A structure theorem for shape functions defined on submanifolds

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Abstract

In this paper, we study shape functions depending on closed submanifolds. We prove a new structure theorem that establishes the general structure of the shape derivative for this type of shape function. As a special case we obtain the classical Hadamard-Zolésio structure theorem, but also the structure theorem for cracked sets can be recast into our framework. As an application we investigate several unconstrained shape functions arising from differential geometry and fracture mechanics.

1 Introduction

The classical structure theorem \cite{4,5} for real valued shape functions plays a crucial role in shape optimization both from the numerical and the theoretical point of view. Given a shape function $J$, the structure theorem states that the shape derivative $X \mapsto \frac{d}{d}(\Omega)(X)$ at an open or closed set $\Omega$ has support in the boundary $\partial \Omega$. This is a consequence of Nagumo’s invariance theorem for ordinary differential equation. If the boundary of $\Omega$ is additionally of class $C^{k+1}$, $k \geq 0$, and $X \mapsto \frac{d}{d}(\Omega)(X)$ is linear and continuous, then it can be shown that there is a linear and continuous function $g : C^k(\partial \Omega) \to \mathbb{R}$ such that

$$\frac{d}{d}(\Omega)(X) = g(X|_{\partial \Omega} \cdot \nu),$$

(1.1)

where $\nu$ a normal vector field along $\partial \Omega$.

In \cite{10} the structure theorem was extended to subsets $\Omega$ of the plane that have a (smooth) fissure/crack of codimension one. A smoothly cracked set $\Omega$ in the plane is a smooth set $\Omega$ from which we remove the image $\Sigma := \gamma([0, 1])$ of an embedded $C^{k+1}$ curve $\gamma : [0, 1] \to \mathbb{R}^2$. In other words $\Omega := \Omega \setminus \Sigma$. The set $\Omega$ is no longer of class $C^{k+1}$ and hence the classical structure theorem does not apply. However, it can be shown that in this case the structure of the shape derivative is

$$\frac{d}{d}(\Omega)(X) = h(X|_{\Sigma} \cdot n) + a\gamma'(0) \cdot X_{\gamma(0)} + b\gamma'(1) \cdot X_{\gamma(1)},$$

(1.2)

where $h : C^k(\Sigma) \to \mathbb{R}^2$ is linear and continuous and $a, b$ are two real numbers and $n$ denotes the normal vector field along $\Sigma$. In \cite{12} this theorem was extended to sets $\Omega \subset \mathbb{R}^d$, but still with a crack of codimension one.

Recently, in \cite[18, p. 3 Theorem 1.3]{18} it was shown that if $\Omega$ has merely finite perimeter, then it is still possible to obtain a formula like (1.1). But it is clear that in this case a normal vector field is
not readily available anymore. However, one can use one of the generalisations of the normal vector field from geometric measure theory. Then the structure theorem reads

\[ dJ(\Omega)(X) = g(X|_{\Gamma^*} \cdot \nu_*) \]  

(1.3)

where \( \nu_* \) is the generalized normal and \( \Gamma^* := \partial^* \Omega \) denotes the reduced boundary of \( \partial \Omega \). The cracks and corners are hidden in the notion of generalised normal and the function \( g \) is defined on a bigger space than \( C^k(\Gamma) \).

In this paper, we prove a structure theorem for shape functions defined on closed submanifolds of \( \mathbb{R}^d \) with or without boundary. As a first side product we are now able to extend the structure theorem of \([12]\) to arbitrary codimensions of cracks. A second striking consequence is that our new structure theorem gives the structure of many other functionals occurring in differential geometry. The proof is very different from the one given in \([12]\) and thus also contributes in giving a new perspective on the subject.

In Section 2, we briefly recall some facts about submanifolds with boundary and introduce shape functions and the Eulerian semi-derivative.

In Section 3, we give a detailed reinterpretation of Nagumo’s invariance condition for the case of submanifolds. This version requires some notions from differential geometry.

In Section 4, we are going to revisit the structure theorem for smooth domains and give a slightly different proof, than what is known in the literature as this will be useful for our further study.

In Section 5, the main result is proved by first studying a general splitting of vector fields on submanifolds.

In Section 6, we are presenting several examples.

2 Preleminaries

2.1 Submanifolds of \( \mathbb{R}^d \) with boundary

We begin with the definition of a submanifold \( M \) of \( \mathbb{R}^d \), \( d \geq 1 \). Let us denote the open half space in \( \mathbb{R}^d \) by

\[ \mathbb{H}^d := \{x \in \mathbb{R}^d | x = (x_1, \ldots, x_d), x_d > 0\}. \]

The boundary of the half space \( \partial \mathbb{H}^d = \mathbb{R}^{d-1} \times \{0\} \) is identified with \( \mathbb{R}^{d-1} \). When \( U \) is an open subset of \( \mathbb{H}^d := \mathbb{H}^d = \mathbb{R}^{d-1} \times [0, \infty) \), then we define its interior and boundary as \( \text{int}(U) := U \cap \mathbb{H}^d \) and \( \partial U := U \cap \partial \mathbb{H}^d \), respectively. Note that the boundary \( \partial U \) does not coincide with the topological boundary of \( U \).

**Definition 2.1.** Let \( 1 \leq m \leq d \). A subset \( N \) of \( \mathbb{R}^d \) is called \( m \)-dimensional \( C^k \)-submanifold of \( \mathbb{R}^d \), \( k \geq 1 \), if for each point \( p \) in \( N \) there is an open set \( U \) of \( \mathbb{R}^d \) containing \( p \), an open set \( V \) of \( \mathbb{R}^d \), and a \( C^k \)-diffeomorphism \( \varphi : U \to V \), such that

\[ \varphi(U \cap N) = V \cap (\mathbb{R}^m \times \{0\}). \]

Here, \( 0 = (0, \ldots, 0)^\top \in \mathbb{R}^{d-m} \). The tuple \( (U \cap N, \varphi) \) is called chart and \( \varphi^{-1} \) is called parametrisation.
Definition 2.2 (Submanifolds with boundary). A subset $M$ of an $n$-dimensional $C^k$-submanifold $N$ is called a \textbf{$m$-dimensional $C^k$-submanifold of $N$ with boundary} if for every $p$ in $M$ there is a chart $(U, \varphi)$ of $N$ around $p$, such that

$$\varphi(U \cap M) = \varphi(U) \cap (\mathbb{H}^m \times \{0\}) \subset \mathbb{R}^n.$$ 

Here, $p$ is called the \textbf{boundary point} if $\psi(p)$ lies in $\partial \mathbb{H}^m := \partial \mathbb{H}^m \times \{0\}$. The set of boundary points is denoted by $\partial M$ and we define the \textbf{interior} of $M$ by $\text{int}(M) := M \setminus \partial M$. In order to avoid any confusion, we are going to denote by $\partial M$ the boundary in the above sense and by $\text{fr}(M)$ ($\text{fr} = \text{frontier}$) the topological boundary of the set $M$.

**Remarks 2.3.**

(a) The boundary $\partial M$ is a $m-1$-dimensional submanifold without boundary, that is, $\partial(\partial(M)) = \emptyset$. The interior $\text{int}(M)$ is a $m$-dimensional submanifold without boundary.

(b) Note that the image $\varphi(U \cap M)$ is not open in $\mathbb{R}^d$, but relatively open.

(c) Open subsets $U$ of $\mathbb{R}^d$ are $C^\infty$-submanifolds without boundary. (Note that they do have a topological boundary.)

(d) One and two dimensional submanifolds of $\mathbb{R}^d$ are called \textbf{embedded curve} and \textbf{embedded surface}, respectively. Analogously $d-1$ dimensional submanifolds of $\mathbb{R}^d$ are \textbf{embedded hypersurfaces}.

(f) It is always possible to replace the open set $U$ by another open set $\tilde{U}$ in such a way that $\varphi(\tilde{U})$ is the unit ball $\mathbb{B}_\tilde{U}$ in $\mathbb{R}^d$ centered at the origin.

We introduce the tangent space at a point $p$ of $M$ by $T_p M := d_{\varphi(p)}(\varphi^{-1})(\mathbb{R}^m)$ and similarly the tangent space of $\partial M$ at a point $p$ is given by $T_p(\partial M) := d_{\varphi(p)}(\varphi^{-1})(\mathbb{R}^{m-1})$. This can also be expressed in a different way by ($q = \varphi(p)$)

$$T_p M = \text{span}\{\partial_{x_1} \varphi^{-1}(q), \ldots, \partial_{x_m} \varphi^{-1}(q)\}$$

$$T_p(\partial M) = \text{span}\{\partial_{x_1} \varphi^{-1}(q), \ldots, \partial_{x_{m-1}} \varphi^{-1}(q)\}.$$ 

Here, $\mathbb{R}^m \subset \mathbb{R}^d$ has to be understood as the image of the natural injection $x \mapsto (x, 0) \in \mathbb{R}^d$. Setting $T_p^\pm M := d_{\varphi(p)}(\varphi^{-1})(\pm \mathbb{H}^m)$, we have for $p \in M$ that $T_p M = T_p^+ M \cup T_p^- M$ and $T_p(\partial M) = T_p^+ M \cap T_p^- M$. We call the disjoint collection $TM := \bigcup_{p \in M} T_p M$ of tangent spaces also tangent bundle of $M$. The tangent bundle is a smooth $2m$-dimensional manifold if $M$ is smooth. Similarly, $T(\partial M)$ denotes the $2(m-1)$-dimensional tangent bundle at $\partial M$. Note that for $p \in \partial M$ the tangent space $T_p(\partial M)$ is a $m-1$-dimensional subspace of the $m$-dimensional vector space $T_p M$. As such $T_p(\partial M)$ is also an inner product space with Euclidean scalar product of $\mathbb{R}^d$. Consequently there are exactly two unit vectors $\pm \nu(p)$ in $T_p M$ that are normal to $T_p(\partial M)$. We call $\nu$ outward-pointing unit vector field if for all $p \in \partial M$, $\nu(p) \in T_p^+ M$; cf. [1]. In the sequel, we always denote the outward-pointing unit normal field by $\nu$. Its uniqueness and existence along $\partial M$ is guaranteed by [19, p. 346 Prop. 13.26].
2.2 Eulerian semi-derivative

Let \( X : \mathbb{R}^d \to \mathbb{R}^d \) be a vector field satisfying a global Lipschitz condition: there is a constant \( L > 0 \) such that
\[
|X(x) - X(y)| \leq L|x - y| \quad \text{for all } x, y \in \mathbb{R}^d.
\]

Then we associate with \( X \) the flow \( \Phi_t \) by solving for all \( x \in \mathbb{R}^d \)
\[
\frac{d}{dt} \Phi_t(x) = X(\Phi_t(x)) \quad \text{on } [-\tau, \tau], \quad \Phi_0(x) = x.
\]

The global existence of the flow is ensured by the theorem of Picard-Lindelöf and hence \( \Phi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d \).

Subsequently, we restrict ourselves to a special class of vector fields, namely \( C^k \)-vector fields with compact support in some fixed set. To be more precise for a fixed open set \( D \subset \mathbb{R}^d \), we consider vector fields belonging to \( C^k_c(D, \mathbb{R}^d) \). We equip the space \( C^k_c(D, \mathbb{R}^d) \) respectively \( C^\infty_c(D, \mathbb{R}^d) \) with the topology induced by the following family of semi-norms: for each compact \( K \subset D \) and multi-index \( \alpha \in \mathbb{N}^d \) with \( |\alpha| \leq k \) we define \( \| f \|_{K, \alpha} := \sup_{x \in K} |\partial^\alpha f(x)| \). With this family of norms the space \( C^k_c(D, \mathbb{R}^d) \) becomes a locally convex vector space.

Next, we recall the definition of the Eulerian semi-derivative.

**Definition 2.4.** Let \( D \subset \mathbb{R}^d \) be an open set. Let \( J : \Xi \to \mathbb{R} \) be a shape function defined on a set \( \Xi \) of subsets of \( D \) and fix \( k \geq 1 \). Let \( \Omega \in \Xi \) and \( X \in C^k_c(D, \mathbb{R}^d) \) be such that \( \Phi_t(\Omega) \in \Xi \) for all \( t > 0 \) sufficiently small. Then the Eulerian semi-derivative of \( J \) at \( \Omega \) in direction \( X \) is defined by
\[
dJ(\Omega)(X) := \lim_{t \searrow 0} \frac{J(\Phi_t(\Omega)) - J(\Omega)}{t}.
\]

(i) The function \( J \) is said to be shape differentiable at \( \Omega \) if \( dJ(\Omega)(X) \) exists for all \( X \in C^\infty_c(D, \mathbb{R}^d) \) and \( X \mapsto dJ(\Omega)(X) \) is linear and continuous on \( C^\infty_c(D, \mathbb{R}^d) \).

(ii) The smallest integer \( k \geq 0 \) for which \( X \mapsto dJ(\Omega)(X) \) is continuous with respect to the \( C^k_c(D, \mathbb{R}^d) \)-topology is called the order of \( dJ(\Omega) \).

The set \( D \) in the previous definition is usually called hold-all domain or hold-all set or universe.

2.3 Quotient space

Henceforth, for all structure theorems to be considered, we define for an arbitrary set \( A \subset D \) the linear space
\[
T^k(A) := \{ X \in C^k_c(D, \mathbb{R}^d) | X = 0 \text{ on } A \}.
\]

By definition \( T^k(A) \subset C^k_c(D, \mathbb{R}^d) \) and \( T^k(A) \) is closed. We introduce an equivalence relation on \( C^k_c(D, \mathbb{R}^d) \) by
\[
X \sim Y, \quad X, Y \in C^k_c(D, \mathbb{R}^d) \quad \Leftrightarrow \quad X = Y \text{ on } A
\]
and denote the set of equivalence classes and its elements by \( Q^k(A) := C^k_c(D, \mathbb{R}^d)/T^k(A) \) and \([X] \), respectively.
We denote by $\tilde{J}_A$ the restriction mapping of vector field belonging to $C^k_c(D, \mathbb{R}^d)$ to mappings $A \rightarrow \mathbb{R}^d$, that is,

$$\tilde{J}_A : C^k_c(D, \mathbb{R}^d) \rightarrow A^{\mathbb{R}^d}, \quad X \mapsto X|_A,$$

where $A^{\mathbb{R}^d}$ denotes the space of all mappings from $A$ into $\mathbb{R}^d$. The mapping $\tilde{J}_A$ induces the mapping $\tilde{J}_A : Q^k(A) \rightarrow \mathbb{R}$ as depicted in Figure 2.3. Hence by definition $\tilde{J}_A = \tilde{J}_A \circ \pi$.

The semi-norms on $C^k_c(D, \mathbb{R}^d)$ induce semi-norms on the quotient space $\| [X] \|_{K,\alpha} := \inf_{\tilde{X} \in T^k(A)} \| X - \tilde{X} \|_{K,\alpha} = \inf_{\xi \in C^k_c(D,\mathbb{R}^d)} \{ \| \xi \|_{K,\alpha} : \xi = X \text{ on } A \}$.

Let $f : C^k_c(D, \mathbb{R}^d) \rightarrow \mathbb{R}$ be a linear function respecting the equivalence relation (2.3), that is, if $X \sim Y$ then it follows $f(X) = f(Y)$. Then $f : C^k_c(D, \mathbb{R}^d) \rightarrow \mathbb{R}$ is continuous if and only if its induced function $\tilde{f} : Q^k(A) \rightarrow \mathbb{R}$ is continuous. So if $f$ is continuous, then for every compact $K \subset \mathbb{R}^d$ there is a constant $C > 0$ such that for all $\psi \in T^k(A)$ and all multi-indicies $\alpha$ with $|\alpha| \leq k$ we have

$$|\tilde{f}([X])| = |f(X)| = |f(X - \psi)| \leq C \| X - \psi \|_{K,\alpha}$$

and hence $|\tilde{f}([X])| \leq C \| [X] \|_{K,\alpha}$. Later we will see that the shape derivative $dJ(\Omega)$ in an open or closed set $\Omega \subset \mathbb{R}^d$ respects the above equivalence relation. This will follow from Nagumo’s theorem considered in the next section.

### 3 Nagumo’s theorem

#### 3.1 Nagumo’s invariance condition

Nagumo’s theorem states roughly the following: if a given vector field defined on some closed subset of $\mathbb{R}^d$ is tangent to that set at each point, then the solutions of the associated ordinary differential equation cannot leave this closed set.

In order to make this tangency requirement precise, we define for a given subset $K \subset \mathbb{R}^d$ the Bouligand contingent cone to $K$ at $x \in \overline{K}$:

$$T_K(x) := \{ v \in \mathbb{R}^d \mid v = \lim_{n \rightarrow \infty} (x_n - x)/t_n \text{ for some } x_n \rightarrow_D x, \ t_n \searrow 0 \}.$$ 

Here $x_n \rightarrow_D x$ indicates that $x_n \in D$ and $x_n \rightarrow x$ as $n \rightarrow \infty$. The following result is Nagumo’s classical theorem [2, Theorem 2, p. 180]; cf. also [5, 20].
Theorem 3.1. Let $K$ be a closed subset of a Hilbert space $H$ and $f$ a continuous function from $K$ into $H$ satisfying the tangential condition $\forall x \in K, \ f(x) \in T_K(x)$. Then for each $x_0 \in K$, there exists $T > 0$ such that the ODE $x'(t) = f(x(t)), x(0) = x_0$ has a viable trajectory on $[0, T]$.

By “viable solution” we means that $x(t) \in K$ for all $t \in [0, T]$.

Corollary 3.2. Let $K \subset \mathbb{R}^d$ be a closed set and $X : K \rightarrow \mathbb{R}^d$ a vector field satisfying a global Lipschitz condition. Assume that for all $x \in K$ we have $\pm X(x) \in T_K(x)$. Then the flow $\Phi_t$ of $X$ is for each $t$ in $[-\tau, \tau]$ a bijection from $K$ onto $K$. In particular, $\Phi_t(K) = K$ for all $t \in \mathbb{R}$.

Proof. By Kirszbraun’s theorem (cf. [16, 25, 26]) we may extend the vector field $X : K \rightarrow \mathbb{R}^d$ to a globally Lipschitz continuous vector field $\tilde{X} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ having the same Lipschitz constant and satisfying $X = \tilde{X}$ on $K$. The Picard-Lindelöf theorem ensures that the flow $\Phi_t$ is globally defined, that is, $\Phi : \mathbb{R} \times \mathbb{R}^d \rightarrow \mathbb{R}^d$. Applying Theorem 3.1 to $K$ yields $\Phi_t(K) \subset K$ for all $t$ in $[0, \infty)$. On the other hand we also have $\Phi_{-t}(K) \subset K$ for all $t$ in $[0, \infty)$ as $-X(x) \in T_K(x)$ for all $x$ in $K$. Together we obtain $K = \Phi_t(\Phi_{-t}(K)) \subset \Phi_t(K)$ for all $t \in \mathbb{R}$ and thus $\Phi_t(K) = K$.

Corollary 3.3. Let $D \subset \mathbb{R}^d$ be an open set with $C^k$-boundary, $k \geq 1$. Suppose that $X : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a vector field satisfying a global Lipschitz condition and $X \cdot \nu = 0$ on $\partial D$. Then $\Phi_t(D) = D$ and $\Phi_t(\partial D) = \partial D$ for all $t$ in $[-\tau, \tau]$.

Proof. We have for all $x \in \partial D$ the inclusion $T_xD \subset T_D(x)$. For all interior points $x \in D$ it is easily checked that $T_D(x) = \mathbb{R}^d$. So the assumptions of Corollary 3.2 are satisfied. Since $D$ is open we have $\overline{D} = \partial D \cup D$. Moreover, since $\partial D$ is closed and $\pm X(x) \in T_{\partial D}(x)$ for all $x \in \partial D$, we also have $\Phi_t(\partial D) = \partial D$ and it follows that $\Phi_t(D) = D$.

3.2 Nagumo’s theorem for submanifolds

In this section we give a proof of the following version of Nagumo’s theorem needed for the further analysis.

Proposition 3.4. Let $M$ be a closed $m$-dimensional $C^k$-submanifold of $\mathbb{R}^d$, $k \geq 1$. Suppose we are given a vector field $X : \mathbb{R}^d \rightarrow \mathbb{R}^d$ of class $C^1$ with compact support satisfying

$$
X_p \in T_p(\text{int}(M)) \quad \text{for all } p \in T_p(\text{int}(M)),
$$

$$
X_p \in T_p(\partial M) \quad \text{for all } p \in \partial M.
$$

Then the flow $\Phi_t = \Phi_t^X$ of $X$ is a $C^k$-diffeomorphism $\Phi_t : M \rightarrow M$ and thus in particular

$$
\Phi_t(\text{int}(M)) = \text{int}(M) \quad \text{for all } t
$$

$$
\Phi_t(\partial M) = \partial M \quad \text{for all } t.
$$

Proof. We first show that for each $p$ in $M$ and each curve $\alpha$ solving

$$
\alpha'(t) = X(\alpha(t)) \quad \text{in } [-\tau, \tau], \ \alpha(0) = p \quad \Rightarrow \quad \alpha(t) \in M \quad \text{for all } t \in [-\tau, \tau].
$$

For each $p$ in $\partial M$, there exist an open neighborhood $U$ of $p$ in $\mathbb{R}^d$, an open set $V$ in $\mathbb{R}^d$ and $C^k$-diffeomorphism $\varphi : U \rightarrow V$, such that $\varphi(U \cap \partial M) = V \cap (\mathbb{R}^{m-1} \times \{0\})$. Let $\alpha$ solve $\alpha'(t) = X(\alpha(t)), \alpha(0) = p$, and define $\tilde{\alpha}(t) := \varphi(\alpha(t))$ and

$$
\tilde{\alpha}(t) := \varphi(\alpha(t)), \quad \tilde{X}(y) := \varphi^{-1}(\partial \varphi X)(y).
$$
Then we compute
\[
\tilde{\alpha}'(t) = \partial\varphi(\alpha(t))\alpha'(t) = \partial\varphi(\alpha(t))X(\alpha(t)) = \tilde{X}(\tilde{\alpha}(t))
\]  
for all \(t\). We have that \(\{v_i := d\varphi^{-1}(e_i), i = 1, \ldots, m - 1\}\) is a basis of \(T_p(\partial M)\) and thus we may write locally
\[
X_p = \sum_{i=1}^{m-1} \alpha_{i,p}v_{i,p} \quad \Rightarrow \quad \tilde{X} \circ \varphi = d_p\varphi(X) = \sum_{i=1}^{m-1} \alpha_{i,p}e_i,
\]
where \(\{e_1, \ldots, e_{m-1}\}\) denotes the canonical basis of \(\mathbb{R}^{m-1}\). But this means that the last \(d - m + 1\) components of \(\tilde{X}\) are zero. In view of (3.5) we obtain \(\tilde{\alpha}'_{m,p} = \cdots = \tilde{\alpha}'_{d,p} = 0\) and taking into account the initial condition we get \(\tilde{\alpha}_{m,p} = \cdots = \tilde{\alpha}_{d,p} = 0\). Define the subinterval \(T := \{t : \alpha(t) \in U \cap \partial M\}\) of \([-\tau, \tau]\). We obtain
\[
\tilde{\alpha}(t) \in \varphi(U) \cap (\mathbb{R}^{m-1} \times \{0\}) \quad \text{for all } t \in T,
\]
which is equivalent to \(\alpha(t) \in \partial M\) for all \(t \in T\). This shows that the curve stays on the boundary of \(M\) as long we are in the chart \(U\). However, if we enter another chart, we can proceed the same argumentation as above and obtain \(T = [-\tau, \tau]\). In a similar way, we may show that if \(p \in \text{int}(M)\) and \(\alpha : [-\tau, \tau] \to M\) is a \(C^1\)-curve, such that \(p = \alpha(0)\), then \(\alpha([-\tau, \tau]) \subset \text{int}(M)\). It follows \(\Phi_t(\partial M) \subset \partial M\) and \(\Phi_{-t}(\partial M) \subset \partial M\), which implies \(\partial M = \Phi_t(\Phi_{-t}(\partial M)) \subset \Phi_t(\partial M)\) and thus \(\Phi_t(\partial M) = \partial M\) for all \(t\). In the same we obtain \(\Phi_t(\text{int}(M)) = \text{int}(M)\) for all \(t\). Now the rest of the statement is clear.

**Remark 3.5.** The invariance \(\Phi_t(M) = M\) can also be proved by directly using Theorem 3.1. It can be shown that for all \(p \in \text{int}(M)\)
\[
\pm X_p \in T_{\text{int}(M)}(x) \iff X_p \in T_p(\text{int}(M))
\]

and for all \(p \in \partial M\)
\[
\pm X_p \in T_M(x) \iff \pm X_p \in T^+_p M \iff X_p \in T^+_p M \cap T^-_p M = T_p(\partial M).
\]

So in fact the conditions (3.1)-(3.2) are reformulations of: for all \(p \in M, \pm X_p \in T_M(x)\). However, in order to give a self contained presentation we gave a direct proof.

**Remarks 3.6.**

(a) The hypothesis that \(M\) be (relatively) closed can not be dropped as can be seen by considering open subsets \(\Omega \subset \mathbb{R}^d\) as submanifolds equipped with the identity chart. In this case the conclusion of the previous proposition does not hold.

(b) Note that the conditions (3.1)-(3.2) state that the map \(p \mapsto X_p\) defines a vector field (smooth section of the tangent bundle) \(X : M \to TM\) such that its restriction to \(\partial M\) is also a vector field on \(\partial M\), that is, \(X : \partial M \to T(\partial M)\). Note that this is not the case in general.

(c) The case \(m = d\) corresponds to the case of the closure of an open set \(M\) in \(\mathbb{R}^d\) with \(C^k\)-boundary \(\partial M = \text{fr}(M)\). The conditions (3.1)-(3.2) reduce to \(X_p \cdot \nu_p = 0\) for all \(p \in \partial M\), where \(\nu\) is the inward pointing normal vector along \(\partial M\). Indeed, for all \(p \in \text{int}(M)\), we have \(X_p \in T_p M = \mathbb{R}^d\) which is always true and for all \(p \in \partial M\), we have \(X_p \in T_p(\partial M)\) if and only if \(X_p \cdot \nu_p = 0\).
(d) Let \( M \) be simply connected. In the case \( m = 1 \) the manifold \( M \) can be described by the image of an embedded curve in \( \mathbb{R}^d \). Let \( \gamma : [a, b] \to \mathbb{R}^d \) be such a curve and put \( M := \gamma([a, b]) \).
Then \( \partial M = \{\gamma(a), \gamma(b)\} \) and the tangent space at \( \gamma(a) \) and \( \gamma(b) \) is simply the zero space, that is, \( T_{\gamma(a)}(\partial M) = T_{\gamma(b)}(\partial M) = \{0\} \). Since \( T_{\gamma(a)}(\partial M)^\perp \oplus T_{\gamma(a)}(\partial M)^\perp = T_{\gamma(a)}(\partial M) \) we obtain \( \nu(a) = \gamma'(a)/|\gamma'(a)| \) and similarly \( \nu(b) = -\gamma'(b)/|\gamma'(b)| \). Compare also Section 6 and [9, 10] for the special case \( m = 1 \) and \( d = 2 \).

4 The classical structure theorem revisited

The following theorem is commonly known as structure theorem; cf. [5, Thm. 3.6, Cor. 1, pp. 479–481]. It gives the general structure of first order shape derivatives of shape functions defined on open or closed subsets \( \Omega \) of \( \mathbb{R}^d \). We make use of the notation and material introduced in Subsection 2.3.

**Theorem 4.1** (General case). Let the hold-all \( D \subset \mathbb{R}^d \) be open and bounded. Let \( \Omega \) be an open or closed set \( \Omega \subset D \) with boundary \( \Gamma := \text{fr}(\Omega) \). Fix \( 1 \leq k < \infty \). Suppose that the Eulerian semi-derivative \( dJ(\Omega)(X) \) exists for all \( X \in C^k_c(D, \mathbb{R}^d) \).

(i) In general we have \( dJ(\Omega)(X) = 0 \) for all \( X \in C^k_c(D, \mathbb{R}^d) \) with \( X = 0 \) on \( \Gamma \).

(ii) If \( X \mapsto dJ(\Omega)(X) \) is linear, then there is a linear mapping \( \tilde{g} : \text{im}(\tilde{\mathcal{J}}_{\Gamma}) \to \mathbb{R} \) such that
\[
dJ(\Omega)(X) = \tilde{g}(X|_{\Gamma}) \tag{4.1}
\]
for all \( X \in C^k_c(D, \mathbb{R}^d) \), where \( \text{im}(\tilde{\mathcal{J}}_{\Gamma}) := \{\tilde{\mathcal{J}}_{\Gamma}(X) \mid X \in Q^k(\Gamma)\} \) denotes the image of \( \tilde{\mathcal{J}}_{\Gamma} \).

(iii) If \( \Omega \) is of class \( C^k \) and \( dJ(\Omega) \) is of order \( k \geq 1 \), then \( \text{im}(\mathcal{J}_{\Gamma}) = C^k(\Gamma, \mathbb{R}^d) \) and \( \tilde{g} : C^k(\Gamma, \mathbb{R}^d) \to \mathbb{R} \) is a continuous functional.

**Proof.** (i) Let \( X \in C^k_c(D, \mathbb{R}^d) \) be such that \( X = 0 \) on \( \text{fr}(\Omega) \). If \( \Omega \) is closed, then \( \pm X(x) \in T_{\Omega}(x) \) for all \( x \in \Gamma \) by definition and obviously \( \pm X(x) \in T_{\Omega}(x) = \mathbb{R}^d \) for all \( x \in \text{int}(\Omega) \). So it follows from Corollary 3.2 that \( \Phi_t(\Omega) = \Omega \) for all \( t \). On the other hand if \( \Omega \) is open, then it follows from Corollary 3.3 that \( \Phi_t(\Omega) = \Omega \) for all times \( t \). So in either cases \( dJ(\Omega)(X) = 0 \) for all \( X \in C^k_c(D, \mathbb{R}^d) \) with \( X = 0 \) on \( \Gamma \).

(ii) Let \( \Omega \) be an open or closed subset of \( \mathbb{R}^d \) and fix an integer \( k \geq 1 \). The set \( T^k(\Gamma) \) is a closed subspace of the vector space \( C^k_c(D, \mathbb{R}^d) \). Accordingly, the quotient \( Q^k(\Gamma) := C^k_c(D, \mathbb{R}^d)/T^k(\Gamma) \) is well-defined. By item (i) and the linearity of \( X \mapsto dJ(\Omega)(X) \) the induced mapping \( dJ(\Omega) : Q^k(\Gamma) \to \mathbb{R} \) is well-defined. We define the function \( \tilde{g} : \text{im}(\tilde{\mathcal{J}}_{\Gamma}) \to \mathbb{R} \) by the following commuting diagram.

\[
\begin{array}{ccc}
C^k_c(D, \mathbb{R}^d) & \xrightarrow{\pi} & \text{im}(\tilde{\mathcal{J}}_{\Gamma}) \\
\downarrow \mathcal{J}_{\Omega} \quad \downarrow \tilde{\mathcal{J}}_{\Gamma} & & \downarrow \tilde{g} \\
Q^k(\Gamma) & \xrightarrow{\tilde{\mathcal{J}}_{\Gamma}} & \text{im}(\tilde{\mathcal{J}}_{\Gamma}) \\
\end{array}
\]
By definition $\tilde{g} \circ \tilde{3}_\Gamma = dJ(\Omega)$. Now $\tilde{3}_\Gamma$ is injective and hence invertible on $\text{im}(\tilde{3}_\Gamma)$. Therefore we obtain $\tilde{g} = dJ(\Omega) \circ \tilde{3}_\Gamma^{-1}$ and by definition $dJ(\Omega)(X) = \tilde{g}(X|_\Gamma)$.

(ii) Now suppose that $\Gamma = \text{fr}(\Omega)$ is of class $C^k$, $k \geq 1$. Denote by $E : C^k(\Gamma, \mathbb{R}^d) \rightarrow C^k(D, \mathbb{R}^d)$ the extension operator. Then it is readily seen that $\tilde{3}^{-1}_\Gamma = \pi \circ E$, so that $\tilde{3}_\Gamma : Q^k(\Gamma) \rightarrow C^k(\Gamma, \mathbb{R}^d)$ is surjective. Hence we get $\text{im}(\tilde{3}_\Gamma) = C^k(\Gamma, \mathbb{R}^d)$. From this it follows that $\tilde{g}$ is a linear and continuous functional on $C^k(\Gamma, \mathbb{R}^d)$.

Nagumo’s theorem allows us to show that the distribution given by (4.1) depends explicitly on normal perturbations $X \cdot \nu$ if we require the boundary to be smoother.

**Corollary 4.2** (Smooth case). Let $\Omega$ be open in $\mathbb{R}^d$ with a compact $C^{k+1}$-boundary $\Gamma := \text{fr}(\Omega)$, $1 \leq k < \infty$. Suppose that $J$ is shape differentiable at $\Omega$ and that $dJ(\Omega)$ is of order $k$. Then there exists a linear and continuous function $g : C^k(\Gamma) \rightarrow \mathbb{R}$, such that

$$dJ(\Omega)(X) = g(X|_\Gamma \cdot \nu) \quad \text{for all } X \in C^k_c(D, \mathbb{R}^d).$$

(4.2)

**Proof.** As $\Gamma := \text{fr}(\Omega)$ is of class $C^k$, $k \geq 1$, we know by Theorem 4.1 that there is a linear and continuous functional $\tilde{g} : C^k(\Gamma, \mathbb{R}^d) \rightarrow \mathbb{R}$, such that

$$dJ(\Omega)(X) = \tilde{g}(X|_\Gamma) \quad \text{for all } X \in C^k_c(D, \mathbb{R}^d).$$

(4.3)

We split $X$ into normal and tangential part along $\Gamma$, that is, $X|_\Gamma = X_t + (X|_\Gamma \cdot \nu)\nu$, where $\nu$ is the normal vector along $\Gamma$ and $X_t := X|_\Gamma - (X|_\Gamma \cdot \nu)\nu$. As the boundary $\Gamma$ is of class $C^{k+1}$ the normal $\nu$ is of class $C^k(\Gamma, \mathbb{R}^d)$. Then it follows from Corollary 3.3 that $dJ(\Omega)(X) = 0$ for all $X$ in $C^k_c(D, \mathbb{R}^d)$ with $X \cdot \nu = 0$ on $\Gamma$. Therefore extending $\nu$ to a function $\tilde{\nu} \in C^k_c(D, \mathbb{R}^d)$ and defining $\tilde{X}_t := X + (\tilde{\nu} \cdot X)\tilde{\nu}$ shows that $0 = dJ(\Omega)(\tilde{X}_t) = g(X_t)$. So inserting $X$ into (4.1), we find

$$dJ(\Omega)(X) = \tilde{g}(X_t) + \tilde{g}((X|_\Gamma \cdot \nu)\nu) = \tilde{g}((X|_\Gamma \cdot \nu)\nu).$$

(4.4)

The mapping $g(\nu) := \tilde{g}(\nu\nu)$ is continuous on $C^k(\Gamma)$.

**Remarks 4.3.**

(a) Corollary 4.2 is usually referred to as structure theorem.

(b) If $g$ in Theorem 4.2 belongs to $L_1(\Gamma)$, then we have the typical boundary expression

$$dJ(\Omega)(X) = \int_\Gamma g X \cdot \nu \, ds.$$  

(4.5)

This expression of the derivative is usually referred to as Hadamard or Hadamard-Zolésio formula.

(c) It is important to note that if one wants a formula like (4.2) for the shape derivative, then the smoothness of the boundary $\text{fr}(\Omega)$ has to be one order higher than the order $k$ of $dJ(\Omega)$. The reason is that in order to have the unit normal vector field in $C^k$, we need the boundary $\text{fr}(\Omega)$ to be of class $C^{k+1}$. However, to obtain that the derivative actually “lives” on the boundary it is no regularity on the boundary necessary. In less regular situations, that is, when $\Omega$ has less regularity, it is still possible to obtain a formula in the spirit of (4.2). However, this requires notions from geometric measure theory; cf. [18].
5 Structure theorem for $C^k$-submanifold

In this section, we study the structure of the shape derivative of real-valued shape functions

$$J : \Xi \to \mathbb{R}, \quad M \mapsto J(M),$$

where $\Xi \subset \mathcal{A}_m^k$, $1 \leq k, m < \infty$, is some admissible set and

$$\mathcal{A}_m^k = \{ M \subset \mathbb{R}^d | M \text{ is closed and bounded } m\text{-dimensional } C^k\text{-submanifold of } \mathbb{R}^d \}.$$ 

5.1 Splitting of vector fields

Let $M$ be a $m$-dimensional closed and bounded $C^k$-submanifold of $\mathbb{R}^d$. We use the notation $\mathcal{X}^k(M) := \{ X : M \to TM | X \text{ is of class } C^k \}$ for the space of $C^k$-vector fields on $M$. Similarly, $\mathcal{X}_\perp^k(M)$ denotes the normal fields along $M$. We introduce the orthogonal projection $p_{T_pM} : T_p\mathbb{R}^d \to T_pM$ by

$$(p_{T_pM}(X) - X, V) = 0 \quad \text{for all } V \in T_pM.$$ 

Then defining $p_{T_pM}^\perp(x) := x - p_{T_pM}(x)$ we have $\ker p_{T_pM} = \operatorname{im} p_{T_pM}^\perp = (T_pM)^\perp$. Note that the projection depends on $p \in M$ as the tangent space varies when $p$ changes.

Now given a function $X \in C^k(M, \mathbb{R}^d)$, we define its orthogonal projection onto the vector bundle $TM^\perp := \cup_{p \in M} (T_pM)^\perp$ pointwise by

$$X \mapsto p_{T_pM}^\perp(X)|_p =: X_p^\perp.$$ 

This defines a mapping

$$p_{T_pM}^\perp : C^k(M, \mathbb{R}^d) \to \mathcal{X}_\perp^k(M).$$

As $\mathbb{R}^d = T_p\mathbb{R}^d = T_pM \oplus (T_pM)^\perp$ for all $p$ in $M$, we may write $X = \check{X} + \check{X}^\perp$, where $\check{X} \in \mathcal{X}^k(M)$ and $\check{X}^\perp \in \mathcal{X}_\perp^k(M)$ and then by definition $p_{T_pM}^\perp(X) = \check{X}^\perp$.

Definition 5.1. A subset $S \subset M$ of a $m$-dimensional submanifold is called embedded submanifold if the inclusion map $i : S \to M$, $x \mapsto x$ is an embedding. We call $S$ closed, embedded submanifold if $i : S \to M$ is proper, that is, $i^{-1}(A)$ is compact for all $A \subset M$ compact.

The following two lemmas will be crucial for our investigation. The first one can be established using local charts; cf. [19].

Lemma 5.2. Let $M$ be a $m$-dimensional $C^k$-submanifold $M$ and let $S \subset M$ be a $s$-dimensional closed, embedded submanifold of $M$. Then every vector field $X \in \mathcal{X}^k(S)$ can be extended to $M$, that is, there is a vector field $\check{X} \in \mathcal{X}^k(M)$ satisfying $\check{X}|_S = X$.

Remark 5.3. • If $M$ is a $m$-dimensional submanifold with boundary $\partial M$, then $\partial M$ is a closed, embedded submanifold of $M$. Hence every vector field defined on the boundary can be extended to all of $M$.

• If $M = \mathbb{R}^d$ and $S \subset \mathbb{R}^d$ is a closed, embedded $C^k$-submanifold, then every vector field defined on $S$ can be extended to a $C^k$-vector field on $\mathbb{R}^d$. In particular, if $S$ is compact then the support of the vector field can be chosen to lie in some open set $D$ containing $S$. 
Lemma 5.4. Let $M$ be a closed and bounded $m$-dimensional $C^{k+1}$-submanifold of $\mathbb{R}^d$ contained in an open set $D \subset \mathbb{R}^d$. Let us denote by $\nu$ the unique outward-pointing unit vector field on $\partial M$. Then to each vector field $X \in C^k_c(D, \mathbb{R}^d)$, we find vector fields $X^\perp, X^i, X^\nu \in C^k_c(D, \mathbb{R}^d)$ satisfying

$$X = X^\perp + X^i + X^\nu \quad \text{in } M,$$

and

$$X^i_p \in T_p M \quad \text{for all } p \in M, \quad (5.1)$$

$$X^\perp_p \in T_p(\partial M) \quad \text{for all } p \in \partial M, \quad (5.2)$$

$$X^\nu_p = (X \cdot \nu) \nu \quad \text{for all } p \in \partial M, \quad (5.3)$$

$$X^\perp_p \in (T_p M)^\perp \quad \text{for all } p \in M. \quad (5.4)$$

Proof. At first, we define

$$\hat{X}^\xi_p := X_p - \hat{X}^\perp_p \quad (5.5)$$

for all $p \in M$, where $\hat{X}^\perp = p^\perp_{T_p M}(X|_M)$. Since by definition we have the decomposition $\mathbb{R}^d = (T_p M)^\perp \oplus T_p M$ for all points $p \in M$, we obtain $\hat{X}^\xi_p \in T_p M$ for all $p \in M$. By definition we have

$$(\hat{X}^\xi_p - X_p, v_p) = 0 \quad \text{for all } v_p \in T_p M, \quad p \in M,$$

and this shows that $\hat{X}^\xi \in C^k(M, \mathbb{R}^d)$ by using local charts. It follows that $\hat{X}^\perp \in C^k(M, \mathbb{R}^d)$. According to Lemma 5.2, we may extend $\hat{X}^\xi$ and $\hat{X}^\perp$ to functions $X^\xi, X^\perp \in C^k_c(D, \mathbb{R}^d)$. On the other hand we have for all boundary points $p \in \partial M$

$$\mathbb{R}^d = (T_p M)^\perp \oplus T_p M = (T_p M)^\perp \oplus T_p(\partial M) \oplus T_{p, M}(\partial M)^\perp. \quad (5.6)$$

Denote by $\nu \in \mathfrak{X}^k(\partial M)$ the outward-pointing unit normal field along $\partial M$. As the injection $i : \partial M \rightarrow M$ is proper we may apply Lemma 5.2 and extend the vector field $\hat{X}^\nu := (\hat{X} \cdot \nu) \nu$ on $\partial M$, to a vector field $X^\nu \in \mathfrak{X}^k(M)$, which itself can be extended to a vector field in $C^k_c(D, \mathbb{R}^d)$, (still keeping the same notation). Finally, we put

$$X^i := X^\xi - X^\nu \quad (5.5) \quad X^i = X^\perp - X^\nu.$$

In view of the fact that $T_p M$ is a linear space, we obtain $X^i|_M = (\hat{X}^\xi - \hat{X}^\nu)|_M \in T_p M$ for all $p \in M$ and because of (5.6) it follows $X^i_p \in T_p(\partial M)$ for all $p \in M$. Hence we obtain the required decomposition $X = X^i + X^\perp + X^\nu$ on $M$. $\blacksquare$

### 5.2 The structure theorem for submanifolds

With the preparations of the previous section we are now able to state our main result.

Theorem 5.5 (Structure theorem for submanifolds). Let $M$ be a bounded and closed $m$-dimensional $C^{k+1}$-submanifold of $\mathbb{R}^d$ contained in a bounded and open set $D \subset \mathbb{R}^d$. Suppose that $J$ is shape differentiable at $M$ and assume that $dJ(M)$ is of order $k$. Then there exist continuous functionals $h : C^k(M, \mathbb{R}^d) \rightarrow \mathbb{R}$ and $g : C^k(\partial M) \rightarrow \mathbb{R}$ such that

$$dJ(M)(X) = h(X^\perp) + g(X|_{\partial M} \cdot \nu) \quad \text{for all } X \in C^k_c(D, \mathbb{R}^d), \quad (5.7)$$

where $X^\perp := p^\perp_{T_p M}(X|_M)$ and $\nu$ is the unique outward-pointing unit vector field along $\partial M$. 

**Proof.** Recall definition (2.2) namely \( T^k(M) = \{ X \in C_c^k(D, \mathbb{R}^d) | X|_M = 0 \} \). The set \( T^k(M) \) is a closed linear subspace of \( C_c^k(D, \mathbb{R}^d) \). Recall the definition of the quotient \( Q^k(M) = C_c^k(D, \mathbb{R}^d)/T^k(M) \) and consider similarly to Theorem 4.1 we have a commuting diagram:

\[
\begin{array}{ccc}
C_c^k(D, \mathbb{R}^d) & \xrightarrow{\pi} & C^k(M, \mathbb{R}^d) \\
\downarrow & & \downarrow \\
Q^k(M) & \xrightarrow{\tilde{h}} & \tilde{h}
\end{array}
\]

By definition we have \( \tilde{J}(M) = \hat{h} \circ \tilde{3}_M \). We see that \( \tilde{3}_M^{-1} = \pi \circ E \), where \( E : C^k(M, \mathbb{R}^d) \to C_c^k(D, \mathbb{R}^d) \) denotes the continuous extension operator. It follows that \( \hat{h} = \tilde{J}(M) \circ \tilde{3}_M^{-1} : C^k(M, \mathbb{R}^d) \to \mathbb{R} \) is continuous. By construction \( \hat{h}(X|_M) = \hat{h}(\tilde{3}_M(\pi(X))) = \tilde{J}(M) \circ \pi(X) = \tilde{J}(M)(X) \).

Now we apply Lemma 5.4 to \( X \) and find \( X^\perp, X^\nu, X^t \in C_c^k(D, \mathbb{R}^d) \) satisfying (5.1)-(5.4) and \( X = X^\perp + X^\nu + X^t \) on \( M \). As \( X_p^t \in T_p M \) for all \( p \in M \) and \( X_p^t \in T_p(\partial M) \) for all \( p \in \partial M \), we get from Proposition 3.4 that \( 0 = \hat{h}(X^t) = dJ(M)(X^t) \), which implies

\[
dJ(M)(X) = h(X^\nu|_M) + h(X^\perp) \quad \text{for all } X \in C_c^k(D, \mathbb{R}^d).
\]

Consequently \( dJ(M)(X) = h(X^\nu|_M) \) for all \( X \in C_c^k(D, \mathbb{R}^d) \) with \( X|_M \in \mathfrak{X}^k(M) \). To further process the right hand side of (5.8) we introduce the linear and continuous mapping

\[
\mathcal{I}_\nu : \mathfrak{X}^k(M) \to C^k(\partial M), \quad [X] \mapsto X|_{\partial M} \cdot \nu
\]

and the linear space \( \tilde{T}^k(M) := \{ X \in \mathfrak{X}^k(M) : X|_{\partial M} \cdot \nu = 0 \text{ on } \partial M \} \). This space is a linear subspace of \( \mathfrak{X}^k(M) \). We define \( g : \mathfrak{X}^k(M) \to \mathbb{R} \) by letting the following diagram commute:

\[
\begin{array}{ccc}
\mathfrak{X}^k(M) & \xrightarrow{\mathcal{I}_\nu} & C^k(\partial M) \\
\downarrow & & \downarrow \\
\mathfrak{X}^k(M)/\tilde{T}^k(M) & \xrightarrow{\tilde{h}} & \mathbb{R}
\end{array}
\]

By definition \( \tilde{h} = g \circ \mathcal{I}_\nu \) on \( \mathfrak{X}^k(M)/\tilde{T}^k(M) \). As before we extend \( \nu : \partial M \to TM \) to a vector field \( \tilde{\nu} : M \to TM \). Moreover denote by \( \tilde{E} : C^k(\partial M) \to C^k(M) \) the usual extension operator. Then we see that \( \tilde{T}^{-1}_\nu(f) = \pi \circ (\tilde{\nu} \cdot \tilde{E}(f)) \). Therefore \( g : C^k(\partial M) \to \mathbb{R} \) is continuous and for every \( X \in \mathfrak{X}^k(M) \), we obtain

\[
g(X|_{\partial M} \cdot \nu) = g(\tilde{T}^{-1}_\nu(\pi(X|_M)))
= \hat{h}(\pi(X|_M))
= h(X|_M)
\]
and thus \( g(\mathbf{X}|_{\partial M} \cdot \nu) = h(\mathbf{X}^\nu|_M) = dJ(M)(\mathbf{X}^\nu|_M) \). Plugging this into (5.8) we recover (5.7). The continuity of \( g \) follows from the continuity of the extension operator. 

We conclude this section with the following two special cases of our main result.

**Corollary 5.6.** Let \( M \) be a closed and bounded \( m \)-dimensional \( C^{k+1} \)-submanifold of \( \mathbb{R}^d \) without boundary, that is, \( \partial M = \emptyset \). Suppose that \( J \) is shape differentiable at \( M \) and assume that \( dJ(M) \) is of order \( k \). Then there exists a continuous functional \( h : C^k(M, \mathbb{R}^d) \to \mathbb{R} \), such that

\[
dJ(M)(\mathbf{X}) = h(\mathbf{X}^\perp) \quad \text{for all } \mathbf{X} \in C^k_c(D, \mathbb{R}^d).
\]

**Corollary 5.7.** Let \( M \) be a closed and bounded \( d \)-dimensional \( C^{k+1} \)-submanifold of \( \mathbb{R}^d \). Suppose that \( J \) is shape differentiable at \( M \) and assume that \( dJ(M) \) is of order \( k \). Then there exists a continuous functional \( g : C^k(\partial M) \to \mathbb{R} \), such that

\[
dJ(M)(\mathbf{X}) = g(\mathbf{X}|_{\partial M} \cdot \nu) \quad \text{for all } \mathbf{X} \in C^k_c(D, \mathbb{R}^d).
\]

## 6 Application to shape functions

### 6.1 Shape functions defined on smoothly cracked sets

Cracked sets naturally arise in fracture mechanics, where they model damage of solids; cf. [11]. Cracked sets are highly irregular and do not even satisfy the cone property, but the crack itself is often assumed to be Lipschitz continuous or smoother. In order to forecast the propagation of a crack it is essential to compute shape derivative in cracked sets. For PDE constrained shape functions, the derivation of the shape differentiability at a cracked set [13–15] or smooth sets [6–8, 22–24] is a challenge itself. Here we are interested in the exact structure of the shape derivative in cracked sets and will assume that the shape function is shape differentiable.

**Definition 6.1.** Let \( \Omega \subset \mathbb{R}^d \) be an open and bounded set.

(i) The set \( \Omega \) is called **crack free** if \( \text{int}(\overline{\Omega}) = \Omega \), otherwise we call \( \Omega \) cracked.

(ii) The set \( \Omega \subset \mathbb{R}^d \) is said to be **smoothly \( l \)-cracked**, \( l \geq 1 \), if there is an open subset \( \tilde{\Omega} \subset \mathbb{R}^d \) with \( C^k \)-boundary \( \text{fr}(\tilde{\Omega}) \), \( k \geq 1 \), and a closed, bounded and simply connected \( l \)-dimensional \( C^k \)-submanifold \( \Sigma \subset \tilde{\Omega} \) of \( \mathbb{R}^d \), such that \( \Omega = \tilde{\Omega} \setminus \Sigma \).

**Remark 6.2.** Note that every open subset \( \Omega \subset \mathbb{R}^d \) with \( C^k \)-boundary \( \text{fr}(\Omega) \) is crack-free, so that part (ii) of Definition 6.1 makes sense. In particular, a smoothly cracked set can not have any further cracks except \( \Sigma \).

Now we want to verify that the shape derivative in a smoothly cracked set can be obtained as the shape derivative of a shape function depending on the only depending the on the crack itself.

**Lemma 6.3.** Suppose that \( \Omega \subset \mathbb{R}^d \) is smoothly \( l \)-cracked of class \( C^k \) with \( C^k \)-set \( \tilde{\Omega} \subset \mathbb{R}^d \) and a \( l \)-dimensional \( C^k \)-submanifold \( \Sigma \subset \mathbb{R}^d \), \( k \geq 1 \), such that \( \Omega = \tilde{\Omega} \setminus \Sigma \). Set \( M := \Sigma \). Let \( \Omega \mapsto J(\Omega) \) be a shape functions and define \( J(M) := J(\Omega \setminus M) \). Then

\[
dJ(M)(\mathbf{X}) = dJ(\Omega)(\mathbf{X}),
\]

where \( \mathbf{X} \in C^k_c(\tilde{\Omega}, \mathbb{R}^d), \) if either of the two expressions exists.
Proof. As \( X \in C^k_c(\bar{\Omega}, \mathbb{R}^d) \) it evident that for all \( t \)
\[
\Phi_t(\Omega) = \Phi_t(\bar{\Omega} \setminus \Sigma) = \Phi_t(\bar{\Omega}) \setminus \Phi_t(\Sigma) = \bar{\Omega} \setminus \Phi_t(\Sigma).
\]
From this the conclusion of the lemma follows.

This lemma shows that shape functions depending on smoothly cracked sets can be seen as shape functions only depending on the crack itself. Next, we consider the special situation of a shape function defined on smoothly 1-cracked sets in \( \mathbb{R}^2 \); cf. [10].

Lemma 6.4. Let \( \Omega \) be a smoothly \( l \)-cracked subset of \( \mathbb{R}^2 \) of class \( C^2 \). By definition there are an open and bounded set \( C^2 \)-set \( \bar{\Omega} \subset \mathbb{R}^2 \) and a closed, bounded, and simply connected \( l \)-dimensional submanifold \( \Sigma \subset \bar{\Omega} \) of class \( C^2 \), such that \( \Omega = \bar{\Omega} \setminus \Sigma \). Set \( M := \Sigma, \partial M = \{A, B\} \), and suppose that \( dJ(\Omega) : C^1_c(\bar{\Omega}, \mathbb{R}^2) \to \mathbb{R} \) is linear and continuous. Then there are real numbers \( \alpha_1, \alpha_2 \) and a linear and continuous functional \( h : C^1(M) \to \mathbb{R} \), such that
\[
dJ(\Omega)(X) = \alpha_1(X \cdot \nu)(A) + \alpha_2(X \cdot \nu)(B) + h(X_{|M} \cdot n)
\]
for all \( X \in C^k_c(\bar{\Omega}, \mathbb{R}^2) \), where \( n \) is a unit normal field along \( M \) and \( \nu \) the unit normal vector field on \( \partial M \).

Proof. Taking into account Lemma 6.3 we see that we can apply Theorem 5.5 to \( M \mapsto \bar{J}(M) := J(\bar{\Omega} \setminus M) \) and obtain linear functionals \( g : C^1(\partial M) \to \mathbb{R} \) and \( h : C^1(M, \mathbb{R}^d) \to \mathbb{R} \), such that
\[
d\bar{J}(M)(X) = g(X_{|\partial M} \cdot \nu) + h(X_{|M} \cdot n) = dJ(\Omega)(X).
\]
We have \( \partial M = \{A, B\} \) and thus \( C^k(\partial M) = \{f : \{A, B\} \to \mathbb{R}\} \). We may define a basis \( f_1, f_2 : \partial M \to \mathbb{R} \) of \( C^k(\partial M) \) by \( f_1(A) := 1, f_1(B) := 0 \) and \( f_2(A) := 0, f_2(B) := 1 \). Then every \( f \in C^k(\partial M) \) can be written as \( f = \alpha_1 f_1 + \alpha_2 f_2 \). In particular, we have \( X_{|\partial M} \cdot \nu = (X \cdot \nu)(A) f_1 + (X \cdot \nu)(B) f_2 \) so that
\[
g(X_{|\partial M} \cdot \nu) = \alpha_1 (X \cdot \nu)(A) + \alpha_2 (X \cdot \nu)(B),
\]
where \( \alpha_1 := g(f_1) \) and \( \alpha_2 := g(f_2) \). Denote by \( n \) the unit normal field along \( M \). Then \( X_{|M} \cdot n = (X_{|M} \cdot \nu)n \) and thus
\[
h(X_{|M} \cdot n) = h((X_{|M} \cdot \nu)n)
\]
for all \( X \in C^k_c(\bar{\Omega}, \mathbb{R}^2) \). Setting \( \bar{h}(\nu) := h(\nu n) \), we recover (6.1).

Remark 6.5. We may describe the crack \( \Sigma \) by an embedded curve \( \gamma : [a, b] \to \mathbb{R}^d \) of class \( C^2 \), that is, \( \gamma([a, b]) =: \Sigma \subset \bar{\Omega} \) and \( \gamma(a) = A \) and \( \gamma(b) = B \). Then \( \nu \circ \gamma(a) = \gamma'(a)/|\gamma'(a)| \) and \( \nu \circ \gamma(b) = -\gamma'(b)/|\gamma'(b)| \).

Corollary 6.6. Let \( \Omega \subset D \subset \mathbb{R}^d \) be a smoothly 1-cracked set such that \( \Omega = \bar{\Omega} \setminus \Sigma \), where \( \bar{\Omega} \) is an open and bounded set of class \( C^\infty \) and \( M := \Sigma \) is a closed, bounded and simply connected \( l \)-dimensional submanifold of \( \mathbb{R}^d \) of class \( C^\infty \). Let \( J \) be a shape function and suppose that \( dJ(\Omega) : C^1_c(\bar{\Omega}, \mathbb{R}^d) \to \mathbb{R} \) is continuous and linear. Let \( X \in C^1_c(D, \mathbb{R}^d) \). Then there are continuous and linear functionals \( \bar{h}_1, \ldots, \bar{h}_{d-1} : C^1(M) \to \mathbb{R} \) and real numbers \( \alpha_1, \alpha_2 \) such that
\[
dJ(\Omega)(X) = \alpha_1(X \cdot \nu)(A) + \alpha_2(X \cdot \nu)(B) + \sum_{i=1}^{d-1} \bar{h}_i(X_{|M} \cdot n_i)
\]
for all \( X \in C^k_c(\bar{\Omega}, \mathbb{R}^d) \), where \( (n_1, \ldots, n_{d-1}) \) is an orthonormal frame along \( M \) satisfying \( \text{span}\{n_1(p), \ldots, n_{d-1}(p)\} = (T_pM)^\perp \) for all \( p \in M \).
Proof. From the previous lemma, we obtain 
\[ dJ(\Omega)(X) = \alpha_1(X \cdot \nu)(A) + \alpha_2(X \cdot \nu)(B) + h(X^\perp), \]
and hence taking into account 
\[ X^\perp = (X \cdot n_1)n_1 + \cdots + (X \cdot n_{d-1})n_{d-1}, \]
we arrive at 
\[ dJ(\Omega)(X) = \alpha_1(X \cdot \nu)(A) + \alpha_2(X \cdot \nu)(B) + \sum_{i=1}^{d-1} h((X \cdot n_i)n_i). \]
So setting \( h_i := h(n_i) \), we recover (6.5).

6.2 Shape functions defined on submanifolds of dimension one and two

Length variation of a curve in \( \mathbb{R}^3 \) Let \( \gamma : [a, b] \to \mathbb{R}^3 \) be an embedded curve of class \( C^2 \) so that \( M := \gamma([a, b]) \) becomes a one dimensional \( C^2 \)-submanifold of \( \mathbb{R}^3 \) with boundary \( \partial M = \{\gamma(a), \gamma(b)\} \). We consider the shape function

\[ J(M) := \int_a^b |\gamma'(t)| \, dt \]
and denote by \( T(t) := \gamma'(t)/|\gamma'(t)|, N(t) := T'(t)/|T'(t)|, \) and \( B(t) := T(t) \times N(t) \) the tangential, normal and binormal vector field along \( \gamma \), respectively. If \( \gamma \) is arc-length parametrised, then we define the curvature \( \kappa \) of \( \gamma \) by \( T' = \kappa N \). If \( \gamma \) is not arc-length parametrised, then we have \( T' = v\kappa N \) on \([a, b]\), where \( v(t) := |\gamma'(t)| \). Let \( n, t, b : M \to \mathbb{R}^3 \) be unit vector fields, such that \( T = t \circ \gamma \), \( N = n \circ \gamma \), and \( B = b \circ \gamma \).

**Lemma 6.7.** Let \( D \) be an open and bounded set of \( \mathbb{R}^3 \) containing \( M \) and let \( X \in C^2_c(D, \mathbb{R}^3) \). Then

\[ dJ(M)(X) = \int_a^b \frac{\kappa(t)(X^\perp \cdot n) \circ \gamma(t) |\gamma'(t)| \, dt + (X \cdot t)(\gamma(b)) - (X \cdot t)(\gamma(a))}{|\gamma'(t)|}, \]

where \( X^\perp = (X \cdot n)n + (X \cdot b)b \).

**Proof.** We compute

\[ dJ(M)(X) = \frac{d}{ds} \left( \int_a^b |(\partial \Phi_s \circ \gamma(t))\gamma'(t)| \, dt \right) \bigg|_{s=0} \]
\[ = \int_a^b \frac{\gamma'(t) \cdot (\partial X \circ \gamma(t))\gamma'(t)}{|\gamma'(t)|} \, dt \]
\[ = \int_a^b \frac{(X(\gamma(t))) \cdot \gamma'(t)}{|\gamma'(t)|} \, dt \]
\[ = \int_a^b |\gamma'(t)| \kappa(t)(X \circ \gamma(t)) \cdot N(t) \, dt + X(\gamma(b)) \cdot T(b) - X(\gamma(a)) \cdot T(a). \]

From this the result follows.

**Corollary 6.8.** Let \( D \) be an open and bounded set in \( \mathbb{R}^3 \) containing \( M \) and let \( X \in C^2_c(D, \mathbb{R}^3) \). Suppose that \( \gamma : [a, b] \to \mathbb{R}^2 \) is a simply closed \( C^2 \)-curve. Then

\[ dJ(M)(X) = \int_a^b \kappa(X^\perp \cdot n) \circ \gamma(t) |\gamma'(t)| \, dt. \]
Variation of the surface integral in $\mathbb{R}^3$. As a two dimensional example, we consider the variation of the surface integral of a cylinder-like surface in $\mathbb{R}^3$. We define $Q := [a, b] \times [c, d]$ and let $\varphi : Q \to \mathbb{R}^3$ be a $C^2$-embedding and put $M := \varphi(Q)$. We assume that $\varphi(u, c) = \varphi(u, d)$, $\partial_u \varphi(u, c) = \partial_u \varphi(u, d)$ and $\partial_v \varphi(u, c) = \partial_v \varphi(u, d)$ for all $u \in [a, b]$. Since $\varphi$ is an embedding $\varphi_u := \partial_u \varphi$ and $\varphi_v := \partial_v \varphi$ are linearly independent at each point $(u, v)$ of $Q$. Hence the unit normal vector to the surface $M$ is given by

$$N(u, v) := \frac{\varphi_u \times \varphi_v}{|\varphi_u \times \varphi_v|}.$$ 

Recall that the classical surface integral of $\varphi(Q)$ is defined by

$$J(M) := \int_a^b \int_c^d |\varphi_u \times \varphi_v| \, dudv.$$ 

**Lemma 6.9.** Let $D$ be an open and bounded set containing $M$. Suppose that $X \in C^2_c(D, \mathbb{R}^3)$. Then

$$dJ(M)(X) = \int_a^b \int_c^d \partial_u(X \circ \varphi) \times \varphi_v \cdot N \, dudv + \int_a^b \int_c^d \varphi_u \times \partial_v(X \circ \varphi) \cdot N \, dudv$$

which is equivalent to

$$dJ(M)(X) = \int_a^b \int_c^d H(u, v)X(\varphi(u, v)) \cdot N(u, v)|\varphi_u \times \varphi_v| \, dudv$$

$$+ \left[ \int_c^d (X \cdot \nu)\varphi_v \, d\nu \right]_a^b,$$

where $H(u, v)$ is the mean curvature at the surface point $\varphi(u, v)$ and $\nu$ the outward-pointing unit normal along $\partial M$.

**Proof.** We compute

$$dJ(M)(X) = \frac{d}{dt} \left( \int_a^b \int_c^d |(\partial \Phi_t \circ \varphi)\varphi_u \times (\partial \Phi_t \circ \varphi)\varphi_v| \, dudv \right) |_{t=0}$$

$$= \int_a^b \int_c^d \frac{(\partial X \circ \varphi)\varphi_u \times \varphi_v \cdot \varphi_u \times \varphi_v}{|\varphi_u \times \varphi_v|} \, dudv + \int_a^b \int_c^d \varphi_u \times (\partial X \circ \varphi)\varphi_v \cdot \varphi_u \times \varphi_v \, dudv$$

$$= \int_a^b \int_c^d \partial_u(X \circ \varphi) \times \varphi_v \cdot N \, dudv + \int_a^b \int_c^d \varphi_u \times \partial_v(X \circ \varphi) \cdot N \, dudv$$

$$= - \int_a^b \int_c^d (X \circ \varphi) \times \varphi_v \cdot N_u \, dudv - \int_a^b \int_c^d \varphi_u \times (X \circ \varphi) \cdot N_v \, dudv$$

$$+ \left[ \int_c^d (X \circ \varphi) \times \varphi_v \cdot N \, d\nu \right]_a^b,$$

where we used $N(u, c) = N(u, d)$ for all $a \leq u \leq b$ which follows from $\partial_v \varphi(u, c) = \partial_v \varphi(u, d)$ for all $a \leq u \leq b$. Now since $N^2 = 1$ we have $N_u \cdot N = 0$ and $N_v \cdot N = 0$, which means that $N_u, N_v \in d_p \varphi(T_p Q)$. Thus we can write (Weingarten equations)

$$N_u = \alpha_1 \varphi_u + \alpha_2 \varphi_v$$

$$N_v = \alpha_3 \varphi_u + \alpha_4 \varphi_v$$
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for smooth functions $\alpha_i$. Note that $H(u, v) = \alpha_1 + \alpha_4$ (that is the trace of the Weingarten mapping). Therefore using $(a \times b) \cdot c = (c \times a) \cdot b = (b \times c) \cdot a$, we get

\[
(X \circ \varphi) \times \varphi_v \cdot N_u = -\alpha_1 \varphi_u \times \varphi_v \cdot X \circ \varphi = -\alpha_1 N \cdot (X \circ \varphi)|\varphi_u \times \varphi_v|
\]
\[
\varphi_u \times (X \circ \varphi) \cdot N_v = -\alpha_4 \varphi_u \times \varphi_v \cdot X \circ \varphi = -\alpha_4 N \cdot (X \circ \varphi)|\varphi_u \times \varphi_v|.
\]

(6.10)

Note also that the outward-pointing unit normal field $\nu$ satisfies $\nu \circ \varphi = \varphi_v \times N/|\varphi_v \times N| = \varphi_v \times N/|\varphi_v|$ as $|\varphi_v \times N| = |\varphi_v|$. Then

\[
(X \circ \varphi) \times \varphi_v \cdot N = (X \cdot \nu) \circ \varphi|\varphi_v|.
\]

(6.11)

So inserting (6.11) and (6.10) into (6.9) we obtain (6.8).

**Remark 6.10.** Formula (6.8) may be rewritten as

\[
dJ(M)(X) = \int_M \mathcal{H}(X \cdot n) \, ds + \int_{\partial M} X \cdot \nu \, ds,
\]

(6.12)

where $n$ and $\mathcal{H}$ are the unit normal field and mean curvature on $M$, respectively. So by definition $n \circ \varphi = N$ and $\mathcal{H} \circ \varphi = H$. Also in this case our main theorem is satisfied and we recover (5.7) with

\[
h(X/\perp) = \int_M \mathcal{H}(X/\perp \cdot n) \, ds, \quad g(X|_{\partial M} \cdot \nu) = \int_{\partial M} X|_{\partial M} \cdot \nu \, ds.
\]

### 6.3 A shape gradient of order one

Provided that the manifold $M$ is smooth enough we have seen in the examples from the previous sections that the shape derivative was always a distribution of order zero in the sense that $g$ and $h$ were linear functionals on $C^0(\partial M)$ respectively $C^0(M)$.

Let $\gamma : [0, L] \to \mathbb{R}^2$ an arc-length parametrised regular curve. Then $M := \gamma([0, L])$ is a closed submanifold of $\mathbb{R}^2$. We define the elastic energy associated with $\gamma$ as

\[
E(M) := \int_0^L \kappa^2 \, ds,
\]

where $\kappa$ denotes the curvature of $\gamma$. Here we are interested in the unconstrained case, where we do not impose any further conditions at the end points of the curve.

Let us introduce some notation. We define the tangent vector field along $\gamma$ by $T := \gamma'$ and $N := RT$ where $R$ denotes the 90 degrees counter-clockwise rotation matrix in $\mathbb{R}^2$. Further we denote by $n : M \to \mathbb{R}^2$ the unit normal field and by $t : M \to \mathbb{R}^2$ the tangent field 'living' on $M$ so that by definition $N = n \circ \gamma$ and $T = t \circ \gamma$. Note that by definition $T' = \kappa N$ and $N' = -\kappa T$.

For the derivation of the first variation of the anisotropic elastic energy with fixed end points, we refer the reader to [3, Lem. 2.2, p. 502].

**Lemma 6.11.** Let $\gamma : [0, L] \to \mathbb{R}^2$ be a $C^2$-regular arc-length parametrised embedded curve such that $M := \gamma([0, L]) \subset D$. For every $X \in C^2_c(D, \mathbb{R}^4)$, we have

\[
dE(M; X) = \int_0^L (2\kappa'' + \kappa^3)(X \cdot n) \circ \gamma \, ds + \left[ 2\kappa\nabla_{T}(X \cdot n) \circ \gamma \cdot \gamma' - 2\kappa'(X \cdot n) \circ \gamma \right]_0^L.
\]
Remark 6.12. We see that also in this case (5.7) is satisfied. We have

\[
h(X^\perp) = \int_0^L (2\kappa'' + \kappa^3)(X^\perp \cdot \nabla) \circ \gamma \, ds - \left[ 2\kappa'(X^\perp \cdot \nabla) \circ \gamma \right]_0^L + \left[ 2\kappa \nabla (X^\perp \cdot \nabla) \circ \gamma \cdot \gamma' \right]_0^L
\]

and \( g = 0 \). Note that \( h : C^1(M) \to \mathbb{R} \) is a distribution of order \( k = 1 \). This well-known result is interesting as it gives an example for which \( g = 0 \) although the manifold \( M \) has non-empty boundary \( \partial M \neq \emptyset \); compare Corollary 5.6. Note that if we fixed the end points of \( \gamma \), then the term \( [2\kappa'(X \cdot \nabla) \circ \gamma]_0^L = 0 \) because \( X(\gamma(0)) = X(\gamma(L)) = 0 \).
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