the higher generality, a benefit is a unified view on the different cases of shape derivatives, which are traditionally treated by separate computations. We also put emphasis on the use of quantities, that are intrinsic to the given problem.

Much care is taken to the derivation and geometrical interpretation of the Hadamard form of the second derivative which includes a splitting into normal and tangential components of the vector fields. This allows to give each term of the Hadamard form a specific geometric interpretation, which we try to illuminate, also with the help of geometric examples. Of particular interest is the occurence of generalizations of the Gauss curvature of S and the Laplace-Beltrami operator on S. The use of only one perturbation field v instead of two is very helpful here, in order to keep the involved computations as concise as possible.

1.1 Embedding of the problem

Consider a one-parameter family of orientation preserving diffeomorphisms

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

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

$$\begin{aligned} v : I \times S &\to \mathbb{R}^d & \qquad v_t : I \times S &\to \mathbb{R}^d \\ v(t, x) &= \phi_t(t, x) & v_t(t, x) &= \phi_{tt}(t, x). \end{aligned}$$

For brevity, we will write $v = v(0)$ and $v_t = v_t(0)$ as mappings $S \to \mathbb{R}^d$. Thus, local Taylor expansion around $t = 0$ yields:

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

For a 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 $f : I \times S \to \mathbb{R}$, such that

$$F(t, \phi(t, x)) = f(t, x) \quad \forall (t, x) \in I \times S$$

and thus consequently

$$F(0,x) = f(0,x) \quad \forall x \in S.$$

By the chain rule we easily derive relations between the derivatives of F and f at $t = 0$:

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

The expression F_t is commonly called *shape derivative* of f, 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 the notation $f' := F_t$ for the shape derivative and $\dot{f} := f_t$ for the material derivative of f is used frequently.

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:

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

Here the well known measure tensor occurs:

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

with $B(x) \in \mathbb{R}^{d\times k}$ being a matrix whose columns consist an orthonormal basis $\{b_i\}_{i=1\ldots k}$ of the tangent space of S at x. It is easy to see that J is independent of the choice of basis.

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:*

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

$$I_{tt}(0) = \int_S f_{tt} + 2f_tJ_t + fJ_{tt}\,dx. \tag{5}$$

Proof. Straightforward application of the product rule to

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

taking into account that $J(0,x) = \sqrt{\det B(x)^T B(x)} = 1$. □

The most involved part of this computation will be the derivation of J_{tt}. Of course, 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 (cf. e.g. [3, 4, 6]), where, however, a different representation of J, via a unit normal field is employed. Our approach treats all cases in a unified way, which yields insights about the common structure of first and second shape derivatives.

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 manifold, since, e.g., curvature terms occur, but in turn yields additional geometrical understanding.

Special care will be taken to use intrinsic quantities only. In particular, ϕ and thus also v and v_t are only defined on S, and thus, the spatial derivatives v_x and v_{xx} only make sense on S and only in tangential direction. Similarly, f is only defined on S. However, F has to be defined on $\mathbb{R}^d$, or at least in a neighbourhood of S. We also stress that we do not need any extension of normal fields from S onto a neighbourhood of S.

1.2 General structure

Before we carry out our computations 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 there F is constant in time, 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 quadratic function of v so that $l(v_t(v))$ is quadratic in v and we can define the following quadratic form in v:

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

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.

Relation to known approaches. 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:

i) The *perturbation of identity method* [13, 5] chooses $\phi(t, x) := x + tv_0(x)$, where $v_0 : S \to \mathbb{R}^d$. 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* [3] defines $\phi(t,x)$ via the following modified initial value problem:

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

In this construction we need $V : \mathbb{R}^d \to \mathbb{R}^d$ as a velocity field "in the back-ground" and $\phi(t,x)$ as the trajectory of a particle that moves in this field. More generally, V may also depend on t. It follows $v(0,x) = V(x)$ and

$$\begin{aligned} v_t &= \frac{d}{dt} V(\phi(t,\cdot))|_{t=0} = V_x \phi_t = V_x v = V_x V, \\ \tilde{q}(V) &= q(V) + l(V_x V), \\ b(V,W) &= \frac{1}{2} q''(0)(V,W) + \frac{1}{2} l(V_x W + W_x V). \end{aligned}$$

The non-symmetric shape hessian discussed in [3] 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 [11]. 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 a spray (cf. e.g. [8, 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 obtain

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

2 Shape derivatives in weak form

Throughout this paper we consider $\mathbb{R}^d$ equipped with the canonical basis $\{e_i\}_{i=1\ldots d}$ of unit vectors and the standard scalar product

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

Let $S \subset \mathbb{R}^d$ be a smooth, ortiented, k-dimensional submanifold. We denote by T_xS the tangent space of S at $x \in S$ and by TS the tangent bundle of S. Similarly $N_xS = (T_xS)^\perp$ is its orthogonal complement, the normal space of S at x and NS the normal bundle of S.

Using local charts on S we can define differentiability and derivatives of mappings $g : S \to Y$, where Y is some vector space. At a given point x we then obtain a linear mapping $T_xg : T_xS \to Y$, which we sometimes denote by g_x or g_s.

2.1 Projection onto the tangent space

A central quantity in the differential geometry of submanifolds is the *orthogonal projection* $P(x)$ onto T_xS at a given point $x \in S$. We associate to each $x \in S$ an orthonormal basis $\{b_1, \ldots, b_k\}$ of T_xS, whose members form the columns of a matrix $B = B(x)$. Then we define the unique 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 $P(x)P(x) = P(x)$, $\operatorname{ran} P(x) = T_xS$, and $\ker P(x) = N_xS$. 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 $P(x)$.

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

$$\operatorname{tr} A := \sum_{i=1}^{d} e_i \cdot Ae_i.$$

The *tangential trace* at a point x of a matrix $A \in \mathbb{R}^{d\times d}$ (or more generally of a linear mapping $A : T_xS \to \mathbb{R}^d$) can be defined as:

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

Obviously tr_S does not depend on the particular choice of B and $\operatorname{tr}_S A = \operatorname{tr}_S A^T$. With its help we define corresponding *symmetric non-negative bilinear forms* for linear mappings:

$$\langle A_1, A_2\rangle_{S\to S} := \operatorname{tr}_S(A_1^T PA_2) = \sum_{i=1}^{k} PA_1b_i \cdot PA_2b_i, \tag{9}$$

$$\langle A_1, A_2\rangle_{S\to N} := \operatorname{tr}_S(A_1^T(I - P)A_2) = \sum_{i=1}^{k}(I - P)A_1b_i \cdot (I - P)A_2b_i. \tag{10}$$

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

$$\langle A_1^T, A_2\rangle_{S\to S} = \operatorname{tr}(A_1PA_2P) = \operatorname{tr}(A_2PA_1P) = \langle A_2^T, A_1\rangle_{S\to S} = \langle A_1, A_2^T\rangle_{S\to S}. \tag{11}$$

Application of the tangential trace to the derivative $v_x : T_xS \to \mathbb{R}^d$ of a differentiable vector field $v : S \to \mathbb{R}^d$ yields the *tangential divergence*:

$$\operatorname{div}_S v := \operatorname{tr}_S v_x = \sum_{i=1}^{k} b_i \cdot v_xb_i. \tag{12}$$

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

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

Observe that $J(t,x)$ can be evaluated, using $\phi_x(t,x) = T_x\phi(t,\cdot)$ in tangential direction, i.e. in $\operatorname{ran} B(x)$, only. Similarly, the expressions of its derivatives in Lemma 2.1 depend on $v_x = \phi_{tx}(t,\cdot)$ and $v_{tx} = \phi_{ttx}(0,\cdot)$ in tangential direction only.

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

$$J_t := J_t(0,\cdot) = \operatorname{div}_S v \tag{13}$$

$$J_{tt} := J_{tt}(0,\cdot) = (\operatorname{div}_S v)^2 - \langle v_x^T, v_x\rangle_{S\to S} + \langle v_x, v_x\rangle_{S\to N} + \operatorname{div}_S v_t. \tag{14}$$

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 $G(t,x) = B^T(x)C(t,x)B(x)$ so that $J(t,x) = \sqrt{\det G(t,x)}$.

$$\begin{aligned}(\det G)_t &= \operatorname{tr}((\det G)G^{-1}G_t) = \det G \operatorname{tr}(G^{-1}G_t)\\ \operatorname{tr}(G^{-1}G_t)_t &= \operatorname{tr}(-G^{-1}G_tG^{-1}G_t + G^{-1}G_{tt}),\end{aligned}$$

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

$$G_t = B^TC_tB = B^T(\phi_x^T\phi_{xt} + \phi_{xt}^T\phi_x)B = B^T(v_x + v_x^T)B$$

and

$$G_{tt} = B^TC_{tt}B = B^T(\phi_x^T\phi_{xtt} + \phi_{xtt}^T\phi_x + 2\phi_{xt}^T\phi_{xt})B = B^T(v_{xt} + v_{xt}^T + 2v_x^Tv_x)B$$

we get

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

$$\begin{aligned}J_{tt} &= ((\det G)^{1/2})_{tt} = \frac{1}{2}((\det G)^{1/2})_t\operatorname{tr}(G^{-1}G_t) + \frac{1}{2}(\det G)^{1/2}\operatorname{tr}(G^{-1}G_t)_t\\ &= \frac{1}{4}\det G^{1/2}\operatorname{tr}(G^{-1}G_t)^2 + \frac{1}{2}(\det G)^{1/2}\operatorname{tr}(-G^{-1}G_tG^{-1}G_t + G^{-1}G_{tt})\\ &\overset{G\equiv I}{=} \frac{1}{4}\operatorname{tr}(G_t)^2 - \frac{1}{2}\operatorname{tr}(G_tG_t) + \frac{1}{2}\operatorname{tr}(G_{tt})\\ &= (\operatorname{div}_S v)^2 - \frac{1}{2}\operatorname{tr} B^TC_tBB^TC_tB + \frac{1}{2}\operatorname{tr}_S(v_{xt} + v_{xt}^T + 2v_x^Tv_x)\\ &= (\operatorname{div}_S v)^2 - \frac{1}{2}\langle C_t, C_t^T\rangle_{S\to S} + \operatorname{div}_S v_t + \operatorname{tr}_S v_x^Tv_x.\end{aligned}$$

We continue

$$\langle C_t, C_t^T\rangle_{S\to S} = \langle v_x + v_x^T, v_x + v_x^T\rangle_{S\to S} \overset{(11)}{=} \langle v_x + v_x^T, v_x + v_x\rangle_{S\to S} = 2\operatorname{tr}_S(v_x + v_x^T)Pv_x.$$

Hence,

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

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

As a short hand notation we introduce the bilinear form:

$$Q(v,w) = \operatorname{div}_S v \operatorname{div}_S w - \langle v_x^T, w_x\rangle_{S\to S} + \langle v_x, w_x\rangle_{S\to N}, \tag{15}$$

which is symmetric by (10) and (11). Observe again that v_x, and w_x only have to be evaluated in tangential direction here. This follows from the explicit expressions in (9), (10) and (12). We obtain:

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

2.3 First and second shape derivatives

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

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

As already mentioned, v only needs to be defined on S to evaluate these expressions. Also, up to now f, f_t and f_{tt} only need to be defined on S.

Classical shape sensitivity analysis often uses a time-independent integrand $F : \mathbb{R}^d \to \mathbb{R}$ as data. Thus, we formulate our derivatives in terms of F. Since $f = F$ and $f_t = F_t + F_x v$ on S we obtain

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

If we define

$$l(F,v) := \int_S F_x v + F \operatorname{div}_S v \, dx \tag{16}$$

we can write

$$I_t(0) = \int_S F_t \, dx + l(F,v). \tag{17}$$

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

$$F_{tt} + 2F_{tx} v + F_{xx} v^2 + F_x v_t = f_{tt}. \tag{18}$$

This yields a volume formulation of the second derivative:

$$I_{tt}(0) = \int_S F_{tt} + 2(F_{tx} v + F_t \operatorname{div}_S v) + (F_x v_t + F \operatorname{div}_S v_t)\, dx$$
$$+ \int_S F_{xx}(v,v) + 2F_x v \operatorname{div}_S v + FQ(v,v)\, dx.$$

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

$$q(F,v) := \int_S F_{xx}(v,v) + 2F_x v \operatorname{div}_S v + F\big((\operatorname{div}_S v)^2 - \langle v_x^T, v_x\rangle_{S\to S} + \langle v_x, v_x\rangle_{S\to N}\big)\, dx \tag{19}$$

and l is given by (16) we obtain:

$$I_{tt}(0) = \int_S F_{tt}\, dx + 2l(F_t, v) + l(F, v_t) + q(F,v). \tag{20}$$

The representation of (17) is sometimes called *domain expression* or *weak form* of the shape derivative. We stress that $F : I \times \mathbb{R}^d \to \mathbb{R}$ cannot be replaced by $f : I \times S \to \mathbb{R}$ in this expression, since, e.g., $f_x v$ may not be well defined, unless v is a tangential vector field.

3 Concepts from differential geometry

Our next aim is to analyse (16) and (19) 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, reflecting that some deformations leave S invariant. Further, the curvature of S and its boundary ∂S will play an important role.

To carry out this plan we need some concepts from differential geometry of submanifolds. For convenience of the reader we will give a concise self contained exposition (the notation varies in the literature), based on the orthogonal projection $P(x)$ onto T_xS and its derivative T_xP. Readers familiar with these concepts may want to browse quickly over this section.

Orthogonal splittings of vector fields. 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 *split v orthogonally* into a tangential field $s : S \to TS$, where $s(x) \in T_xS$, and a normal field $n : S \to NS$, where $n(x) \in N_xS$:

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

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:

$$F_x = F_xP + F_x(I - P) = F_s + F_n,$$

so that $F_sv = F_xPv = F_xs$ and $F_nv = F_x(I - P)v = F_xn$.

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* $\nabla_s F(x) \in T_xS$ via $\nabla_s F(x) \cdot w = F_s(x)w$ for all $w \in T_xS$.

Derivative of P. 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 with respect to x in tangential direction. The derivative of P at x is a linear mapping

$$T_xP : T_xS \to L(\mathbb{R}^d, \mathbb{R}^d).$$

Thus, for each $b \in T_xS$ the directional derivative $T_xP(b) \in L(\mathbb{R}^d, \mathbb{R}^d)$ is a linear mapping. We write $T_xP(b)v \in \mathbb{R}^d$ to denote the derivative of P at $x \in S$ in direction $b \in T_xS$, 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 $b \in T_xS$:

$$(Pv)_xb = T_xP(b)v + Pv_xb. \tag{21}$$

We summarize some well known results on T_xP from differential geometry:

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

$$T_xP(b)s = (I - P)s_xb \in N_xS, \tag{22}$$

$$T_xP(b)n = -Pn_xb \in T_xS. \tag{23}$$

The following symmetries are valid:

$$s_1, s_2 \in T_xS \quad \Rightarrow \quad T_xP(s_1)s_2 = T_xP(s_2)s_1 \tag{24}$$

$$v_1, v_2 \in \mathbb{R}^d \quad \Rightarrow \quad v_1 \cdot (T_xP(b)v_2) = v_2 \cdot (T_xP(b)v_1) \tag{25}$$

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

$$s_1, s_2 \in T_xS \quad \Rightarrow \quad s_1 \cdot n_xs_2 = s_2 \cdot n_xs_1. \tag{26}$$

Proof. Since $Ps = s$, (21) yields $s_x b = T_x P(b)s + Ps_x b$ and thus (22). Similarly, we use $Pn = 0$ to deduce (23). For (24) 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, (25) 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 (26):

$$\begin{aligned} s_1 \cdot n_x s_2 = s_1 \cdot P n_x s_2 &\overset{(23)}{=} -s_1 \cdot T_x P(s_2)n \overset{(25)}{=} -n \cdot T_x P(s_2)s_1 \\ &\overset{(24)}{=} -n \cdot T_x P(s_1)s_2 \overset{(25)}{=} -s_2 \cdot T_x P(s_1)n \overset{(23)}{=} s_2 \cdot n_x s_1. \end{aligned}$$

□

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

$$0 = \frac{1}{2}(\hat{v} \cdot \hat{v})_x w = \hat{v}_x w \cdot \hat{v} \quad \Rightarrow \hat{v}_x w \perp \hat{v} \quad \forall w \in \mathbb{R}^d. \tag{27}$$

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 Curvature and Laplace Beltrami operator

By (24) we see that the *second fundamental form*:

$$\begin{aligned} h : T_x S \times T_x S &\to N_x S \\ (s_1, s_2) &\mapsto h(s_1, s_2) := -T_x P(s_1)s_2 \end{aligned} \tag{28}$$

is well defined as a symmetric bilinear vector valued mapping (cf. e.g. [8, XIV §1]).

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

$$\kappa := \sum_{i=1}^{k} h(b_i, b_i) = -\sum_{i=1}^{k} T_x P(b_i)b_i \in N_x S. \tag{29}$$

Using the fact that each component of κ can be written as a tangential trace over a matrix that represents h, we see that this expression is independent of the choice of orthonormal basis. We have chosen the sign of $h(\cdot, \cdot)$, such that the corresponding curvature vector points outward, if S is a sphere.

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

$$n \cdot \kappa = \operatorname{div}_S n. \tag{30}$$

For any differentiable scalar function $\alpha : S \to \mathbb{R}$ it holds

$$\operatorname{div}_S \alpha n = \alpha \operatorname{div}_S n. \tag{31}$$

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

If S is a $k = d-1$ dimensional manifold (a hypersurface), then N_xS has dimension 1. Thus we have (due to orientation) a unit normal field $\hat{n}$ on S with $\hat{n} \cdot \hat{n} = 1$ and $h(s_1, s_2)$ 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 $\kappa_1 \dots \kappa_k$, the *principal curvatures*. These are the eigenvectors and eigenvalues of the mapping $-T_xP(\cdot)\hat{n} : T_xS \to T_xS$ (known as the shape operator). Further, we can define the (scalar valued) additive curvature,

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

which is related to the well known mean curvature $H := \hat{\kappa}/k$.

Gaussian curvature. Next, we indicate the geometrical meaning of some expressions that arise in the Hadamard form, derived below. We insert a purely normal field $v = n$ and $v_t = 0$ into (14):

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

We will see that the sum of the first two terms

$$K(n, n) := (\operatorname{div}_S n)^2 - \langle n_x^T, n_x \rangle_{S\to S} \tag{32}$$

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

The first part $K(n, n)$ 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:

$$\langle n_x^T, n_x \rangle_{S\to S} \overset{(26)}{=} \langle n_x, n_x \rangle_{S\to S} \overset{(23)}{=} \langle T_xP(\cdot)n, T_xP(\cdot)n \rangle_{S\to S} = \sum_{i=1}^{k} T_xP(b_i)n \cdot T_xP(b_i)n$$

and thus:

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

$K(n, n)$ does not depend on the derivatives of the normal field n and is thus a tensor field on S. 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 and $\eta : S \to \mathbb{R}$. 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 $k = d$, then $n = 0$ and all terms vanish. For the remaining cases we recall that $T_xP(\cdot)n : T_xS \to T_xS$ is symmetric, and thus there is an orthonormal basis $\{b_i\}_{i=1\dots k}$ of T_xS, consisting of eigenvectors of $T_xP(\cdot)n$ with eigenvalues $\lambda_1, \dots, \lambda_k$. 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 $k = d$, $\langle n_x, n_x\rangle_{S\to N}$ is an empty expression. The case $k = 1$ follows simply from the definition of $\langle\cdot,\cdot\rangle_{S\to N}$ and the relation $n_s = n_xb_1$, 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:

$$\hat{n}\cdot n_xb = (\eta\hat{n})_xb = \hat{n}\cdot\eta_xb\hat{n} + \eta\hat{n}\cdot\hat{n}_xb \overset{(27)}{=} \eta_xb.$$

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

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

□

3.2 Gauss's Divergence Theorem

To formulate Gauss's divergence 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 $\mathbb{R}^d$ with orientation induced from S. 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 oriented, 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:

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

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 $x \in \partial S$ and $n \in N_xS$ and vector fields $v : S \to \mathbb{R}^d$ we have the splittings:*

$$\kappa \cdot n = (\kappa_{\partial S} + h(\hat\nu,\hat\nu)) \cdot n \tag{33}$$

$$\operatorname{div}_S v = \operatorname{div}_{\partial S} v + \hat\nu \cdot v_x\hat\nu. \tag{34}$$

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

$$\begin{aligned} n\cdot h(\sigma_1,\sigma_2) &= -n\cdot(I-P)\sigma_{1,x}\sigma_2 = -(I-P)n\cdot\sigma_{1,x}\sigma_2 = -(I-P_{\partial S})n\cdot\sigma_{1,x}\sigma_2 \\ &= -n\cdot(I-P_{\partial S})\sigma_{1,x}\sigma_2 = n\cdot h_{\partial S}(\sigma_1,\sigma_2). \end{aligned} \tag{35}$$

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:

$$\begin{aligned} \kappa\cdot n &= \sum_{i=1}^{k-1} h(\beta_i,\beta_i)\cdot n + h(\hat\nu,\hat\nu)\cdot n \\ &\overset{(35)}{=} \sum_{i=1}^{k-1} h_{\partial S}(\beta_i,\beta_i)\cdot n + h(\hat\nu,\hat\nu)\cdot n = \kappa_{\partial S}\cdot n + h(\hat\nu,\hat\nu)\cdot n. \end{aligned}$$

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 Gauss's integral theorem (or divergence theorem):

$$\int_S \operatorname{div}_S s\,dx = \int_{\partial S} \hat\nu\cdot s\,d\xi. \tag{36}$$

In addition the following well known product rule with a scalar function f holds:

$$\operatorname{div}_S(fv) = f_s v + f\operatorname{div}_S v. \tag{37}$$

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

$$\int_S \operatorname{div}_S v\,dx = \int_S \kappa\cdot n\,dx + \int_{\partial S}\hat\nu\cdot s\,d\xi = \int_S \kappa\cdot v\,dx + \int_{\partial S}\hat\nu\cdot v\,d\xi. \tag{38}$$

If f is a scalar function on S then we have

$$\int_S f\operatorname{div}_S v\,dx = \int_S f\kappa\cdot n - f_x s\,dx + \int_{\partial S} f\hat\nu\cdot s\,d\xi. \tag{39}$$

Proof. (38) follows from (30) by linearity of div_S and (36). For the second identity in (38) we note that $\kappa \in N_xS$, so $v\cdot\kappa = n\cdot\kappa$ and $\hat\nu \in T_xS$, so that $v\cdot\hat\nu = s\cdot\hat\nu$. Finally, (36) follows from (38) and the product rule (37). □

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

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

A lemma on nested divergence. In the derivation of the Hadamard form we will observe the nested occurrence of div_S. The following lemma yields a useful formula that preceeds the application of Gauss's theorem.

Lemma 3.7. *For a vector field v on S and a tangential vector field s on 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. Using a local chart φ of $\mathbb{R}^d$ around a given point x_0, which maps S to a k-dimensional linear subspace $\bar{S}$ of $\mathbb{R}^d$, we may extend $v : S \to \mathbb{R}^d$ locally to a smooth vector field in a neighbourhood of x_0 in $\mathbb{R}^d$ by setting $v(x) := v(\varphi^{-1}(\bar{y}))$, for $\varphi(x) = \bar{y} + y_\perp$, where $\bar{y} \in \bar{S}$ and $y_\perp \in \bar{S}^\perp$. In this way, the expression $v_x w$ is defined at x_0 for all $w \in \mathbb{R}^d$. This simplifies the following computations. Our result, however, is independent of the chosen extension.

By the product rule (37) 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:

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

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:

$$\begin{aligned}\operatorname{tr}(v_x T_x P(s)(I-P)) &\overset{(23)}{=} \operatorname{tr}(v_x P T_x P(s)(I-P)) = \operatorname{tr}(T_x P(s)(I-P)v_x P) \\ &= \langle T_x P(s)^T, v_x\rangle_{S\to N} \overset{(25)}{=} \langle T_x P(s), v_x\rangle_{S\to N} = \langle (I-P)s_x, v_x\rangle_{S\to N} = \langle s_x, v_x\rangle_{S\to N}.\end{aligned}$$

For the second term we obtain:

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

Adding everything up yields the desired result. □

4 Shape derivatives in Hadamard form

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

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

Further, let s be a tangential vector field 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 Gauss's theorem (38) immediately yields the well known Hadamard form of the first shape derivative. Recall the definition of the curvature vector κ in (29) and the outer unit normal $\hat{\nu}$ of ∂S.

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

$$I_t(0) = \int_S F_t \, dx + l(F, v) \tag{40}$$

where

$$l(f, v) = \int_S (F_n + F\kappa\cdot)v \, dx + \int_{\partial S} F\hat{\nu} \cdot v \, d\xi. \tag{41}$$

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

$$\begin{aligned} I_t(0) &= \int_S f_t + f J_t \, dx = \int_S F_t + F_x v + F \operatorname{div}_S v \, dx \\ &\overset{(37)}{=} \int_S F_t + F_x v + \operatorname{div}_S F v - F_s v \, dx = \int_S F_t + F_n v + \operatorname{div}_S F v \, dx \\ &\overset{(38)}{=} \int_S F_t + F_n v + F\kappa \cdot v \, dx + \int_{\partial S} F\hat{\nu} \cdot v \, d\xi. \end{aligned}$$

□

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:

$$I_t(0) = \int_S F_t + (F_x + F\kappa\cdot)n \, dx + \int_{\partial S} F\hat{\nu} \cdot \nu \, d\xi. \tag{42}$$

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 split $v = s + n$ and use the product rule to write as many terms as possible as tangential divergence of some vector fields. Second we apply Gauss's theorem on S to interpret them as boundary terms. Finally, an additional application of Gauss's theorem on ∂S yields further information.

Lemma 4.2. *For $v = s + n$ the integrand in $q(F, v)$ can be split as follows:*

$$\begin{aligned} FQ(v, v) + 2F_x v \operatorname{div}_S v + F_{xx}(v, v) &= FQ(n, n) + 2F_x n(\kappa\cdot n) + F_{xx}(n, n) - F_n(s + 2n)_x s \\ &\quad + \operatorname{div}_S \big(F\big(\operatorname{div}_S(s + 2n) - (s + 2n)_x\big)s + F_x(s + 2n)s\big). \end{aligned} \tag{43}$$

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

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

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:

$$\begin{aligned}
&F\operatorname{div}_S(\operatorname{div}_S(s+2n)s-(s+2n)_x s)-\operatorname{div}_S\big(F(\operatorname{div}_S(s+2n)-(s+2n)_x)s-(F_x s)s\big)\\
&\overset{(37)}{=}-F_s(\operatorname{div}_S(s+2n)s-(s+2n)_x s)+F_x s\operatorname{div}_S s+(F_x s)_s s\\
&=F_s(s+2n)_x s+F_{xx}(s,s)+F_x s_x s-F_x s\operatorname{div}_S(2n)\\
&\overset{(31)}{=}(F_s+F_x)s_x s+2F_s n_x s+F_{xx}(s,s)-\operatorname{div}_S((F_x s)2n)
\end{aligned}$$

and conclude

$$\begin{aligned}
FQ(v,v)=\operatorname{div}_S(F(\operatorname{div}_S(s+2n)-(s+2n)_x)s)+FQ(n,n)\\
-\operatorname{div}_S(F_x s(s+2n))+(F_s+F_x)s_x s+2F_s n_x s+F_{xx}(s,s).
\end{aligned}\tag{44}$$

The terms in the first line of (44) can already be found in (43). Next, we compute:

$$2F_x v\operatorname{div}_S v=2\operatorname{div}_S(F_x vv)-2(F_x v)_s v=2\operatorname{div}_S(F_x vv)-2F_x v_x s-2F_{xx}(v,s).\tag{45}$$

To show (43) we have to add (44), (45), and $F_{xx}(v,v)$, and then simplify the expression. In particular, we observe:

$$\begin{aligned}
&-\operatorname{div}_S(F_x s(s+2n))+2\operatorname{div}_S(F_x vv)=\operatorname{div}_S(-F_x s(s+2n)+2F_x sv+2F_x nv)\\
&=\operatorname{div}_S(F_x ss)+2\operatorname{div}_S(F_x ns)+2\operatorname{div}_S(F_x nn)=\operatorname{div}_S(F_x(s+2n)s)+2F_x n(\kappa\cdot n),\\
&(F_s+F_x)s_x s+2F_s n_x s-2F_x v_x s=(-F_n+2F_x)s_x s-2F_x v_x s+2F_s n_x s\\
&\qquad=-F_n s_x s-2F_x n_x s+2F_s n_x s=-F_n s_x s-2F_n n_x s=-F_n(s+2n)_x s,\\
&F_{xx}(s,s)-2F_{xx}(v,s)+F_{xx}(v,v)=F_{xx}(v,n)-F_{xx}(n,s)=F_{xx}(n,n).
\end{aligned}$$

Taking all this into account finally yields (43). □

Next, we apply Gauss's theorem on S to the second line of (43) and then, in Lemma 4.4, a second time to some terms on ∂S. Although the resulting formulas will be rather lengthy, we will see in the following section that each term can be given a distinct geometric interpretation.

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

$$I_{tt}(0)=\int_S F_{tt}\,dx+2l(F_t,v)+l(F,v_t)+q(F,v)\tag{46}$$

where

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

and

$$\begin{aligned}
q(F,v)=&\int_{\partial S}F\hat{\nu}\cdot\big(h_{\partial S}(\sigma,\sigma)-2(n+\nu)_x\sigma\big)+(F_x+F\kappa_{\partial S}\cdot)(\nu+2n)(\nu\cdot\hat{\nu})\,d\xi\\
&+\int_S(F_n+F\kappa\cdot)(h(s,s)-2n_x s)+F\big(K(n,n)+\langle n_x,n_x\rangle_{S\to N}\big)+2F_x n(n\cdot\kappa)+F_{xx}(n,n)\,dx.
\end{aligned}\tag{47}$$

Proof. We apply Gauss's theorem to the integral over the second line of (43) and obtain, taking into account $\kappa\cdot s=0$:

$$\int_S\operatorname{div}_S\big(F(\operatorname{div}_S(s+2n)-(s+2n)_x)s+F_x(s+2n)s\big)\,dx=\int_S-F\kappa\cdot((s+2n)_x s)\,dx+I_{\partial S}\tag{48}$$

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 right hand side of the first line of (43) to the first integral on the right hand side of (48) we can also define a full term:

$$I_S = \int_S -(F_n + F\kappa\cdot)((s+2n)_x s) + FQ(n,n) + 2F_x n(\kappa\cdot n) + F_{xx}(n,n)\,dx \tag{49}$$

and thus split (43) 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 (47), respectively.

We begin with I_S. Taking into account (15) the last three terms of the integrand in (49) can easily be identified in the second line of (47). 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 (47).

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

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

Now we apply Gauss's theorem to the first integral of the second line, which is performed in detail 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:

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

We observe that the third line of this computation coincides with the first line of (47). To show that the fourth line vanishes, we compute, taking into account that $\hat\nu\in T_xS$:

$$n_x\nu\cdot\hat\nu = Pn_x\nu\cdot\hat\nu \overset{(23)}{=} -T_xP(\nu)n\cdot\hat\nu \overset{(25)}{=} -T_xP(\nu)\hat\nu\cdot n = h(\nu,\hat\nu)\cdot n = (\nu\cdot\hat\nu)h(\hat\nu,\hat\nu)\cdot n.$$

Thus, also $I_{\partial S}$ is equal to the boundary integral that appears in (47), as claimed. □

Lemma 4.4.

$$\begin{aligned} &\int_{\partial S} F\big((\nu\cdot\hat\nu)\operatorname{div}_S s - (s_x s)\cdot\hat\nu\big)\,d\xi \\ &\qquad = \int_{\partial S} F(\kappa_{\partial S}\cdot\nu)(\nu\cdot\hat\nu) + F\hat\nu\cdot\big(h_{\partial S}(\sigma,\sigma) - 2\nu_x\sigma\big) - (F_x\sigma)(\nu\cdot\hat\nu)\,d\xi. \end{aligned} \tag{50}$$

Proof. Application of the splitting formula (34) for div_S on ∂S and Gauss's theorem (39) on ∂S, using $\partial(\partial S) = \emptyset$ yields:

$$\begin{aligned}\int_{\partial S} F(\nu \cdot \hat{\nu}) \operatorname{div}_S s \, d\xi &= \int_{\partial S} F(\nu \cdot \hat{\nu}) \left(\operatorname{div}_{\partial S} s + (\hat{\nu} \cdot s_x \hat{\nu})\right) d\xi \\ &\overset{(39)}{=} \int_{\partial S} F(\nu \cdot \hat{\nu})(\nu \cdot \kappa_{\partial S} + \hat{\nu} \cdot s_x \hat{\nu}) - (F(\nu \cdot \hat{\nu}))_\sigma s \, d\xi.\end{aligned} \tag{51}$$

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 (27) and also $\nu = (\nu \cdot \hat{\nu})\hat{\nu}$, implying $(\nu \cdot \hat{\nu})\hat{\nu} \cdot s_x \hat{\nu} = \hat{\nu} \cdot s_x \nu$. So we obtain

$$F(\nu \cdot \hat{\nu})(\nu \cdot \kappa_{\partial S} + \hat{\nu} \cdot s_x \hat{\nu}) - (F(\nu \cdot \hat{\nu}))_\sigma s = F\big((\nu \cdot \hat{\nu})(\nu \cdot \kappa_{\partial S}) + \hat{\nu} \cdot (s_x \nu - \nu_x \sigma)\big) - F_x \sigma (\nu \cdot \hat{\nu}).$$

Taking into account the term $-s_x s \cdot \hat{\nu}$ in the left hand side of (50) 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 Gauss's 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 Gauss's theorem in the proof of Theorem 4.3 is still feasible.

However, the second application of Gauss's 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 $\hat{\nu}_i$. Then the left hand side in (51) can be replaced by:

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

Assume further that each ∂S_i has a smooth boundary $\partial\partial S_i = \partial(\partial S_i)$ with unit outer normal field $\hat{\mathfrak{n}}_i(x) \in N_x \partial\partial S_i \cap T_x \partial S_i \cap T_x S$. Separate application of Gauss's theorem to each of the summands yields the following sum of boundary terms in addition to (51):

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

This sum then has to be added to (47). 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:

$$\int_{\partial\partial S_i \cap \partial\partial S_j} F\big((s \cdot \hat{\nu}_i)(s \cdot \hat{\mathfrak{n}}_i) + (s \cdot \hat{\nu}_j)(s \cdot \hat{\mathfrak{n}}_j)\big) \, d\mathfrak{x}, \tag{52}$$

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

This section is devoted to the geometric interpretation of our formulas for I_t and I_{tt}. It turns out that each term of the Hadamard form models a distinct geometrical effect that occurs during deformation of S. We will illustrate each of these effects by a simple geometrical example, where we compare the k-volume $I(t)$ with $I_t(0)$ and $I_{tt}(0)$.

5.1 Sensitivity of k-volumes

Of special interest and a little more concise than the general result is the case $F \equiv 1 = \mathit{const}$, which captures changes in the pure k-dimensional volume of S. First of all we note that all terms with derivatives of F drop out in (47) and we obtain the shorter formulas.

The *first shape derivative* is rather straightforward to interpret:

$$I_t(0) = \int_S \kappa \cdot n \, dx + \int_{\partial S} \hat{\nu} \cdot \nu \, dx. \tag{53}$$

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*

$$\begin{aligned} I_{tt}(0) = &\int_S \kappa \cdot (h(s,s) + v_t - 2n_x s) + K(n,n) + \langle n_x, n_x \rangle_{S \to N} \, dx \\ &+ \int_{\partial S} \hat{\nu} \cdot (h_{\partial S}(\sigma,\sigma) + v_t - 2(n+\nu)_x \sigma) + \kappa_{\partial S} \cdot (\nu + 2n)(\nu \cdot \hat{\nu}) \, d\xi. \end{aligned} \tag{54}$$

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.

Indirect normal acceleration. According to (54) the acceleration field v_t contributes to I_{tt} via the linear term

$$l(1, v_t) = \int_S \kappa \cdot v_t \, dx + \int_{\partial S} \hat{\nu} \cdot v_t \, d\xi.$$

Since $\kappa \in N_x S$ and $\hat{\nu} \in N_x \partial S$, only the normal components of v_t contribute to a change of k-volume. In addition, (54) shows terms that have a similar effect on I_{tt} as v_t, namely:

$$\int_S \kappa \cdot (h(s,s) - 2n_x s) \, dx + \int_{\partial S} \hat{\nu} \cdot (h_{\partial S}(\sigma,\sigma) - 2(n+\nu)_x \sigma) \, d\xi.$$

This suggests that these terms reflect some *acceleration* of S and ∂S into *normal direction*, caused *indirectly* by tangential movement, which contributes to the change of k-volume of S in a similar way as v_t does.

Let us discuss the contributions of $h(s,s)$ and $-2n_x s$ individually. The presence of the terms $h(s,s)$ and $h_{\partial S}(\sigma,\sigma)$ indicates that *straight* movement along a purely tangential field in the presence of curvature may result in an indirect acceleration of S and ∂S into normal direction. The resulting change of k-volume is reflected by the terms $\kappa \cdot h(s,s)$ and $\hat{\nu} \cdot h_{\partial S}(\sigma,\sigma)$.

We illustrate this by an example: let $S \subset \mathbb{R}^2$ be a *circle* around 0 with radius r_0 and unit tangent field $\hat{s}$. Its second fundamental form is known as $\hat{h}(\alpha\hat{s}, \beta\hat{s}) = \alpha\beta/r_0$. For $\tau \in \mathbb{R}$ consider the purely tangential deformation

$$\phi(t,x) = x + t\tau\hat{s}(x) = x + ts(x).$$

Since $x \cdot \hat{s}(x) = 0$ we 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 $r_{tt}(0) = \tau^2/r_0 = \hat{h}(s,s)$. This is the acceleration of S in normal direction, predicted by our formula.

The remaining terms $-2n_x s$ and $-2(n+\nu)_x\sigma$ describe that tangential transport of non-constant normal velocity also induces acceleration of S and ∂S into normal direction, indirectly. Let us point out the perfect analogy of these two terms:

$$-2n_x s = -2((I-P)v)_x Pv \quad \text{and} \quad -2(n+\nu)_x\sigma = -2((I-P_{\partial S})v)_x P_{\partial S}v.$$

For illustration consider the *horizontal line* $S = \operatorname{span}\{e_1\} \subset \mathbb{R}^2$, so $\hat{n} \equiv e_2$ and introduce cartesian coordinates $x = \xi_1 e_1 + \xi_2 e_2$. For $\tau, \eta > 0$ we define

$$\phi(t,x) := x + t(\tau e_1 + \eta\xi_1 e_2) = x + t(s + n(x)).$$

Each point of S moves to the right with tangential velocity $s = \tau e_1$ and with normal velocity $n(x) = \eta\xi_1 e_2$. We observe that $\phi(t,S)$ is the graph of the linear function

$$\xi_2 = q(t,\xi_1) = (\xi_1 - \tau t)\eta t,$$

evolving in t, where $q_t(0,\xi_1) = \eta\xi_1$ and $q_{tt}(0,\xi_1) = -2\tau\eta = -2n_x s$. This indicates an acceleration of S *downwards*, i.e., in negative normal direction.

Our considerations suggest the introduction of a *modified acceleration field* $\tilde{v}_t$ on $S \times \partial S$ as follows:

$$\tilde{v}_t(x) := \begin{cases} h(s,s) + v_t - 2n_x s & : \quad x \in S \setminus \partial S \\ h_{\partial S}(\sigma,\sigma) + v_t - 2(n+\nu)_x\sigma & : \quad x \in \partial S. \end{cases} \tag{55}$$

Now we can write the second shape derivative in (54) more concisely:

$$I_{tt}(0) = l(1,\tilde{v}_t) + \int_S K(n,n) + \langle n_x, n_x\rangle_{S\to N}\, dx + \int_{\partial S} \kappa_{\partial S}\cdot(\nu + 2n)(\nu\cdot\hat{\nu})\, d\xi, \tag{56}$$

and only three terms remain to be discussed.

Gaussian curvature. By Proposition 3.3 we can interpret the term $K(n,n)$ in (56) as a sum of increase of two-dimensional area. Recall that K describes the Gauss curvature $\hat{K}$ for $d = 3$ and $k = 2$. Together with its first order 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.

Let us illustrate the role of $\hat{K}$ with an example: let S be a *sphere* in $\mathbb{R}^3$ around 0 with radius r_0, so $\partial S = \emptyset$. For $\eta \in \mathbb{R}$ define

$$\phi(t,x) := x + t\eta\hat{n}(x) = x + tn(x).$$

Since $\hat{n}$ points in radial direction, the radius $r(t)$ of the sphere changes in time as $r(t) = r_0 + t\eta$. We compute for the surface area $I(t)$:

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

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 and confirm that they coincide with the second order expansion of $I(t)$:

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

Laplace-Beltrami operator. The term $\langle n_x, n_x\rangle_{S\to N}$ is present in (56) 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.

For illustration, let S be a relatively open subset of span$\{e_1, e_2\} \subset \mathbb{R}^3$, $\eta : S \to \mathbb{R}$ a smooth function and

$$\phi(t,x) := x + t\eta(x)e_3 = x + n(x)$$

so that $\phi(t,S)$ is the graph of $t\eta$. Then by the well known formula for the surface of graphs we obtain:

$$I(t) = \int_S \sqrt{1+t^2(\nabla_s\eta\cdot\nabla_s\eta)}\,dx = \int_S 1 + \frac{t^2}{2}(\nabla_s\eta\cdot\nabla_s\eta)\,dx + o(t^2),$$

to be compared to $I_t(0) = 0$ and

$$I_{tt}(0) = \int_S \langle n_x\cdot n_x\rangle_{S\to N}\,dx = \int_S (\nabla_s\eta\cdot\nabla_s\eta)\,dx.$$

Boundary stretch and shift. The boundary integral term $\kappa_{\partial S}\cdot(\nu+2n)(\nu\cdot\hat\nu)$ in (56) describes change of k-volume of S that is caused by a combination of shifting ∂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. We illustrate this term and the occurence of the factor 2 by two examples.

To illustrate $(\kappa_{\partial S}\cdot\nu)(\nu\cdot\hat\nu)$ let S be a *disc* in $\mathbb{R}^2$ with center 0 and radius r_0, so ∂S is a circle. For $\eta\in\mathbb{R}$ we define

$$\phi(t,x) := x + t(\eta/r_0\,x) = x + tv(x).$$

Then $r(t) = r_0 + t\eta$ and

$$I(t) = \pi r(t)^2 = \pi(r_0+t\eta)^2 = \pi r_0^2 + t\,2\pi r_0\eta + \frac{t^2}{2}2\pi\eta^2. \tag{57}$$

Using $\kappa_{\partial S} = 1/r_0\,\hat\nu$, and $v = \eta\hat\nu$ on ∂S we compute via (56) in accordance with (57):

$$I_t(0) = \int_{\partial S}\hat\nu\cdot v\,d\xi = \int_{\partial S}\eta\,d\xi = 2\pi r_0\,\eta,$$
$$I_{tt}(0) = \int_{\partial S}(\kappa_{\partial S}\cdot\nu)(\nu\cdot\hat\nu)\,d\xi = \int_{\partial S}\frac{1}{r_0}\eta\,\eta\,d\xi = 2\pi\,\eta^2.$$

To illustrate $2(\kappa_{\partial S}\cdot n)(\nu\cdot\hat\nu)$ let S be the *lateral surface of a right circular cylinder* of radius r_0 and height h_0. We choose the center line of the cylinder as $[0, h_0e_3]$, where e_3 points upwards in vertical direction. Its boundary consists of two circles of radius r_0: $\underline{\partial S}$ at height 0 and $\overline{\partial S}$ at height h_0. We expand the radius and the height of the cylinder using the deformation

$$\phi(t,x) = x + t\begin{pmatrix}\eta/r_0 & & \\ & \eta/r_0 & \\ & & \tau/h_0\end{pmatrix}x = x + tv(x), \tag{58}$$

This yields $r(t) = r_0 + \eta t$ and $h(t) = h_0 + \tau t$ for the expanded surface. Hence, its surface area can be computed as

$$I(t) = 2\pi r(t)h(t) = 2\pi(r_0+\eta t)(h_0+\tau t) = 2\pi h_0 r_0 + t\,2\pi(\eta h_0 + \tau r_0) + \frac{t^2}{2}4\pi\eta\tau.$$

We have $\kappa = 1/r_0\,\hat n$, $\hat K = 0$, and $h(s,s) = 0$ on S, $\kappa_{\partial S} = 1/r_0\,\hat n$, $\hat\nu = e_3$, $n = \eta\hat n$, and $\nu = s = \tau\hat\nu$ on $\overline{\partial S}$ and $\nu = 0$ on $\underline{\partial S}$, with which we compute via (56):

$$I_t(0) = \int_S \kappa\cdot n\,dx + \int_{\partial S}\nu\cdot\hat\nu\,d\xi = \int_S\frac{1}{r_0}\eta\,dx + \int_{\overline{\partial S}}\tau d\xi = 2\pi r_0 h_0\frac{\eta}{r_0} + 2\pi r_0\tau = 2\pi(h_0\eta + r_0\tau)$$
$$I_{tt}(0) = \int_{\overline{\partial S}}\kappa_{\partial S}\cdot(\nu+2n)(\hat\nu\cdot\nu)d\xi = 2\pi\,r_0\frac{1}{r_0}(0+2\eta)\tau = 4\pi\eta\tau.$$

An example with piecewise smooth boundary. We illustrate the significance of (52) in the presence of a boundary that is only piecewise smooth. Let S be a *solid right circular cylinder* with radius r_0, height h_0 and centerline $[0, h_0 e_3]$. Its boundary is the union of its lateral surface ∂S_L and two discs of radius r_0: its bottom $\underline{\partial S}$ at height 0 and its top $\overline{\partial S}$ at height h_0. In view of the additional terms in (52) that we have to take into account, we denote the corresponding boundaries $\overline{\partial\partial S} = \partial(\overline{\partial S})$ and $\underline{\partial\partial S} = \partial(\underline{\partial S})$, which are circles of radius r_0. As above, we expand the cylinder via the same deformation (58) as before, so that again $h(t) = h_0 + \tau t$ and $r(t) = r_0 + \eta t$. Its volume is given as:

$$I(t) = \pi r(t)^2 h(t) = \pi(r_0 + \eta t)^2(h_0 + \tau t) = \pi r_0^2 h_0 + t\pi(2r_0h_0\eta + \tau r_0^2) + \frac{t^2}{2}\pi(2h_0\eta^2 + 4r_0\tau\eta).$$

It is easy to verify that $\kappa_{\partial S_L} = 1/r_0\, \hat{\nu}_{\partial S_L}$ and $\nu = \eta\hat{\nu}_{\partial S_L}$ on ∂S_L, $\kappa_{\underline{\partial S}} = 0$ and $\nu = 0$ on $\underline{\partial S}$, and $\kappa_{\overline{\partial S}} = 0$ and $\nu = \tau\hat{\nu}_{\overline{\partial S}} = \tau e_3$ on $\overline{\partial S}$. So we can evaluate our shape derivatives, which again coincide with the exact formula, if (52) is taken into account:

$$\begin{aligned}
I_t(0) &= \int_{\partial S} \hat{\nu} \cdot \nu \, dx = \int_{\partial S_L} \eta \, dx + \int_{\overline{\partial S}} \tau \, dx = 2\pi r_0 h_0 \eta + \pi r_0^2 \tau, \\
I_{tt}(0) &= \int_{\partial S_L} (\kappa_{\partial S_L} \cdot \nu)(\nu \cdot \hat{\nu}_{\partial S_L}) \, dx + \int_{\overline{\partial\partial S}} (s\cdot\hat{\nu}_{\overline{\partial S}})(s\cdot\hat{\mathfrak{n}}_{\overline{\partial S}}) + (s\cdot\hat{\nu}_{\partial S_L})(s\cdot\hat{\mathfrak{n}}_{\partial S_L}) \, d\mathfrak{x} \\
&= 2\pi r_0 h_0 \frac{1}{r_0}(\nu\cdot\hat{\nu}_{\partial S_L})^2 + 2\pi r_0((s\cdot e_3)(s\cdot\hat{\nu}_{\partial S_L}) + (s\cdot\hat{\nu}_{\partial S_L})(s\cdot e_3)) \\
&= 2\pi h_0 \eta^2 + 2\pi r_0(\tau\eta + \eta\tau) = \pi(2h_0\eta^2 + 4r_0\tau\eta).
\end{aligned}$$

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:

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

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 shift of S by ϕ. 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:

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

In the first line we recognize the second order model F_{tt} for F in time and a mixed term $2l(F_t, v)$, where l is given by (41). This term combines first order temporal change of F and first order change of k-volume of S. Further, the first parts of the second and the third line are modified acceleration fields, discussed in Section 5.1. Using the modified acceleration field $\tilde{v}_t$ from (55) they can be summarized by $l(F, \tilde{v}_t)$. Now our formula looks more concise:

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

This form can be related to the structure theorem of the hessian, presented in [10].

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, as discussed in Section 5.1, scaled by F. 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.

We have written the integrand in the third line as a sum of two products. The first factors $(F_x\nu + F\kappa_{\partial S}{\cdot}\nu)$ and $(F_x n + F\kappa_{\partial S}{\cdot}n)$ approximate to first order the change of $\int_{\partial S} F\,d\xi$, when ∂S is 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.

5.3 Specific dimensions and codimensions

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

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 (27) 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:

$$I_t(0) = \int_{\partial S} F\theta\,d\xi, \tag{59}$$

$$I_{tt}(0) = \int_{\partial S} F(\hat{h}_{\partial S}(\sigma,\sigma) + v_t \cdot \hat{\nu} - 2\theta_x\sigma) + \theta^2(F_{\hat{\nu}} + F\hat{\kappa}_{\partial S})\,d\xi. \tag{60}$$

In $I_{tt}(0)$ we observe a modified acceleration field 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 a closed oriented hypersurface, where $\partial S = \emptyset$, we have a 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

$$n_x s \cdot \kappa = \hat{\kappa}(\eta\hat{n})_x s \cdot \hat{n} = \hat{\kappa}(\eta_x s\hat{n} \cdot \hat{n} + \eta\hat{n}_x s \cdot \hat{n}) \overset{(27)}{=} \hat{\kappa}\eta_x s.$$

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:

$$I_t(0) = \int_S \eta(F_{\hat{n}} + F\hat{\kappa})\,dx,$$

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

The first term in $I_{tt}(0)$ is again caused by a modified acceleration field. 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 [7]. However, the Laplace-Beltrami term seems to be missing there. For normal fields $v = n$ and $v_t = 0$ this formula simplifies to

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

This formula can also be found in [6] for the special case $d = 2$ (so $\hat{K} = 0$).

If S is not closed, then the boundary term in (47) must be added. However, no significant simplifications arise in this case.

Line integrals. In this case we have a unit tangent field $\hat{s}$ and we may write $v = n + \tau\hat{s}$, where $\tau = (s \cdot \hat{s})$. Also we can define the vector $n_s = n_x \hat{s}$. 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

$$I_t(0) = \int_S F_x n + F(\kappa \cdot n)\, dx + F\tau\big|_{x_0}^{x_1}.$$

By Proposition 3.3 we get $K(n, n) = 0$ and by Proposition 3.4 we obtain, setting $\tilde{n}_s := (I - P)n_s$.

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

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

$$\begin{aligned} I_{tt}(0) = &\int_S (F_n + F\kappa\cdot)(\tau^2\kappa + v_t - 2\tau n_s) + \big(F(\tilde{n}_s \cdot \tilde{n}_s) + 2F_x n(\kappa \cdot n) + F_{xx}(n, n)\big)\, dx \\ &+ \big(F_x(\nu + 2n)\tau + v_t \cdot \hat{s}\big)\big|_{x_0}^{x_1}. \end{aligned}$$

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

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:

$$\begin{aligned} I_t(0) &= F_t + F_x v, \\ I_{tt}(0) &= F_{tt} + 2F_{xt}v + F_{xx}(v, v) + F_x v_t, \end{aligned}$$

to be evaluated at x_0.

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