Convergence of Newton’s method in shape optimization via approximate normal functions

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Abstract

This paper is concerned with the convergence study of Newton’s method on the image set generated by the Micheletti group. At first we review the structure of first and second derivatives of shape functions and present a new proof of the structure theorem for second (shape) derivatives. Then we examine a quotient group and compute its tangent space and relate it to the shape derivative.

In the second part of the paper we introduce a class of so-called approximate normal functions using reproducing kernels. The approximate normal functions are then used to define a Newton method. Under suitable assumptions we are able to show the convergence of the Newton method in the Micheletti group. Finally we verify our findings in a number of numerical experiments.

Keywords: shape optimization, Micheletti group, Newton methods, convergence analysis, Banach manifolds, infinite dimensional manifold, numerical mathematics

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Chapter 3 and [23, 16]. The image set consists of all images defined on the image set $X$. Shape optimisation is concerned with the minimisation of real-valued shape or objective functions $J$ and thus it is of paramount importance to find efficient methods to solve these problems numerically.

In order to develop efficient second order methods we study in Section 2 the structure of second (shape) Hessians restricted to the space of approximate normal functions are approximately superlinearly or even quadratically. Despite their importance, the literature on Newton or Newton-like methods for shape optimisation problems is rather thin and only a manageable number of papers exploit second order methods, but also on first order methods, is even thinner; [28, 20, 13].

Newton and Newton-like methods have the great advantage over gradient methods that they converge superlinearly to zero and there is no domain expression of the second shape Hessian is related to the third structure theorem. We refer to [26] and [4] for alternative proofs. After these preparations we investigate the Micheletti group and a quotient group from a geometric perspective and compute their tangent spaces. Our analysis suggests to introduce two types of shape Hessians called first and second shape Hessians on and compute their tangent spaces. Our analysis suggests to introduce two types of shape Hessians called first and second shape Hessians on the structure of second (shape) Hessians restricted to the space of approximate normal functions are approximately superlinearly or even quadratically. Despite their importance, the literature on Newton or Newton-like methods for shape optimisation problems is rather thin and only a manageable number of papers exploit second order methods, but also on first order methods, is even thinner; [28, 20, 13].

One reason for the lack of literature in this field is the nonlinearity of the space of admissible shapes on a (mostly Riemannian) manifold and therefore the tool from differential geometry become accessible. Newton methods, Newton-like and gradient methods on finite dimensional Riemannian manifolds are well-studied [1]. In shape optimisation the spaces of shapes are usually infinite dimensional manifolds and in this situation the analysis is more complicated as one has to account for the infinite dimensionality of the space of admissible shapes on a (mostly Riemannian) manifold and therefore the tool from differential geometry become accessible. Newton methods, Newton-like and gradient methods on finite dimensional Riemannian manifolds are well-studied [1]. In shape optimisation the spaces of shapes are usually infinite dimensional manifolds and in this situation the analysis is more complicated as one has to account for the infinite dimensionality of the manifold; [21, 24]. In the rather recent work [25] the link between shape optimisation problems and a certain infinite dimensional Riemannian manifolds of mappings, also called shape space, has been established. To be more specific the analysis was carried out in the so-called shape space of planar curves studied in [25].

It will be shown in Section 1 that there is a tight relationship between the tangent space of the quotient $F(C^1_b)/G(Ω)$ and the structure theorem. In fact we will see that the (shape) derivative $DJ(F(Ω))$ is a well-defined mapping on the tangent space of $F(C^1_b)/G(Ω)$ at $[F]$. In order to develop efficient second order methods we study in Section 2 the structure of second (shape) derivatives. We give a new proof of what we call third structure theorem and show that it is in fact a direction consequence of the first and second structure theorem. We refer to [26] and [4] for alternative proofs. After these preparations we investigate the Micheletti group and a quotient group from a geometric perspective and compute their tangent spaces. Our analysis suggests to introduce two types of shape Hessians called first and second shape Hessian. The first shape Hessian is related to the second structure theorem and the second shape Hessian is related to the third structure theorem.

In Section 3 we introduce what we call approximate normal basis functions. These functions yield (in a certain sense) an approximation of the tangent space of the quotient $F(C^1_b)/G(Ω)$. It turns out that the first and second shape Hessian restricted to the space of approximate normal functions are approximately the same and this justifies to solve only (0.1). As a result we may use the domain expression of the second derivative without resorting to the boundary expression.

After these preparations we turn our attention to the convergence study of the Newton method (0.1). We will show in Section 4 that under suitable conditions on the first and second derivative of Newton’s method

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**Introduction**

Shape optimisation is concerned with the minimisation of real-valued shape or objective functions $J(Ω)$ depending on subsets $Ω ⊂ R^d$; see [18, 20, 6, 17]. Many tasks in industry lead to shape optimisation problems and thus it is of paramount importance to find efficient methods to solve these problems numerically.

The aim of this paper is to develop Newton algorithms for the minimisation of shape functions $J(·)$ defined on the image set $X(Ω)$ generated by the Micheletti metric group $F(C^1_b) := F(C^1_b(R^d, R^d))$; cf. [9] Chapter 3 and [23, 16]. The image set consists of all images $F(Ω)$ of some fixed subset $Ω ⊂ R^d$, where the transformations $F : R^d → R^d$ belong to $F(C^1_b)$. The key to define a stable Newton algorithm is to introduce for every $C^1$-domain $Ω$ a so-called approximate normal spaces $V^{\beta\Omega}(R^d, R^d) ⊂ C^1_b(R^d, R^d)$ by means of a reproducing kernel $k$. By construction the space $V^{\beta\Omega}(R^d, R^d)$ is contained in the reproducing kernel Hilbert space (RKHS) associated with $k$. The next step is to fix a finite number of points $Χ := \{x_1, \ldots, x_n\} ⊂ \partial Ω$ and to define a finite dimensional subspace $V^{\beta\Omega}(R^d, R^d)$ of the approximate normal space. Under certain conditions on $DJ$ and $D^2J$ we can show the well-posedness of the Newton iterations: find $g_k ∈ V^{\beta\Omega}(R^d, R^d)$ so that

$$D^2J(Ω_k)(g_k)(ϕ) = DJ(Ω_k)(ϕ) \quad \text{for all } ϕ ∈ V^{\beta\Omega}(R^d, R^d),$$

(0.1)

where $F_k := (id + g_{k-1}) \circ F_{k-1}$, $Ω_k := F_k(Ω)$ and $Χ_k := F_k(Χ)$. Moreover we prove that the sequence $g_k$ converges in $C^1_b(R^d, R^d)$ superlinearly to zero and there is $F^* ∈ F(C^1_b)$ so that $F_k → F^*$ in $F(C^1_b)$ and $DJ(F^∗(Ω))(ϕ) = 0$ for all $ϕ ∈ V^{\beta\Omega}(R^d, R^d)$.

Newton and Newton-like methods have the great advantage over gradient methods that they converge superlinearly or even quadratically. Despite their importance, the literature on Newton or Newton-like methods for shape optimisation problems is rather thin and only a manageable number of papers exploit second order information; see [9, 10, 19, 20, 12, 11, 11, 12]. The literature on the convergence analysis of second order methods, but also on first order methods, is even thinner; [25, 20, 13].

One reason for the lack of literature in this field is the nonlinearity of the space of admissible shapes on which a shape function $J$ is minimised. However in certain situations, it is possible to turn the admissible sets into a (mostly Riemannian) manifold and therefore the tool from differential geometry become accessible. Newton methods, Newton-like and gradient methods on finite dimensional Riemannian manifolds are well-studied [1]. In shape optimisation the spaces of shapes are usually infinite dimensional manifolds and in this situation the analysis is more complicated as one has to account for the infinite dimensionality of the manifold; [21, 24]. In the rather recent work [25] the link between shape optimisation problems and a certain infinite dimensional Riemannian manifolds of mappings, also called shape space, has been established. To be more specific the analysis was carried out in the so-called shape space of planar curves studied in [25].

It will be shown in Section 1 that there is a tight relationship between the tangent space of the quotient $F(C^1_b)/G(Ω)$ and the structure theorem. In fact we will see that the (shape) derivative $DJ(F(Ω))$ is a well-defined mapping on the tangent space of $F(C^1_b)/G(Ω)$ at $[F]$. In order to develop efficient second order methods we study in Section 2 the structure of second (shape) derivatives. We give a new proof of what we call third structure theorem and show that it is in fact a direction consequence of the first and second structure theorem. We refer to [26] and [4] for alternative proofs. After these preparations we investigate the Micheletti group and a quotient group from a geometric perspective and compute their tangent spaces. Our analysis suggests to introduce two types of shape Hessians called first and second shape Hessian. The first shape Hessian is related to the second structure theorem and the second shape Hessian is related to the third structure theorem.

In Section 3 we introduce what we call approximate normal basis functions. These functions yield (in a certain sense) an approximation of the tangent space of the quotient $F(C^1_b)/G(Ω)$. It turns out that the first and second shape Hessian restricted to the space of approximate normal functions are approximately the same and this justifies to solve only (0.1). As a result we may use the domain expression of the second derivative without resorting to the boundary expression.

After these preparations we turn our attention to the convergence study of the Newton method (0.1). We will show in Section 4 that under suitable conditions on the first and second derivative of Newton’s method

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Section 5 provides some numerical results comparing gradient and Newton methods. We show numerical evidence that our method outperforms gradient methods and thus justifies the additional effort of the Newton method.

1 The group $\mathcal{F}(C^1_b)$ as a Banach manifold

1.1 Function spaces

Let $D \subset \mathbb{R}^d$ be an open set. We define

$$\tilde{C}(D, \mathbb{R}^d) = \{ f : \tilde{D} \to \mathbb{R}^d : f \text{ is continuous and } f = 0 \text{ on } \partial D \}.$$ 

We denote by $C^{0,1}(\bar{D}, \mathbb{R}^d)$ the space of bounded, Lipschitz continuous functions defined on $\bar{D}$ with values in $\mathbb{R}^d$. We denote by $C^k(D, \mathbb{R}^d)$ with $k \geq 1$ the usual space of $k$-times continuously differentiable functions on $D$ with values in $\mathbb{R}^d$. The space $C^k(\bar{D}, \mathbb{R}^d)$ comprises all functions from $C^k(D, \mathbb{R}^d)$ that admit a uniformly continuous and bounded extensions of its partial derivatives $\partial^\alpha f$ to $\bar{D}$ for all multi-indices $|\alpha| \leq k$. The space $C^k_b(D, \mathbb{R}^d)$ indicates all $k$-times differentiable functions $f$ on $D$ with values in $\mathbb{R}^d$ that have bounded and continuous partial derivatives $\partial^\alpha f$ for all multi-indices $|\alpha| \leq k$. When $D$ is convex, then it is readily checked that for $k \geq 1$,

$$\tilde{C}^k_b(D, \mathbb{R}^d) \subset C^{0,1}(\bar{D}, \mathbb{R}^d). \quad (1.1)$$

For all spaces introduced above we define subspaces: $\tilde{C}^{0,1}(\bar{D}, \mathbb{R}^d) := C^{0,1}(\bar{D}, \mathbb{R}^d) \cap \tilde{C}(D, \mathbb{R}^d)$, $\tilde{C}^k(\bar{D}, \mathbb{R}^d) := C^k(\bar{D}, \mathbb{R}^d) \cap \tilde{C}(D, \mathbb{R}^d)$ and $\tilde{C}^k_b(D, \mathbb{R}^d) := C^k_b(D, \mathbb{R}^d) \cap \tilde{C}(D, \mathbb{R}^d)$.

1.2 Group of transformations and metric distance

At first we recall the definition of the Micheletti group and review some basic its properties. The reader is also referred to [6, Chapter 3] for more information. Following this we prove some further results that are used for our later investigation of Newton’s method.

**Definition 1.1 ([6], p.124).** The Micheletti group associated with the space $C^1_b(\mathbb{R}^d, \mathbb{R}^d)$ is defined by

$$\mathcal{F}(C^1_b) := \{ \text{id} + f \text{ bijective : } f \in C^1_b(\mathbb{R}^d, \mathbb{R}^d), \exists g \in C^1_b(\mathbb{R}^d, \mathbb{R}^d) \text{ so that } (\text{id} + f)^{-1} = \text{id} + g \}. \quad (1.2)$$

This set is a group under composition $(F_1 \circ F_2)(x) := F_1(F_2(x))$.

**Definition 1.2 ([6], p.126).** The metric distance between the identity mapping $\text{id}$ on $\mathbb{R}^d$ and $F \in \mathcal{F}(C^1_b)$ is defined by

$$d(\text{id}, F) := \inf_{F = (\text{id} + f_1) \circ \cdots \circ (\text{id} + f_n)} \sum_{k=1}^n \| f_k \|_{C^1} + \| f_k \circ (\text{id} + f_k)^{-1} \|_{C^1}. \quad (1.3)$$

The metric distance between arbitrary $F_1, F_2 \in \mathcal{F}(C^1_b)$ is defined by

$$d(F_1, F_2) := d(\text{id}, F_2 \circ F_1^{-1}).$$

It is readily checked that $d(\cdot, \cdot)$ is right-invariant, that is, $d(F_1 \circ G, F_2 \circ G) = d(F_1, F_2)$ for all $F_1, F_2, G \in \mathcal{F}(C^1_b)$. For a proof that $(\mathcal{F}(C^1_b)), d(\cdot, \cdot))$ is indeed a complete metric space we refer to [6] p.134, Theorem 2.6.

In shape optimisation the metric space $(\mathcal{F}(C^1_b), d)$ is used as follows. First we fix a set $\Omega \subset \mathbb{R}^d$ and associate with it the image set

$$\mathcal{X}(\Omega) := \{ (\text{id} + f)(\Omega) : \text{id} + f \in \mathcal{F}(C^1_b) \}. \quad (1.4)$$

This set forms the set of all admissible shapes on which a shape function $J(\cdot)$ is minimised. In the following sections we study Newton’s method defined in the Micheletti group that aim to solve

$$\min_{\tilde{\Omega} \in \mathcal{X}(\Omega)} J(\tilde{\Omega}). \quad (1.5)$$
Usually a set \( \tilde{\Omega} \in \mathcal{X}(\Omega) \) does not correspond to a unique \( F \in \mathcal{F}(C_b^1) \) as two elements \( F, \tilde{F} \in \mathcal{F}(C_b^1) \) can have the same image \( F(\Omega) = \tilde{F}(\Omega) \). Therefore it makes sense to quotient out transformations that have the same image. Introduce for \( \Omega \subset \mathbb{R}^d \) the set

\[
\mathcal{G}(\Omega) := \{ F \in \mathcal{F}(C_b^1) : F(\Omega) = \Omega \}.
\]

As can be readily seen \( \mathcal{G}(\Omega) \) is a subgroup of \( \mathcal{F}(C_b^1) \) and hence the quotient group \( \mathcal{F}(C_b^1) / \mathcal{G}(\Omega) \) is well-defined and can be shown to be a complete metric space itself under certain conditions on \( \Omega \). For details we refer to [6, Chapter 3]. We will investigate this quotient in the subsequent sections.

### 1.3 Properties of the metric distance

Let us now extract some refined properties of the metric \( d(\cdot, \cdot) \). The first aim is to show that if the norm of \( f \in C_b^1(\mathbb{R}^d, \mathbb{R}^d) \) is smaller then one, then the metric distance \( d(id + f) \) can be estimated from above in terms of norms of \( f \).

**Lemma 1.3.** Let \( q \in (0, 1) \). For all \( id + f \in \mathcal{F}(C_b^1) \) such that \( \| f \|_{C^1} < q \) we have

\[
d(id, id + f) \leq \| f \|_{C^1} + \| f \|_{\infty} + 1/(1 - q) \| \partial f \|_{\infty} (\| \partial f \|_{\infty} + 1).
\]  

**Proof.** At first by definition of \( d(\cdot, \cdot) \) as an infimum and since \( id + f \in \mathcal{F}(C_b^1) \):

\[
d(id, id + f) \leq \| f \|_{C^1} + \| f \circ (id + f)^{-1} \|_{C^1}.
\]

By the chain rule we obtain

\[
\| \partial (f \circ (id + f)^{-1}) \|_{\infty} \leq \| \partial f \circ (id + f)^{-1} \|_{\infty} (I + \partial f)^{-1} \circ (id + f)^{-1} \|_{\infty}
\]

\[
= \| \partial f \|_{\infty} (I + \partial f)^{-1} \|_{\infty}.
\]

Let \( \text{inv}(A) := A^{-1} \) denote the inverse mapping defined for all invertible \( A \in \mathbb{R}^{d,d} \). For given invertible \( A_0 \in \mathbb{R}^{d,d} \) and \( A \in \mathbb{R}^{d,d} \) with \( \| A - A_0 \| < q/(\| A_0^{-1} \|) \), we get by [3, Satz 7.2] the Lipschitz estimate

\[
\| \text{inv}(A) - \text{inv}(A_0) \| < 1/(1 - q) \| A_0^{-1} \|^2 \| A - A_0 \|. \]

It follows by the triangle inequality \( \| \text{inv}(A) \| < 1/(1 - q) \| A_0^{-1} \|^2 \| A - A_0 \| + \| \text{inv}(A_0) \| \). Hence setting \( A_0 := I \) and \( A := I + \partial f(x) \) for fixed \( x \in \mathbb{R}^d \) yields

\[
\| (I + \partial f)^{-1} \|_{\infty} \leq 1/(1 - q) \| \partial f(x) \| + 1.
\]

Thus using this estimate in (1.9) we arrive at

\[
\| \partial (f \circ (id + f)^{-1}) \|_{\infty} \leq 1/q \| \partial f \|_{\infty} (\| \partial f \|_{\infty} + 1)
\]

and this finishes the proof.

**Remark 1.4.** Although the manifold \( \mathcal{F}(C_b^1) \) is smooth we are not restricted to smooth sets \( \Omega \). Indeed we will see later that when the initial set is not smooth then the set \( \mathcal{F}(C_b^1) / \mathcal{G}(\Omega) \) is in general not nice since differentiable functions on this space can not be associated with normal perturbations on \( \partial \Omega \).

The next lemma shows a similar statement to the previous lemma, but without the assumption that the norms of \( f_i \) be smaller than one. However, the estimate is not as sharp. We also refer to [6, p. 127, Example 2.2] where the space of bounded Lipschitz continuous functions \( C^{0,1}(\mathbb{R}^d, \mathbb{R}^d) \) rather than \( C_b^1(\mathbb{R}^d, \mathbb{R}^d) \) is considered.

**Lemma 1.5.** For all \( (id + f_k) \in \mathcal{F}(C_b^1), k = 1, \ldots, n \), we have

\[
\| (id + f_1) \circ \cdots \circ (id + f_n) - id \|_{C^1} \leq \max\{ 1, e^{\sum_{i=1}^n \| \partial f_i \|_{\infty}} \} \sum_{k=1}^n \| \partial f_k \|_{\infty}.
\]

**Proof.** Define \( \Theta_k := (id + f_k) \circ \cdots \circ (id + f_n) \) for \( k = 1, \ldots, n \). Then it is readily checked that the recursive formula \( \Theta_k = \Theta_{k+1} + f_k \circ \Theta_{k+1} \) for \( k = 1, \ldots, n - 1 \) holds. Summing over \( k = 1, \ldots, n - 1 \) and recalling the telescope sum, we get

\[
\sum_{k=1}^{n-1} f_k \circ \Theta_{k+1} = \sum_{k=1}^{n-1} (\Theta_k - \Theta_{k+1}) = \Theta_1 - \Theta_n.
\]

Then (1.11) together with the fact that \( \Theta_k \) are homeomorphisms yields

\[
\| \Theta_1 - id \|_{\infty} \leq \| f_n \|_{\infty} + \sum_{k=1}^{n-1} \| f_k \circ \Theta_{k+1} \|_{\infty} = \sum_{k=1}^n \| f_k \|_{\infty}
\]
Now observe that for all $k$, we have $\|\partial \Theta_k\|_\infty \leq (1+\|\partial f_k\|_\infty) \cdots (1+\|\partial f_n\|_\infty) \leq e^{\sum_{k=1}^n \|\partial f_k\|_\infty}$ and consequently

$$
\|\partial \Theta_1 - I\|_\infty \leq \|\partial f_n\|_\infty + \sum_{k=1}^{n-1} \|\partial f_k\circ \Theta_{k+1}(\partial \Theta_{k+1})\|_\infty
$$
$$
\leq \|\partial f_n\|_\infty + \sum_{k=1}^{n-1} e^{\sum_{l=k+1}^n \|\partial f_l\|_\infty} \|\partial f_k\|_\infty
$$
$$
\leq \|\partial f_n\|_\infty + e^{\sum_{k=1}^{n-1} \|\partial f_k\|_\infty} \sum_{k=1}^{n-1} \|\partial f_k\|_\infty
$$
$$
\leq \max\{1, e^{\sum_{k=1}^{n-1} \|\partial f_k\|_\infty}\} \sum_{k=1}^{n} \|\partial f_k\|_\infty.
$$

(1.13)

Now (1.12) and (1.13) together yield (1.10). \qed

With the help of the previous lemma we may show that the convergence of $(F_n)$ against $F$ in $\mathcal{F}(C^1_b)$ implies the convergence of $F_n - id$ and $F_n^{-1} - id$ against $F - id$ and $F^{-1} - id$ in $C^1_b(\mathbb{R}^d, \mathbb{R}^d)$, respectively. This statement is summarised in the following lemma.

**Lemma 1.6.** Let $F_n, F \in \mathcal{F}(C^1_b)$ be given and assume $F_n \to F$ in $\mathcal{F}(C^1_b)$ as $n \to \infty$. Then

$$
F_n - id \to F - id \quad \text{and} \quad F_n^{-1} - id \to F^{-1} - id \quad \text{in} \quad C^1_b(\mathbb{R}^d, \mathbb{R}^d) \quad \text{as} \quad n \to \infty.
$$

(1.14)

**Proof.** Thanks to the right invariance of metric $d$ we have $d(F_n, F) = d(id, F \circ F_n^{-1}) = d(id, F_n \circ F^{-1})$. Therefore we may assume without loss of generality $F = id$ and $F_n \to id$ and $F_n^{-1} \to id$ in $\mathcal{F}(C^1_b)$.

By assumption for every $\epsilon > 0$ we find $N \geq 1$ so that $d(F_n, id) < \epsilon$ for all $n \geq N$. By definition of $d(\cdot, \cdot)$ as an infimum we find for every number $n \geq N$ transformations $(id+f^n_i) \in \mathcal{F}(C^1_b)$ with $F_n = (id+f^n_i) \circ \cdots \circ (id+f^n_M)$, so that

$$
d(F_n, id) \leq \sum_{k=1}^{M} \|f^n_k\|_{C^1} + \|f^n_k \circ (id+f^n_{k-1})^{-1}\|_{C^1} < \epsilon.
$$

(1.15)

Now Lemma 1.5 yields $\|F_n - id\|_{C^1} \leq \max\{1, e^{\epsilon}\} \epsilon$ for all $n \geq N$. Since $\epsilon$ was arbitrary we conclude $F_n - id \to 0$ as $n \to \infty$. Noticing $d(id, F_n^{-1}) = d(id, F_n) \to 0$ as $n \to \infty$ shows that the argumentation above can be repeated to prove $F_n^{-1} - id \to 0$ as $n \to \infty$ which finishes the proof. \qed

### 1.4 The Miechletti group as a smooth Banach manifold

**Charts and tangent space** The Miechletti group can be given a manifold structure turning it into a smooth Banach manifold. We refer to [22] for the definition of a Banach manifolds and basic properties.

**Lemma 1.7.** The group $\mathcal{F}(C^1_b)$ is a $C^\infty$-Banach manifold. For each $F \in \mathcal{F}(C^1_b)$ and $q \in (0, 1)$ the mapping

$$
\psi_F : B_{\delta_F}(0) \to \mathcal{F}(C^1_b) : g \mapsto F + g,
$$

(1.16)

where $\delta_F := \|g/\|1 + \|F^{-1} - id\|_{C^1}\|_{C^1}$, is a well-defined parameterization. Differentiable charts may be defined by $\varphi_F := \psi^{-1}_F$ with $U_F := \psi(F_B(0))$ and the chart changes are $C^\infty$. The sets $U_F$ are open in the topology generated by $d(\cdot, \cdot)$.

**Proof.** We first show that for given $F \in \mathcal{F}(C^1_b)$ there is a $\delta > 0$ so that the mapping

$$
\varphi_F : B_{\delta}(0) \to \mathcal{F}(C^1_b) : g \mapsto F + g
$$

(1.17)

is well-defined. Indeed we may write $F + g = (id + g \circ F^{-1}) \circ F$. Now since $\mathcal{F}(C^1_b)$ is a group we only need to show that $id + g \circ F^{-1} \in \mathcal{F}(C^1_b)$. We first show that $S(x) := x + g \circ F^{-1}(x)$ is invertible. Let $y \in \mathbb{R}^d$ be given and define $\Psi(x) := g \circ F^{-1}(x) - y$. Notice that by definition $F^{-1} = id + f$ for some $f \in C^1_b(\mathbb{R}^d, \mathbb{R}^d)$. Then for all $x_1, x_2 \in \mathbb{R}^d$, $|f(x_1) - f(x_2)| \leq \|\partial f\|_{\infty}|x_1 - x_2|$ and $|g(x_1) - g(x_2)| \leq \|\partial g\|_{\infty}|x_1 - x_2|$. Hence

$$
|\Psi(x_1) - \Psi(x_2)| \leq \|\partial g\|_{\infty}|F^{-1}(x_1) - F^{-1}(x_2)| \leq \|\partial g\|_{\infty}(1 + \|\partial f\|_{\infty})|x_1 - x_2|.
$$

(1.18)
Since \( \|g\|_{C^1} < 1/(1 + \|\partial f\|_{\infty}) \) we see that the mapping \( \Psi : \mathbb{R}^d \to \mathbb{R}^d \) is a contraction and thus admits a unique fixed point \( \Psi(x) = x \). But that means there is a unique \( x \in \mathbb{R}^d \) so that \( x + g \circ F^{-1}(x) = y \). This shows that \( id + g \circ F^{-1} \) is a contraction. Finally let us show that the inverse of \( id + g \circ F^{-1} \) is also \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \). Let us set \( S(x) := x + g \circ F^{-1}(x) \) and let \( x_0 \in \mathbb{R}^d \). Then

\[
|S^{-1}(y) - S^{-1}(y_0) - [\partial S(x_0)]^{-1}(y - y_0)| = |x - x_0 - [\partial S(x_0)]^{-1}(S(x) - S(x_0))| \\
\leq |\partial S^{-1}(x_0)||\partial S(x_0)(x - x_0) - (S(x) - S(x_0))|,
\]

(1.19)

where \( y_0 = S(x_0) \) and \( y = S(x) \). Since \( S \) is differentiable the right hand side of (1.19) is \( o(\|x_0 - x\|) \) but since \( S^{-1} \) is continuous this means it is also \( o(\|y_0 - y\|) \) which proves the differentiability of \( S^{-1} \). As expected the derivative is given by \( \partial S^{-1}(y_0) = (\partial S(S^{-1}(y_0)))^{-1} \). It is clear that \( S^{-1} \) is bounded in \( \mathbb{R}^d \). Moreover, in view of the definition of \( \delta_F \), for all \( y_0 \in \mathbb{R}^d \) (and hence all \( x_0 = S^{-1}(y_0) \)),

\[
\partial S^{-1}(y_0) = (I + (\partial g \circ F^{-1})\partial F^{-1}(x_0))^{-1} \leq \frac{1}{1 - \|(\partial g \circ F^{-1})\partial F^{-1}(x_0)\|} \leq \frac{1}{q},
\]

(1.20)

Consequently \( id + g \circ F^{-1} \) belongs to \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \).

Next we show that the chart change is smooth. Let \( F_1, F_2 \in \mathcal{F}(C^1_b) \). The chart change is given by

\[
\varphi_{F_1} \circ \varphi_{F_2}^{-1} : \varphi_{F_1}(B_{\delta_F}(0) \cap B_{\delta_{F_2}}(0)) \to \varphi_{F_1}(B_{\delta_{F_1}}(0) \cap B_{\delta_{F_2}}(0)), f \mapsto F_1 - F_2 + f
\]

(1.21)

which is obviously \( C^\infty \). Recall that \( B_0(0) \) denotes the open ball of radius \( \delta \) at the origin in \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \).

It remains to show that \( U_{F} \subset \mathcal{F}(C^1_b) \) is indeed open. Let \( F_0 = F + f_0 \in U_{F}, f_0 \in C^1_b(\mathbb{R}^d, \mathbb{R}^d) \) be given. We choose \( \epsilon > 0 \) so that \( \epsilon \max\{1, \epsilon\} \leq \min\{\delta_F - \|f_0\|_{C^1}, (\delta_F - \|f_0\|_{C^1})/\|(\partial F_0)^{-1}\|_{\infty}\} \). Suppose \( G \in \mathcal{F}(C^1_b) \) is so that \( d(F_0, G) < \epsilon \). We need to show \( \|G - F\| < \delta_F \). The definition of \( d(\cdot, \cdot) \) and Lemma 1.5 yield

\[
\|id - G \circ F_0^{-1}\|_{C^1} \leq \epsilon \max\{1, \epsilon\}
\]

(1.22)

Now the fact that \( F_0 \) is a homeomorphism and (1.22) yields \( \|F_0 - G\|_{\infty} = \|id - G \circ F_0^{-1}\|_{\infty} \leq \epsilon \max\{1, \epsilon\} \) and

\[
\|I - \partial G \circ F_0^{-1}\|_{\infty} = \|(\partial F_0 - \partial G)(\partial F_0)^{-1}\|_{\infty} = \|(I - \partial G(\partial F_0)^{-1}\|_{\infty} \leq \epsilon \max\{1, \epsilon\}
\]

(1.23)

Hence by our choice of \( \epsilon \),

\[
\|G - F\|_{\infty} \leq \|G - F_0\|_{\infty} + \|f_0\|_{\infty} < \delta_F
\]

(1.24)

and similarly

\[
\|\partial G - \partial F\| \leq \|\partial G - \partial F_0\|_{\infty} + \|\partial f_0\|_{\infty} \leq \|(\partial F_0)^{-1}\|_{\infty} \|(\partial G - \partial F_0)(\partial F_0)^{-1}\|_{\infty} + \|\partial f_0\|_{\infty} < \delta_F
\]

(1.25)

and this finishes the proof.

The following definitions are taken from [3] pp. 43

**Definition 1.8.** Let \( U \subset \mathcal{F}(C^1_b) \) be open. Given \( F \in \mathcal{F}(C^1_b), C^k(U, \{F\}) \), \( k \geq 0 \) denotes the set of all real-valued \( C^k \)-functions \( f : U \to \mathbb{R} \), so that dom(\( f \)) is an open subset of \( U \) and contains \( F \).

**Definition 1.9.** We denote by \( S^1(U, \{F\}) \) the set of all \( C^1 \) curves \( \gamma : (-\delta, \delta) \to \mathcal{F}(C^1_b) \), (the positive numbers \( \delta, \epsilon \) depend on \( \gamma \)) with \( \gamma(0) = F \).

**Definition 1.10.** Let \( F \in \mathcal{F}(C^1_b) \) be given and suppose that \( U \) is an open neighborhood of \( F \). Let \( \gamma_1, \gamma_2 \in S^1(U, \{F\}) \) be two \( C^1 \) curves with \( \gamma_2(0) = \gamma_1(0) = F \). We say that \( \gamma_1 \) and \( \gamma_2 \) are equivalent if

\[
\frac{d}{dt} f(\gamma_1(t))_{|t=0} = \frac{d}{dt} f(\gamma_2(t))_{|t=0}
\]

(1.26)

for all \( f \in C^\infty(U, \{F\}) \). The equivalence relation is denoted \( \sim \) and the equivalence classes by \( \langle \gamma \rangle_F \).
Definition 1.11. The tangent space of $F(C^b_1)$ at the point $F \in F(C^b_1)$ is defined by

$$T_F(F(C^b_1)) := S(U_F, \{F\})/\sim. \quad (1.27)$$

The tangent bundle is defined as disjoint union of all tangent space, that is, $T(F(C^b_1)) := \cup_{F \in F(C^b_1)} T_F(F(C^b_1))$.

Lemma 1.12. Let $(\varphi_F, U_F)$ be the chart defined in (1.16). If $h \in C^b_1(\mathbb{R}^d, \mathbb{R}^d)$ is such that

$$\partial(f \circ \varphi_F^{-1})(0)(h) = 0 \quad \text{for all } f \in C^\infty(U_F, \{F\}) \quad (1.28)$$

then we must have $h = 0$.

Proof. For every bounded and open set $\Omega \subset \mathbb{R}^d$ and for every $f \in C^\infty(\mathbb{R}^d)$ the function $f_\Omega(\hat{F}) := \int_{\hat{F}(\Omega)} f \, dx$ belongs to $C^\infty(U, \{F\})$. Indeed let $(\varphi_F, U_F)$ be the chart defined in (1.16), then $f_\Omega(h) := f_\Omega \circ \varphi_F^{-1}(h) = \int_{(F + h)(\Omega)} f \, dx$ and this function belongs to $C^\infty(B_{d_F}(0), B_{d_F}(0) \subset C^b_1(\mathbb{R}^d, \mathbb{R}^d)$.

Now let $x \in \mathbb{R}^d$ be fixed and choose an arbitrary unit vector $\hat{\nu} \in S^{d-1}$. Define the $C^1$-domain $\Omega_\nu := F^{-1}(\hat{\nu} + B(x)) = F^{-1}(B(x + \hat{\nu}))$, where $B(x)$ is the open unit ball in $\mathbb{R}^d$ centered at $x$. Notice that the outward pointing unit normal field along the ball $\hat{\nu} + B(x)$ is given by $\nu(x) = \frac{z - (x + \hat{\nu})}{|z - (x + \hat{\nu})|}$. Then by our assumption (1.28) yields

$$\partial f_{\Omega_\nu}(0)(h) = \int_{\partial(F(\Omega_\nu))} (h \circ F^{-1}) \cdot \nu \, ds = \int_{\partial(\hat{\nu} + B(x))} (h \circ F^{-1}) \cdot \nu \, ds = 0 \quad (1.29)$$

for all $f \in C^\infty(\mathbb{R}^d)$. The fundamental theorem of calculus of variations yields $(h \circ F^{-1}) \cdot \nu = 0$ on $\partial(\hat{\nu} + B(x))$. Observe $\nu(x) = -\hat{\nu}$ and thus $(h \circ F^{-1})(x) \cdot \nu = 0$. Since $\hat{\nu}$ was arbitrary we conclude $h \circ F^{-1}(x) = 0$ and since also the point $x$ was arbitrary we get $h \circ F^{-1} = 0$ on $\mathbb{R}^d$. Finally the bijectivity of $F$ yields $h = 0$ on $\mathbb{R}^d$ and we obtain the desired claim.

\[ \square \]

The previous lemma allows us for a fixed chart $(\varphi_F, U_F)$ to identify the tangent space $T_F(F(C^b_1))$ with a subspace of $C^b_1(\mathbb{R}^d, \mathbb{R}^d)$ via the mapping

$$T_F(F(C^b_1)) \rightarrow C^b_1(\mathbb{R}^d, \mathbb{R}^d) : \langle \gamma \rangle_F \mapsto \frac{d}{dt} \langle \varphi_F \circ \gamma \rangle|_{t=0}. \quad (1.30)$$

Indeed if $\gamma_1 \sim \gamma_2$, then the chain rule gives

$$\partial(f \circ \varphi_F^{-1})(0) \frac{d}{dt} \langle \varphi_F \circ \gamma_1 \rangle|_{t=0} = \frac{d}{dt} f(\gamma_1(t))|_{t=0} = \frac{d}{dt} f(\gamma_2(t))|_{t=0} \quad (1.31)$$

for all $f \in C^\infty(U_F, \{F\})$. Now an application of Lemma 1.12 yields

$$\frac{d}{dt} \langle \varphi_F \circ \gamma_1 \rangle|_{t=0} = \frac{d}{dt} \langle \varphi_F \circ \gamma_2 \rangle|_{t=0}. \quad (1.32)$$

This shows that (1.30) is well-defined and injective. It is also easily seen to be surjective. So we have proved:

Lemma 1.13. We have $T_F(F(C^b_1)) \simeq C^b_1(\mathbb{R}^d, \mathbb{R}^d)$ for all $F \in F(C^b_1)$ via the mapping (1.30).

Tangent space of quotient group Let $\Omega \subset \mathbb{R}^d$ be a set that is either closed or open and crack free. Recall that an open subset $\Omega \subset \mathbb{R}^d$ is called crack-free if $\text{int}(\Omega) = \Omega$. An important class of crack-free domains constitute $C^k_k$, $k \geq 1$ and polygonal domains. Under this assumption \[ \[ p.138, \text{Lemma 2.3} \] shows that the set $G(\Omega)$, defined in (1.6), is a closed subgroup of $F(C^b_1)$ (closed with respect to the topology defined by $d(\cdot, \cdot)$). Hence the quotient group $F(C^b_1)/G(\Omega)$ is well-defined.

The next definition tells us when functions are differentiable on the quotient group.

Definition 1.14. A function $f : F(C^b_1)/G(\Omega) \rightarrow \mathbb{R}$ is said to be differentiable if $F \mapsto f([F])$ is differentiable on $F(C^b_1)$. 

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Since our definition of tangent space only involves differentiable functions we may prove the following lemma.

**Lemma 1.15.** Let $\Omega$ be a $C^1$-domain. Then for every $[F] \in \mathcal{F}(C^1_b)/\mathcal{G}(\Omega)$ we have

\[ T_{[F]}(\mathcal{F}(C^1_b)/\mathcal{G}(\Omega)) \simeq \{(X, \dot{X}) : X, \dot{X} \in C^1_b(\mathbb{R}^d, \mathbb{R}^d) : (X \circ F^{-1}) \cdot \nu_F = (\dot{X} \circ F^{-1}) \cdot \nu_F \text{ on } F(\partial \Omega)\}. \]  

where $\nu_F$ is the unit normal field along $F(\partial \Omega)$. The latter set is isomorphic to the set of equivalence classes of $[X]$ where $X, \dot{X} \in C^1_b(\mathbb{R}^d, \mathbb{R}^d)$ are equivalent if and only if $X \circ \nu_F = \dot{X} \circ \nu_F$ on $F(\partial \Omega)$.

**Proof.** As in the proof of Lemma 1.12 we define for every open set $\Omega \subset \mathbb{R}^d$ and for every $f \in C^\infty_c(\mathbb{R}^d)$ the function $f_\Omega(F) := \int_{F(\Omega)} f \, dx$. It is clear that the mapping $F \mapsto f_\Omega([F])$ is well defined on $\mathcal{F}(C^1_b)$ and smooth.

Two curves $\gamma_1, \gamma_2 \in S^1(U_F, \{F\})$ are equivalent if $\frac{d}{dt} f(\gamma_1(t))|_{t=0} = \frac{d}{dt} f(\gamma_2(t))|_{t=0}$ for all $f \in C^\infty_c(U, \{F\})$. Therefore $\frac{d}{dt} f_\Omega([\gamma_1(t)])|_{t=0} = \frac{d}{dt} f_\Omega([\gamma_2(t)])|_{t=0}$ leads to

\[ \int_{F(\partial \Omega)} \frac{d}{dt} f(\gamma_1(t)) \cdot \nu_F \, ds = \int_{F(\partial \Omega)} \frac{d}{dt} f(\gamma_2(t)) \cdot \nu_F \, ds \quad \text{for all } f \in C^\infty_c(\mathbb{R}^d). \]  

The fundamental theorem of calculus of variations yields $\gamma_1(t) \circ F^{-1} \cdot \nu_F = \gamma_2(t) \circ F^{-1} \cdot \nu_F$ on $F(\partial \Omega)$. Since this relation only depends on the derivative of the curves $\gamma_1, \gamma_2$ at $t = 0$ we may choose without loss of generality the special curves $\gamma_1(t) := F + th_1$ and $\gamma_2(t) := F + th_2$, $h_1, h_2 \in C^1_b(\mathbb{R}^d, \mathbb{R}^d)$ yielding $(h_1 \circ F^{-1}) \cdot \nu_F = (h_2 \circ F^{-1}) \cdot \nu_F$ on $F(\partial \Omega)$.

\[ \square \]

# 2 Structure of first and second derivatives

## 2.1 Definition of first and second derivatives

The following definition recalls the standard notion of derivative of shape functions using perturbation of identity. For given set $D \subset \mathbb{R}^d$ we denote by $\mathcal{P}(D)$ the powerset of $D$.

**Definition 2.1.** Let $D \subset \mathbb{R}^d$ be an open set and $J : \Xi \subset \mathcal{P}(D) \to \mathbb{R}$ a shape function. Let $\Omega \in \Xi$ and $X, Y \in C^1_b(D, \mathbb{R}^d)$ be given.

(i) If $(\text{id}+tX)(\Omega) \in \Xi$ for all $t > 0$ sufficiently small, then the derivative of $J$ at $\Omega$ in direction $X$ is defined by

\[ DJ(\Omega)(X) := \lim_{t \searrow 0} \frac{J((\text{id}+tX)(\Omega)) - J(\Omega)}{t}. \]  

(ii) Suppose that $(\text{id}+tX+sY)(\Omega) \in \Xi$ for all sufficiently small $s$ and $t$. Then the second derivative of $J$ at $\Omega$ in direction $(X, Y)$ is defined by

\[ D^2J(\Omega)(X)(Y) = \frac{d^2}{dsdt} J((\text{id}+tX+sY)(\Omega))|_{s=t=0}. \]  

(iii) If $DJ((\text{id}+tX)(\Omega))(X)$ exists for all $t > 0$ sufficiently small, then the second Euler derivative of $J$ at $\Omega$ in direction $(X, Y)$ is defined by

\[ D^2J(\Omega)(X)(Y) = \lim_{t \searrow 0} \frac{DJ((\text{id}+tY)(\Omega))(X) - DJ(\Omega)(X)}{t}. \]  

**Definition 2.2.** Let $D \subset \mathbb{R}^d$ be an open and convex set and $J : \Xi \subset \mathcal{P}(D) \to \mathbb{R}$ be a shape function. Let $\Omega \in \Xi$ and $X, Y \in C([-\tau, \tau]; C^1_b(D, \mathbb{R}^d))$. Denote by $\Phi_t^X$ and $\Phi_t^Y$ the flow associated with $X$ and $Y$, respectively.

(i) If $\Phi_t^X(\Omega) \in \Xi$ for all $t > 0$ sufficiently small, then the Euler derivative of $J$ at $\Omega$ in direction $X$ is defined by

\[ dJ(\Omega)(X) = \lim_{t \searrow 0} \frac{J(\Phi_t^X(\Omega)) - J(\Omega)}{t}. \]  

(ii) If $\Phi_t^Y(\Omega) \in \Xi$ for all $t > 0$ sufficiently small, then the Euler derivative of $J$ at $\Omega$ in direction $Y$ is defined by

\[ dJ(\Omega)(Y) = \lim_{t \searrow 0} \frac{J(\Phi_t^Y(\Omega)) - J(\Omega)}{t}. \]  

(iii) If both $\Phi_t^X$ and $\Phi_t^Y$ exist and are continuous for all $t > 0$ sufficiently small, then the second Euler derivative of $J$ at $\Omega$ in direction $(X, Y)$ is defined by

\[ d^2J(\Omega)(X)(Y) = \lim_{t \searrow 0} \frac{dJ(\Omega)(\Phi_t^Y(\Omega))(X) - dJ(\Omega)(X)}{t}. \]  

(iv) If $\Phi_t^X$ and $\Phi_t^Y$ are both convex for all $t > 0$, then the second Euler derivative of $J$ at $\Omega$ in direction $(X, Y)$ is defined by

\[ d^2J(\Omega)(X)(Y) = \lim_{t \searrow 0} \frac{F_\Omega(\Phi_t^X(\Omega))(\Phi_t^Y(\Omega))(\Omega) - F_\Omega(\Omega)(\Omega)}{t}. \]  

where $F_\Omega(\cdot)$ is the Euler derivative of $J$ at $\Omega$.
(ii) If \( dJ(\Phi^Y_t(\Omega))(X) \) exists for all \( t > 0 \) sufficiently small, then the second Euler derivative of \( J \) at \( \Omega \) in direction \((X, Y)\) is defined by

\[
d^2 J(\Omega)(X)(Y) = \lim_{t \to 0} \frac{dJ(\Phi^Y_t(\Omega))(X) - dJ(\Omega)(X)}{t}.
\]

Remark 2.3. In order to have a well-defined flow \( \Phi^X_t \) for a vector field \( X \in C([-\tau, \tau]; \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d)) \), we assumed the convexity of the set \( \mathbb{D} \). Indeed the inclusion (1.1) shows that \( X(t, x) \) satisfies a Lipschitz condition on \([-\tau, \tau] \times \mathbb{D}\) with respect to the second argument. Then we may extend this function to a function \( \Phi^X_t \) defined on \([-\tau, \tau] \times \mathbb{R}^d\) satisfying a Lipschitz conditions with respect to the second argument. Then the flow of \( \Phi^X \) is globally well-defined thanks to the theorem of Picard-Lindelöf.

The next lemma provides a link between the Euler derivative and the derivative of \( J \).

Lemma 2.4. Let \( \Omega \subset \mathbb{D} \) and suppose \( \mathbb{D} \subset \mathbb{R}^d \) is convex. Suppose the Euler derivative \( dJ(\Omega) : C([-\tau, \tau]; \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d)) \to \mathbb{R} \) exists and is continuous.

(i) We have \( dJ(\Omega)(X) = dJ(\Omega)(0) \) for all \( X \in C([-\tau, \tau]; \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d)) \). So the Euler derivative only depends on the vector field \( X \) at time \( t = 0 \).

(ii) Let \( Y \in \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \). Then the flow \( T_t := \text{id} + tY \) is generated by the vector field \( X(t, x) := Y \circ (\text{id} + tY)^{-1}(x) \in \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \) and

\[
dJ(\Omega)(X) = dJ(\Omega)(X) = dJ(\Omega)(X(0)) = dJ(\Omega)(Y).
\]

(iii) Suppose \( \Omega \) is of class \( C^1 \). Then

\[
DJ(\Omega)(Y) = 0 \quad \forall Y \in \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \text{ with } Y \cdot \nu = 0 \text{ on } \partial\Omega,
\]

where \( \nu \) denotes the outward pointing normal vector field along \( \partial\Omega \).

Proof. (i) This directly follows from (ii) p.474, Theorem 3.1, item (ii).

(ii) Equation (2.6) is a direct consequence of (i).

(iii) Let \( \Omega \) be of class \( C^1 \) and suppose \( Y \in \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \) is such that \( Y \cdot \nu = 0 \) on \( \partial\Omega \). By Nagumo’s theorem \( \Phi^Y_t(\Omega) = \Omega \) for all \( t \) and hence \( dJ(\Omega)(Y) = 0 \) which in view of (2.6) yields \( DJ(\Omega)(Y) = 0 \).

Definition 2.5. Let \( \mathbb{D} \subset \mathbb{R}^d \) be an open set and \( J : \Xi \subset \varphi(\mathbb{D}) \to \mathbb{R} \) a shape function. Let \( X, Y \in \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \).

(i) The function \( J \) is said to be differentiable at \( \Omega \in \Xi \) if:

- \( DJ(\Omega)(X) \) exists for all \( X \in \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \), and
- the mapping \( DJ(\Omega) : \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \to \mathbb{R} \) is linear and continuous.

We say \( J \) is differentiable if it is differentiable at all \( \Omega \in \Xi \).

(ii) The function \( J \) is said to be twice differentiable at \( \Omega \in \Xi \) if:

- \( J \) is differentiable at \( \Omega \),
- \( D^2 J(\Omega)(X)(Y) \) exists for all \( X, Y \in \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \), and
- the mapping \( D^2 J(\Omega) : \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \times \tilde{C}^1_b(\mathbb{D}, \mathbb{R}^d) \to \mathbb{R} \) is bilinear and continuous.

We say \( J \) is twice differentiable if it is twice differentiable at all \( \Omega \in \Xi \).

Example 2.6. As an illustration of the previous definition consider \( J(\Omega) = \int_\Omega f \, dx \), where \( \Omega \subset \mathbb{R}^d \) is bounded and open. If \( f \in C^1(\mathbb{R}^d) \), then \( J \) is differentiable at \( \Omega \) with derivative in direction \( X \in \tilde{C}^1_b(\mathbb{R}^d, \mathbb{R}^d) \) given by

\[
DJ(\Omega)(X) = \int_\Omega S_1 : \partial X + S_0 \cdot X \, dx, \quad S_1(x) := f(x)I, \ S_0(x) := \nabla f(x).
\]
Part (iii) follows since by Lemma 2.4 we have

\[ \mathbf{D}^2 J(\Omega)(X)(Y) = \int_{\Omega} T_1(X) : \partial Y + T_0(X) \cdot Y \, dx, \]

where \( X, Y \in \mathcal{C}_b^1(\mathbb{R}^d, \mathbb{R}^d) \) and \( T_1(X) := (\partial \text{div} f + \nabla f \cdot X) - \partial X^T f, T_0(X) := \nabla^2 f X + \text{div}(X)\nabla f. \) Notice that \( \mathbf{D}^2 J(\Omega)(X)(Y) \) exists for all \( X, Y \in \mathcal{C}_b^2(\mathbb{R}^d, \mathbb{R}^d) \) and is given by

\[ \mathbf{D}^2 J(\Omega)(X)(Y) = \mathbf{D}^2 J(\Omega)(X)(Y) + D\mathbf{J}(\Omega)(\partial XY). \]  

It will be shown in Lemma 2.10 that under suitable conditions this identity always holds. From (2.9) it can be seen that the second Euler derivative may fail to exist for \( X \) only being \( C^1 \)-regular, however, \( J(\cdot) \) can still be twice differentiable. Also notice that the computation of \( \mathbf{D}^2 J(\Omega)(X)(Y) \) requires the vector fields \( X, Y \) to belong to \( \mathcal{C}_b^2(\mathbb{R}^d, \mathbb{R}^d) \) while the computation of \( \mathbf{D} J^2(\Omega)(X)(Y) \) only requires the vector fields to be in \( \mathcal{C}_b^1(\mathbb{R}^d, \mathbb{R}^d) \).

### 2.2 Quotient space and restriction mapping

Let \( D \subset \mathbb{R}^d \) be a given open set. We define for every set \( \Omega \subset D \) and integer \( k \geq 0 \) the linear space

\[ T^k(\partial \Omega) := \{ X \in \mathcal{C}_b^k(D, \mathbb{R}^d) | X = 0 \text{ on } \partial \Omega \}. \]  

By definition \( T^k(\partial \Omega) \subset \mathcal{C}_b^k(D, \mathbb{R}^d) \) and \( T^k(\partial \Omega) \) is closed. We introduce an equivalence relation on \( \mathcal{C}_b^k(D, \mathbb{R}^d) \) as follows: two vector fields \( X, Y \in \mathcal{C}_b^k(D, \mathbb{R}^d) \) are equivalent, written \( X \sim Y \), if and only if \( X = Y \) on \( \partial \Omega \). In other words two vector fields are equivalent if their restriction at \( \partial \Omega \) coincides. We denote the set of equivalence classes and its elements by \( Q^k(\partial \Omega) \) and \( [X] \), respectively. We denote by \( \tilde{\mathfrak{J}}_{\partial \Omega} \) the restriction mapping of vector field belonging to \( \mathcal{C}_b^k(D, \mathbb{R}^d) \) to mappings \( \partial \Omega \rightarrow \mathbb{R}^d \), that is,

\[ \tilde{\mathfrak{J}}_{\partial \Omega} : \mathcal{C}_b^k(D, \mathbb{R}^d) \rightarrow \partial \Omega^{\mathbb{R}^d}, \quad X \mapsto X_{|\partial \Omega}. \]

where \( \partial \Omega^{\mathbb{R}^d} \) denotes the space of all mappings from \( \partial \Omega \) into \( \mathbb{R}^d \). The mapping \( \tilde{\mathfrak{J}}_{\partial \Omega} \) induces the mapping

\[ \hat{\mathfrak{J}}_{\partial \Omega} : Q^k(\partial \Omega) \rightarrow \partial \Omega^{\mathbb{R}^d} \]

and by definition \( \tilde{\mathfrak{J}}_{\partial \Omega} = \hat{\mathfrak{J}}_{\partial \Omega} \circ \pi \).

### 2.3 First structure theorem

The following theorem provides the structure of the first shape derivative of a shape function \( J : \Xi \subset \varphi(D) \rightarrow \mathbb{R} \).

**Theorem 2.7.** Let \( \Omega \) be an open and bounded subset of the open hold-all \( D \subset \mathbb{R}^d \). Suppose that \( D\mathbf{J}(\Omega)(X) \) exists for all \( X \in \mathcal{C}_b^1(D, \mathbb{R}^d) \) and assume that \( X \mapsto D\mathbf{J}(\Omega)(X) \) is linear.

(i) Then there is a linear mapping \( \hat{g} : \text{im}(\tilde{\mathfrak{J}}_{\partial \Omega}) \rightarrow \mathbb{R} \) such that

\[ D\mathbf{J}(\Omega)(X) = \hat{g}(X_{|\partial \Omega}) \]  

for all \( X \in \mathcal{C}_b^1(D, \mathbb{R}^d) \), where \( \text{im}(\tilde{\mathfrak{J}}_{\partial \Omega}) := \{ \tilde{\mathfrak{J}}_{\partial \Omega}(X) | X \in Q^1(\partial \Omega) \} \) denotes the image of \( \tilde{\mathfrak{J}}_{\partial \Omega} \).

(ii) Suppose \( \Omega \) is of class \( C^1 \) and \( D\mathbf{J}(\Omega) : \mathcal{C}_b^1(D, \mathbb{R}^d) \rightarrow \mathbb{R} \) is continuous. Then \( \text{im}(\tilde{\mathfrak{J}}_{\partial \Omega}) = C^1(\partial \Omega, \mathbb{R}^d) \) and \( \hat{g} : C^1(\partial \Omega, \mathbb{R}^d) \rightarrow \mathbb{R} \) is a continuous functional.

(iii) Suppose \( \Omega \) is of class \( C^2 \) and \( D \) is convex. Assume the Euler derivative \( d\mathbf{J}(\Omega) : C([-\tau, \tau]; \mathcal{C}_b^1(D, \mathbb{R}^d)) \rightarrow \mathbb{R} \) exists and is continuous and linear. Then \( g(v) := \hat{g}(v\nu) \), where \( \hat{g} \) is the function from item (ii), is continuous on \( C^1(\partial \Omega) \) and satisfies

\[ D\mathbf{J}(\Omega)(X) = g(X_{|\partial \Omega} \cdot \nu) \]  

for all \( X \in \mathcal{C}_b^1(D, \mathbb{R}^d) \).

**Proof.** This is a version of the structure theorem from [30]. Part (i) and (ii) follow the lines of the proof of [30]. Part (iii) follows since by Lemma 2.4 we have \( d\mathbf{J}(\Omega)(X) = D\mathbf{J}(\Omega)(X) \) for all \( X \in \mathcal{C}_b^1(D, \mathbb{R}^d) \). \( \square \)
2.4 Second structure theorem

This section is devoted to the second structure theorem that provides a structure of $D^2J(\Omega)$. For more information we refer to [4, 20] and [3] pp. 501.

**Lemma 2.8.** Let $X, Y \in \mathcal{C}_b^2(D, \mathbb{R}^d)$. Suppose that $f(s, h) := J((\text{id} + sX + hY)(\Omega))$ is well defined on $U := (-\tau, \tau) \times (-\tau, \tau)$, $\tau > 0$, and continuously partially differentiable at zero. Then

$$D^2J(\Omega)(X)(Y) = D^2J(\Omega)(Y)(X).$$

(2.14)

*Proof.* This is a consequence of Schwarz’s theorem. Particularly $f$ is twice continuously differentiable on $U$. \qed

**Remark 2.9.** If the function $f$, defined in Lemma 2.8, is not twice continuously differentiable the derivative $D^2J(\Omega)$ may be non-symmetric. Consider for instance $J(\Omega) = \int_{\Omega} f \, dx$ with $f$ only twice differentiable on $\mathbb{R}^d$. Then $\nabla^2 f(x)$ is not necessarily symmetric which destroys the symmetry of $D^2J(\Omega)$.

The following theorem is called second structure theorem as it provides the structure of $D^2J(\Omega)$.

**Theorem 2.10.** Suppose the following conditions are satisfied at an open set $\Omega \subset \mathbb{R}^d$.

(a) The shape function $J$ is twice differentiable at $\Omega$.

(b) There is $\epsilon > 0$ so that $J$ is differentiable at $(\text{id} + X)(\Omega)$ for all $X \in B_{\epsilon}(0) \subset \mathcal{C}^1_b(D, \mathbb{R}^d)$. Moreover, $X \mapsto DJ((\text{id} + X)(\Omega)) : B_{\epsilon}(0) \to \mathcal{L}(C^1_b(D, \mathbb{R}^d), \mathbb{R})$ is continuous at $X = 0$.

Then we have for all $X, Y \in \mathcal{C}^2_b(\mathbb{D}, \mathbb{R}^d)$,

$$D^2J(\Omega)(X)(Y) = D^2J(\Omega)(Y)(X) + DJ(\Omega)(\partial XY)$$

(2.15)

and

$$\lim_{s \to 0} DJ((\text{id} + sX)(\Omega)) \left( \frac{X \circ (\text{id} + sY)^{-1} - X}{s} \right) = -DJ(\Omega)(\partial XY).$$

(2.16)

The symmetrical part is given by

$$D^2J(\Omega)(X)(Y) = \frac{d}{ds} DJ((\text{id} + sY)(\Omega))(X \circ (\text{id} + sY)^{-1})|_{s=0}. \quad (2.17)$$

*Proof.* At first since $X, Y \in \mathcal{C}^2_b(\mathbb{D}, \mathbb{R}^d)$, we conclude

$$\left\| \frac{X \circ (\text{id} + sY)^{-1} - X}{s} + \partial XY \right\|_{C^1} \to 0 \quad \text{as} \ s \to 0. \quad (2.18)$$

Then by direct estimation for $s > 0$

$$|DJ((\text{id} + sY)(\Omega)) \left( \frac{X \circ (\text{id} + sY)^{-1} - X}{s} \right) + DJ(\Omega)(\partial XY)|$$

$$\leq |DJ((\text{id} + sY)(\Omega)) \left( \frac{X \circ (\text{id} + sY)^{-1} - X}{s} + \partial XY \right) | + |DJ((\text{id} + sY)(\Omega))(\partial XY) - DJ(\Omega)(\partial XY)|$$

$$\leq \|DJ((\text{id} + sY)(\Omega))\|_{\mathcal{L}(C^1, \mathbb{R})} \left\| \frac{X \circ (\text{id} + sY)^{-1} - X}{s} + \partial XY \right\|_{C^1} + \|DJ((\text{id} + sY)(\Omega)) - DJ(\Omega)\|_{\mathcal{L}(C^1, \mathbb{R})} \|\partial XY\|_{C^1}. \quad (2.19)$$

Taking into account assumption (b) and (2.18) we see that the right hand side tends to zero as $s \to 0$ and this shows (2.16).
Consider from the definition of the derivative, 
\[
\mathcal{D}^2 J(\Omega)(X)(Y) = \frac{d^2}{dsdt} J((id+sY + tX)(\Omega))|_{t=s=0} = \frac{d}{ds} DJ((id+sY)(\Omega))(X \circ (id+sY)^{-1})|_{s=0}.
\]  
(2.20)

Now on a account of (2.16) and (2.20), we get
\[
D^2 J(\Omega)(X)(Y) = \lim_{s \to 0} \frac{DJ((id+sY)(\Omega))(X) - DJ(\Omega)(X)}{s} = -\lim_{s \to 0} \frac{DJ((id+sY)(\Omega))\left(\frac{X \circ (id+sY)^{-1} - X}{s}\right)}{s} + \lim_{s \to 0} \frac{DJ((id+sY)(\Omega))(X \circ (id+sY)^{-1}) - DJ(\Omega)(X)}{s}
\]
\[
= DJ(\Omega)(\partial XY) + \mathcal{D}^2 J(\Omega)(X)(Y).
\]

Example 2.11. Consider \( J(\Omega) := \int_\Omega f \, dx \) with \( f \in C_c^\infty(\mathbb{R}^d) \). Then \( h \mapsto J((id+h)(\Omega)) : B_\epsilon(0) \subset C^1_b(\mathbb{R}^d, \mathbb{R}^d) \to \mathbb{R} \) is infinitely often differentiable for all \( \epsilon > 0 \) small enough. However, \( D^2 J(\Omega)(X)(Y) \) does not exist in general for \( X, Y \in C^1_b(\mathbb{R}^d, \mathbb{R}^d) \).

2.5 Third structure theorem

In this section proof a third structure theorem that provides a generic form of the symmetrical part of the second Euler derivative. We will derive this theorem with the help of the first and second structure theorem. We refer the reader to [26] for a different proof of the following theorem.

In the following we use the notation \( X_\tau := X_{\nu_{\Omega}} - (X_{\nu_{\Omega}} \cdot \nu)\nu \) and \( A_\tau := A_{\nu_{\Omega}} - (A_{\nu_{\Omega}} \cdot \nu) \otimes \nu \) to indicate the tangential part of the vector fields \( X \in \mathcal{C}^1_b(\mathbb{D}, \mathbb{R}^d) \) and \( A \in \mathcal{C}^1_b(\mathbb{D}, \mathbb{R}^{d \times d}) \) restricted to \( \partial \Omega \). Here \( \nu \) is a unit vector field along \( \partial \Omega \) and \( \otimes \) denotes the tensor product defined by \( (a \otimes b)c := (c \cdot b)a \) for all \( a, b, c \in \mathbb{R}^d \). The tangential gradient of \( f \in C^1(\partial \Omega) \) and Jacobian and divergence of \( g \in C^1(\partial \Omega, \mathbb{R}^d) \) can then be defined by \( \nabla^r f := (\nabla f)_\tau \), \( \partial^r g := (\partial g)_\tau \), and \( \div^r : g = \partial^r g : I \).

The following theorem will be referred to as third structure theorem.

Theorem 2.12. Let \( \Omega \) be an open and bounded subset of the open and convex hold-all set \( \mathcal{D} \subset \mathbb{R}^d \). Suppose that \( J \) satisfies the assumptions (a) and (b) of Theorem 2.10 at \( \Omega \).

(i) There are mappings \( \bar{g} : \text{im}(\nu_{\partial \Omega}) \to \mathbb{R} \) and \( \bar{l} : \text{im}(\nu_{\partial \Omega}) \times \text{im}(\nu_{\partial \Omega}) \to \mathbb{R} \), so that
\[
\mathcal{D}^2 J(\Omega)(X)(Y) = \bar{l}(X_{\nu_{\Omega}}, Y_{\nu_{\Omega}}) \quad \text{and} \quad DJ(\Omega)(\partial XY) = \bar{g}((\partial XY)_{\nu_{\Omega}})
\]  
(2.21)

and hence
\[
D^2 J(\Omega)(X)(Y) = \bar{l}(X_{\nu_{\Omega}}, Y_{\nu_{\Omega}}) + \bar{g}((\partial XY)_{\nu_{\Omega}})
\]  
(2.22)

for all \( X, Y \in \mathcal{C}^2(\mathbb{D}, \mathbb{R}^d) \).

(ii) If \( \partial \Omega \in C^1 \), then \( \text{im}(\nu_{\partial \Omega}) = C^1(\partial \Omega, \mathbb{R}^d) \) and \( \bar{g} \) and \( \bar{l} \) are continuous on \( C^1(\partial \Omega, \mathbb{R}^d) \).

(iii) Suppose \( \partial \Omega \in C^2 \). Assume that for all \( X \in \mathcal{C}^1_b(\mathbb{D}, \mathbb{R}^d) \) the mappings \( dJ(\Omega), d^2 J(\Omega)(X) : C([-\tau, \tau]; \mathcal{C}^1_b(\mathbb{D}, \mathbb{R}^d)) \to \mathbb{R} \) are continuous and linear. Then \( g(\nu) := \bar{g}(\nu \nu) \) and \( l(\nu, w) := \bar{l}(\nu \nu, \nu w) \) are continuous on \( C^1(\partial \Omega) \) and satisfy
\[
\mathcal{D}^2 J(\Omega)(X)(Y) = l(X_{\nu_{\Omega}} \cdot \nu, Y_{\nu_{\Omega}} \cdot \nu) - g(\nabla^r (Y_{\nu_{\Omega}} \cdot \nu) \cdot X_\tau) - g(\nabla^r (X_{\nu_{\Omega}} \cdot \nu) \cdot Y_\tau)
\]  
(2.23)

valid for all \( X, Y \in \mathcal{C}^2(\mathbb{D}, \mathbb{R}^d) \).
Proof. (i): At first on account of Theorem \[2.10\] we have

\[
D^2J(\Omega)(X)(Y) = \mathfrak{D}^2J(\Omega)(X)(Y) + DJ(\Omega)\partial XY
\]

for all \(X, Y \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d)\). Let \(X, Y \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d)\). The Banach fix point theorem shows that \(T_{s,\tau} := \text{id} + sX + tY\) is bijective on \(\mathbb{R}^d\) for all \(|s| + |t| < 1/\max\{\|X\|_{C^1}, \|Y\|_{C^1}\}\). Moreover if \(X = Y = 0\) on \(\partial \Omega\), then \(T_{s,\tau}(\Omega) = \Omega\) for all such \(s, t\). Thus we have

\[
\mathfrak{D}^2J(\Omega)(X)(Y) = 0 \quad \text{for all } X, Y \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d) \quad \text{with } X = Y = 0 \text{ on } \partial \Omega.
\]

Hence the mapping \(h([X], [Y]) := \mathfrak{D}^2J(\Omega)(X)(Y)\) is well defined for all \([X], [Y] \in Q^1(\partial \Omega)\). Since \(\mathfrak{D}^2J(\Omega)\) is a bijection on its image \(\text{im}(\mathfrak{D}^2J(\Omega))\), we may define \(\tilde{h}(V, W) := h(\tilde{\mathfrak{D}}^{-1}(V), \tilde{\mathfrak{D}}^{-1}(W))\) which satisfies by definition

\[
\tilde{h}(X, Y) := \tilde{h}(\tilde{\mathfrak{D}}(X), \tilde{\mathfrak{D}}(Y)) = h([X], [Y]) = \mathfrak{D}^2J(\Omega)(X)(Y)
\]

for all \(X, Y \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d)\). Finally by the first structure theorem (Theorem \[2.7\]), we have \(DJ(\Omega)(X) = \tilde{g}(X)\) for all \(X \in C^1(\partial \Omega)\) and plugging this and (2.26) into (2.24) we recover (2.22) and also (2.21).

(ii) This follows from the continuity of the extension operator.

(iii) At first note that since \(\Omega\) is \(C^2\), Theorem \[2.7\] item (iii) yields that \(g(v) := \tilde{g}(v\nu)\) is continuous on \(C^1(\partial \Omega)\) and satisfies \(DJ(\Omega)(Z) = g(Z \cdot \nu)\) for all \(Z \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d)\). Notice that \(T_{\nu}\) is the flow of the vector field \(Y(t, z) := Y \circ (id + tY)^{-1}(z) \in C([-\tau, \tau]; \hat{C}^1_b(\mathfrak{D}, \mathbb{R}^d))\). Therefore Lemma \[2.4\] shows \(0 = d^2J(\Omega)(X)(Y) = d^2J(\Omega)(X)(Y) = D^2J(\Omega)(X)(Y)\) for all \(X, Y \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d)\) with \(Y \cdot \nu = 0\) on \(\partial \Omega\). In view of (2.22) this yields

\[
\tilde{h}(X, Y) = -g((\partial X) Y, Y, \nu) \quad \text{for all } X, Y \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d) \quad \text{with } Y \cdot \nu = 0 \text{ on } \partial \Omega.
\]

Now (2.22) with \(\nu = 0\) on \(\partial \Omega\) follows from the continuity of the extension operator.

Remark 2.13. Notice that the second part of formula (2.23) can be written by noting that

\[
0 = g(\partial^\tau X, Y) = g(\partial^\tau XY, Y) - g(\partial^\tau((X \cdot \nu)Y), Y)
\]

\[
= g(\partial^\tau XY, Y) - g(\partial^\tau(X \cdot \nu, Y), Y)
\]

\[
g(\nabla^\tau(Y) \cdot X) = g(\nu, \partial^\tau Y X) + g(Y \cdot \partial^\tau X)
\]

for all \(X, Y \in \hat{C}^2(\mathfrak{D}, \mathbb{R}^d)\). The continuity of \(l\) follows from the continuity of the extension operator.
where we used \((\partial^r \nu)\)\(\nu = 0\). Substituting this into \((2.23)\) we obtain

\[
\Delta^2 J(\Omega)(X)(Y) = l(X \cdot \nu, Y \cdot \nu) - g(\nu \cdot \partial^r Y X_{\tau}) - g(Y_{\tau} \cdot \partial^r \nu X_{\tau}) - g(\nu \cdot \partial^r Y Y_{\tau})
\]  

(2.34)

which is precisely equation (2.7) in [26].

**Remark 2.14.** Notice that to get the explicit structure \((2.23)\) of the second derivative we need the vector fields \(X, Y\) to belong to \(C^2\). However, the second derivative \(\Delta^2 J(\Omega)(X)(Y)\) is already well-defined for \(X, Y \in C^1\). This can explicitly be seen from Example 2.7.

**Remark 2.15.** At a stationary point \(\Omega^*\) of \(J\), we have by definition \(DJ(\Omega^*)(X) = 0\) for all \(X \in \tilde{C}_b^2(D, R^d)\), which implies \(g = 0\) when \(\partial \Omega^*\) belongs to \(C^2\). In this case the previous theorem shows \(\Delta^2 J(\Omega^*)(X)(Y) = l(X_{\tau}, Y_{\tau}, \nu)\) for all \(X, Y \in \tilde{C}_b^2(D, R^d)\). So even though werestrict ourselves to the boundary \(\partial \Omega^*\), the second derivative can only be positive semi-definite on the hole space \(C^1(\partial \Omega^*, R^d)\).

### 2.6 First and second shape Hessian

**First shape Hessian** We have seen that \(\mathcal{F}(C_b^1)\) is a smooth Banach manifold. So we may define a Hessian on it as follows.

**Definition 2.16.** Let \(D \subset R^d\) be open. Let \(J : \Xi \subset \varphi(D) \to R\) be a twice shape differentiable. The first shape Hessian \(H_{\Omega,J}^1 : C_b^2(D, R^d) \times C_b^2(D, R^d) \to R\) at \(\Omega \in \Xi\) is defined by

\[
H_{\Omega,J}^1(X, Y) := \Delta^2 J(\Omega)(X)(Y).
\]  

(2.35)

Notice that if the hypotheses of Lemma 2.8 are satisfied for \(J\) at \(\Omega\) then the first shape Hessian is symmetric.

**Remark 2.17.** (i) Fix a set \(\Omega \subset R^d\) and let a shape function \(J : \chi(\Omega) \subset \varphi(R^d) \to R\) be given, where the set \(\chi(\Omega)\) was introduced in (1.4). Then we may identify the shape function \(J\) with functions \(\tilde{J} \in C^1(\mathcal{F}(C_b^1))\) via \(F \mapsto \tilde{J}(F) := J(F(\Omega))\). The first shape Hessian can be identified as an object \(\mathcal{F}(C_b^1) \to (T\mathcal{F}(C_b^1) \times T\mathcal{F}(C_b^1))^*, F \mapsto H_{\tilde{J}(F)}^1\), where \((T\mathcal{F}(C_b^1) \times T\mathcal{F}(C_b^1))^*\) denote the union of all cotangent spaces \(\mathcal{L}(T_F\mathcal{F}(C_b^1) \times T_F\mathcal{F}(C_b^1)), F \in \mathcal{F}(C_b^1)\).

(ii) In view of identity \((2.24)\) (valid under the assumptions stated in the theorem) the shape Hessian has the form \(H_{\Omega,J}^1(X, Y) = D^2 J(\Omega)(X)(Y) - DJ(\Omega)(\partial XY)\) valid for \(X, Y \in C_b^2(D, R^d)\). Now \(T\mathcal{F}(C_b^1) \times T\mathcal{F}(C_b^1) \to T\mathcal{F}(C_b^1), (X, Y) \mapsto \nabla_X Y := \partial XY\) is the Euclidean connection on \(R^d\) and \(D^2 J(\Omega)(X)(Y)\) can be interpreted as the second Lie derivative. Hence this observation and (i) let us conclude that our definition of the shape Hessian coincides with the typical definition of the Hessian on the manifold \(\mathcal{F}(C_b^1)\).

**Second shape Hessian** As we have seen at a fixed point \(F \in \mathcal{F}(C_b^1)\) the first shape Hessian \(H_{\Omega,J}^1\) cannot be positive definite on \(T_F\mathcal{F}(C_b^1) = C_b^1(R^d, R^d)\), but only on a subspace. The reason for that is that the function \(F \mapsto J(F(\Omega))\) has the same value for transformations \(F, \tilde{F}\) that are equivalent and thus belong to the same equivalence class of \(\mathcal{F}(C_b^1)/\mathcal{G}(\Omega)\). Therefore it makes sense to define a shape Hessian on \(\mathcal{F}(C_b^1)/\mathcal{G}(\Omega)\) that quotients out those transformations. In view of the third structure theorem (Theorem 2.12) we know how define such a Hessian (called second shape Hessian).

**Definition 2.18.** Let \(D \subset R^d\) be open and convex. Suppose \(J : \Xi \subset \varphi(D) \to R\) is twice differentiable. Let \(\Omega \in \Xi\) be an open and bounded set with \(C^2\)-boundary. Let \(g : C^1(\partial \Omega) \to R\) be the function obtained from the first structure theorem (Theorem 2.7). Then the second shape Hessian at \(\Omega\) is defined by

\[
H_{\Omega,J}^2(X)(Y) := H_{\Omega,J}^1(X)(Y) + g(\nabla^\tau (Y \cdot \nu) \cdot X_{\tau} + \nabla^\tau (X \cdot \nu) \cdot Y_{\tau})
\]  

(2.36)

for all \(X, Y \in \tilde{C}_b^2(D, R^d)\).

**Remark 2.19.** By construction the first and second shape Hessian coincide in a stationary point \(\Omega^*\) since then \(g = 0\).
Remark 2.20. If \( F \in \mathcal{F}(C^1_0) \) is so that \( F - \text{id} \in C^2 \), then the second Hessian is a well-defined mapping \( H^2_{\tau(F)}(\mathcal{F}(C^1_0)/\mathcal{G}(\Omega)) \to \mathbb{R} \). In fact according to Theorem 2.12 the second shape Hessian depends only on normal components \( X \cdot \nu \) and \( Y \cdot \nu \) on \( \partial \Omega \) so it is well-defined on \( T_{\tau(F)}(\mathcal{F}(C^1_0)/\mathcal{G}(\Omega)) \).

Remark 2.21. In \([3]\) a special second derivative along normal perturbations is computed to rule out tangential perturbations. The authors obtain a boundary expression of the second derivative which is extended to the whole domain \( \mathbb{R}^d \). This is in contrast to our approach where we choose special basis functions to rule out "pure" tangential perturbations. Our Hessian only depends on normal perturbations by definition.

Example of first and second shape Hessians  Let us again consider \( J(\Omega) := \int_{\Omega} f \, dx \), where \( f \in C^2(\mathbb{R}^d) \) and \( \Omega \subset \mathbb{R}^d \) is open and bounded. In Example 2.6 we computed the first shape Hessian of \( J \), namely

\[
H_{\Omega,1}(X)(Y) = \int_{\Omega} T_1(X) : \partial Y + T_0(X) \cdot Y \, dx,
\]

(2.37)

where \( X, Y \in \mathcal{C}^1_0(\mathbb{R}^d, \mathbb{R}^d) \) and \( T_1(X) := (f(\nabla f) + \nabla f \cdot X)I - \partial X^T f \) and \( T_0(X) = \nabla^2 f(X) + \text{div}(X) \nabla f \).

Since \( \mathcal{D}^2 J(\Omega)(X)(Y) = 0 \) for all \( X \in C^2(\mathbb{R}^d, \mathbb{R}^d) \) with \( \text{supp}(X) \subset \Omega \), we conclude by partial integration \(- \text{div}(T_1(X)) + T_0(X) = 0 \) everywhere in \( \Omega \) which shows by partial integration \( \mathcal{D}^2 J(\Omega)(X)(Y) = \int_{\partial \Omega} T_1(X) \nu \cdot Y \, ds \) for all \( X \in C^2(\mathbb{R}^d, \mathbb{R}^d) \). Then by splitting the restrictions of \( X, Y \) to \( \partial \Omega \) into normal and tangential part and assuming \( \partial \Omega \) is of class \( C^2 \) we may check

\[
\mathcal{D}^2 J(\Omega)(X)(Y) = \int_{\partial \Omega} T_1(X) \nu \cdot Y \, ds
\]

(2.38)

\[
= \int_{\partial \Omega} (f(\nabla f(X) + \nabla X \cdot Y)(Y \cdot \nu) - fX^T \nu \cdot Y \, ds
\]

\[
= \int_{\partial \Omega} (\nabla f \cdot X + \kappa f)(X \cdot Y) \, ds - \int_{\partial \Omega} fX^T(Y \cdot \nu) \cdot X + fX^T(Y \cdot \nu) \cdot Y \, ds,
\]

where \( \kappa := \text{div}_r(\nu) \) is the mean curvature of \( \partial \Omega \) and in the last step we used the tangential Stokes formula \([6] \text{p.} 498\). Notice that (2.38) has the predicted form (2.23). From (2.38) we also see that the second shape Hessian is given by

\[
H^2_{\Omega,1}(X)(Y) = \int_{\partial \Omega} (\nabla f \cdot X + \kappa f)(X \cdot Y) \, ds
\]

(2.39)

for all \( X, Y \in C^2(\mathbb{R}^d, \mathbb{R}^d) \).

Remark 2.22 (Positive definiteness). As a conclusion we see that the second shape Hessian of \( J \) will be positive definite on the quotient \( T_{\tau(F)}(\mathcal{F}(C^1_0)/\mathcal{G}(\Omega)) \) if \( \nabla f \cdot \nu + \kappa c > \epsilon \) on \( \partial \Omega \) for some constant \( \epsilon > 0 \). Then

\[
H^2_{\Omega,1}(J)(X)(X) \geq \epsilon \|X \cdot \nu\|^2 L_{\tau(\partial \Omega)}.
\]

(2.40)

Of course the Hessian does not need to be positive definite in a stationary point as illustrated by the following example.

Remark 2.23 (Saddle points). Consider \( \Omega^* = (-1,1) \) and define \( f \in C^3(\mathbb{R}) \) by

\[
f(x) := \begin{cases} 
(x-1)^4 & \text{if } x > 1, \\
0 & \text{if } x \in [-1,1], \\
-(x+1)^4 & \text{if } x < 1,
\end{cases}
\]

(2.41)

Then \( \Omega^* \) is a stationary point since \( DJ(\Omega^*)(X) = 0 \) for all \( X \in C^1_0(\mathbb{R}, \mathbb{R}) \). But also the second derivative vanishes identically \( \mathcal{D}^2 J(\Omega^*)(X)(X) = 0 \) for all \( X, Y \in C^2_0(\mathbb{R}, \mathbb{R}) \). As a conclusion a set \( \Omega \) may be a stationary point, but not a local minimum. Let us slightly modify the above function \( f \) to \( \tilde{f} \):

\[
\tilde{f}(x) := \begin{cases} 
(x-1)^4 & \text{if } x > 1, \\
0 & \text{if } x \in [-1,1], \\
(x+1)^4 & \text{if } x < 1,
\end{cases}
\]

(2.42)

Then \( DJ(\Omega^*) = 0 \) and \( \mathcal{D}^2 J(\Omega^*) = 0 \), but \( \Omega^* \) is even a global minimum of \( J \).
2.7 Relation between quotient space and first derivative

Let $J$ be a shape function that is differentiable at $F(\Omega)$, where $\Omega$ is a $C^2$-domain and $F \in \mathcal{F}(C^1_b)$. Recall that $T_F(\mathcal{F}(C^1_b)) = C^1_b(R^d, R^d)$ and $T_{\pi(F)}(\mathcal{F}(C^1_b)/\mathcal{G}(\Omega)) = C^1_b(R^d, R^d)/\sim$, where $\sim$ is defined by $X \sim \tilde{X}$ if and only if $X \cdot \nu = \tilde{X} \cdot \nu$ on $F(\partial \Omega)$. Here $\nu$ is the normal vector field along $F(\partial \Omega)$. Then the link between the shape derivative, structure theorem and the tangent space is given by Figure 1, we have the following diagram.

The function $\overline{DJ}(F(\Omega))$ in Figure 1 is defined by $\overline{DJ}(F(\Omega))(\lfloor X \rfloor) := DJ(F(\Omega))(X)$ for all $\lfloor X \rfloor \in T_{\pi(F)}(\mathcal{F}(C^1_b)/\mathcal{G}(\Omega))$. Notice that if $F - \text{id}$ is only of class $C^1$ the normal vector field along $F(\partial \Omega)$ is only continuous and we can not apply the structure theorem to $DJ(\Omega)$ (unless $DJ(F(\Omega))$ is continuous on $C^0_b(R^d, R^d)$).

3 Approximate normal basis functions

This section is devoted to the construction of basis functions with which we can approximate the first and second shape Hessian.

3.1 Reproducing kernel Hilbert spaces

We begin with the definition of matrix-valued reproducing kernels.

**Definition 3.1.** Let $\mathcal{X} \subset R^d$ be an arbitrary set. A function $K : \mathcal{X} \times \mathcal{X} \to R^{d,d}$ is called matrix-valued reproducing kernel for the Hilbert space $\mathcal{H}(\mathcal{X}, R^d)$ of functions $\mathcal{X} \to R^d$, if for all $x \in \mathcal{X}, a \in R^d$ and $f \in \mathcal{H}(\mathcal{X}, R^d)$,

(a) $K(x,\cdot)a \in \mathcal{H}(\mathcal{X}, R^d)$

(b) $(K(x,\cdot)a, f)_{\mathcal{H}(\mathcal{X}, R^d)} = (a \otimes \delta_x)f = a \cdot f(x)$.

In case $d = 1$ we call $K$ scalar reproducing kernel and in order to distinguish the matrix and scalar case we set $k(x, y) := K(x, y)$ and $\mathcal{H}(\mathcal{X}) := \mathcal{H}(\mathcal{X}, \mathbb{R})$.

**Remark 3.2.**

• Notice that in case $d = 1$ the items (a) and (b) of the previous definition reads: for all $x \in \mathcal{X}, a \in R^d$ and $f \in \mathcal{H}(\mathcal{X}, R^d)$,

(a) for all $k(x, \cdot) \in \mathcal{H}(\mathcal{X})$

(b) $(k(x, \cdot), f\cdot)_{\mathcal{H}(\mathcal{X})} = f(x)$.

• Notice that items (a) and (b) together imply that the point evaluation $\delta_x(f) := f(x)$ is a continuous functional on a reproducing kernel Hilbert space.

The following remark collects a few interesting properties of reproducing Hilbert spaces; cf. [33].
Remark 3.3. • It is readily checked that a (scalar) reproducing kernel is symmetric, $k(x,y) = k(y,x)$ for all $x,y \in X$. It is also positive semi-definite, that is, for all mutually distinct $\{x_1, \ldots, x_N\}$ the matrix $(k(x_i,x_j))$ is positive semidefinite. When this latter matrix is positive definite for all mutually distinct $x_i$ we call $k$ positive definite reproducing kernel.

• If a kernel $k$ is positive definite then it is linearly linearly independent in the following sense: for all $M \geq 1$, all mutually distinct $\{y_1, \ldots, y_M\} \subset \mathbb{R}^d$ and arbitrary $\alpha_1, \ldots, \alpha_M \in \mathbb{R}$ we have

$$
\sum_{l=1}^M \alpha_l k(x,y_l) = 0 \quad \text{for all } x \in \mathbb{R}^d \quad \Rightarrow \quad \alpha_1 = \cdots = \alpha_M = 0. \quad (3.1)
$$

• Suppose $X = \Omega$, $\Omega \subset \mathbb{R}^d$ open, and $k(x,\cdot) \in C(\Omega)$ for all $x \in \Omega$. Then we have the inclusion $\mathcal{H}(\Omega) \subset C(\Omega)$; cf. [15, pp.133].

• When we start with a scalar reproducing kernel $k$ on $X \subset \mathbb{R}^d$ with RKHS $\mathcal{H}(X)$, then $K(x,y) := k(x,y)I$ is a matrix-valued reproducing kernel with RKHS $[\mathcal{H}(X)]^d$. Moreover, the inner product is given by $(f,g)_{\mathcal{H}(X,\mathbb{R}^d)} := (f_1,g_1)_{\mathcal{H}(X)} + \cdots + (f_d,g_d)_{\mathcal{H}(X)}$ for all $f = (f_1,\ldots,f_d)$ and $g = (g_1,\ldots,g_d)$ with $f_1,\ldots,f_d,g_1,\ldots,g_d \in \mathcal{H}(X)$. A proof may be found in [15].

Next we define what we understand by a bounded kernel in $C_b^k(\mathbb{R}^d)$.

**Definition 3.4.** We say that a reproducing kernel $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is bounded in $C_b^k(\mathbb{R}^d)$, $k \geq 0$, if for all $x \in \mathbb{R}^d$ the function $k(x,\cdot)$ belongs to $C_b^k(\mathbb{R}^d)$ and there is a constant $C > 0$ so that

$$
\|k(x,\cdot)\|_{C_b^k} \leq C \quad \text{for all } x \in \mathbb{R}^d. \quad (3.2)
$$

**Example 3.5.** An example of positive definite kernel is the Gaussian kernel $k^\sigma(x,y) := e^{-|x-y|^2/\sigma^2}$, $\sigma > 0$; cf. [14]. Another important compactly supported radial kernel that is positive definite and bounded in $C_b^k(\mathbb{R}^d)$ is $k^\sigma(x,y) := (1 - |x-y|^2/\sigma^2)^{+} (4|x-y|^2/\sigma^2 + 1)$, $\sigma > 0$; [13, pp.119]. (Here bounded means bounded for fixed $\sigma$.)

### 3.2 General approximate normal basis functions

At next we define for every $C^1$-submanifold $M \subset \mathbb{R}^d$ of codimension one special basis functions. These new basis functions are vector fields $\mathbb{R}^d \rightarrow \mathbb{R}^d$ with the pleasing property that their restriction to $M$ is approximately normal in a certain sense (cf. Lemma 3.12).

**Definition 3.6** (Approximate basis functions). Let $M \subset \mathbb{R}^d$ be a $C^1$-submanifold (without boundary) of codimension one and denote by $\nu$ a continuous unitary normal field along $M$. Suppose that $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is a positive definite reproducing kernel that is bounded in $C_b^k(\mathbb{R}^d)$. Then we define approximate normal basis functions $v^\nu : \mathbb{R}^d \rightarrow \mathbb{R}^d$ at the point $x \in M$ by

$$
v^\nu_M(y) := \nu(x)k(x,y). \quad (3.3)
$$

For arbitrary points $X := \{x_1, \ldots, x_N\} \subset M$, $N \geq 1$, we define the finite dimensional space

$$
\mathcal{V}^d_M(\mathbb{R}^d,\mathbb{R}^d) := \text{span}\{v^\nu_M(\cdot) : x \in X\}. \quad (3.4)
$$

Since $\mathcal{V}^d_M(\mathbb{R}^d,\mathbb{R}^d)$ is a subset of the reproducing kernel Hilbert space $[\mathcal{H}(\mathbb{R}^d)]^d$ associated with $K(x,y) = k(x,y)I$ we may define the approximate normal space

$$
\mathcal{V}_M^d(\mathbb{R}^d,\mathbb{R}^d) := \overline{\text{span}\{v^\nu_M(\cdot) : x \in X\}}, \quad (3.5)
$$

where the closure is taken in $[\mathcal{H}(\mathbb{R}^d)]^d$. In case $X = M$ we set $\mathcal{V}^d_M(\mathbb{R}^d,\mathbb{R}^d) := \mathcal{V}_M^d(\mathbb{R}^d,\mathbb{R}^d)$.

When no confusion is possible we simply write $v^\nu(y)$ instead of $v^\nu_M$. Notice that we have the inclusion $\mathcal{V}_M^d(\mathbb{R}^d,\mathbb{R}^d) \subset C(\mathbb{R}^d,\mathbb{R}^d)$ as $[\mathcal{H}(\mathbb{R}^d)]^d$ is compactly embedded in $C(\mathbb{R}^d,\mathbb{R}^d)$; cf. Remark 3.3.

**Example 3.7.** We are particularly interested in radial kernels $k$ like the ones from Example 3.5. In Figure 2 the (compact) support of a basis function $v^\nu$ at a point $x \in \partial M$ is depicted.
3.3 Inner products on approximate normal spaces

In this subsection let $M$, $k$ and $\mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$ be defined as in Definition 3.6.

**Lemma 3.8.** The vector fields $\{v^z, \ldots, v^N\}$ defined in (3.3) are linearly independent if and only if $\{x_1, \ldots, x_N\} \subset \mathcal{X}$ are pairwise distinct.

**Proof.** Suppose $\alpha_1, \ldots, \alpha_N \in \mathbb{R}$ are such that $\sum_{i=1}^N \alpha_i v^i(x) = 0$ for all $x \in \mathcal{X}$. Since $\{k(x_1, x), \ldots, k(x_N, x)\}$ are linearly independent on $\mathcal{X}$, we obtain $\alpha_1 v(x_1) = \cdots = \alpha_N v(x_N) = 0$. But at each point $x$, one component of $v_i(x)$ must be non-zero since $|v(x_0)| = 1$ and hence we conclude $\alpha_i = 0$ for all $i = 1, \ldots, N$. \hfill \qed

Next we want to compute the orthogonal complement of $\mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$ in $[\mathcal{H}(\mathbb{R}^d)]^d$.

**Lemma 3.9.** We have for arbitrary subset $\mathcal{X} \subset M$,

$$\mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d) = \{f \in [\mathcal{H}(\mathbb{R}^d)]^d : f(x) \cdot \nu(x) = 0 \text{ for all } x \in \mathcal{X}\}. \quad (3.6)$$

**Proof.** Let $x \in \mathcal{X}$ and $v^z \in \mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$ be given. Set $f := v^z$. We have by definition $(f, \varphi)_{\mathcal{H}} = \sum_{i=1}^d (f_i, \varphi_i)_{\mathcal{H}} = 0$ for all $\varphi \in \mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$, where $f_i, \varphi_i$ are the components of $\varphi$ and $f$, respectively. Now we choose $\varphi = v^z$ and obtain

$$0 = (f, v^z)_{\mathcal{H}} = \sum_{l=1}^d (f_l, \nu_l(x))_{\mathcal{H}} = \sum_{l=1}^d \nu_l(x)f_l(x) = \nu(x) \cdot f(x), \quad (3.7)$$

where in the penultimate step we used the reproducing property of $k(x, y)$. \hfill \qed

The previous lemma tells us that $f(x) \cdot \nu(x) = 0$ for all $f \in \mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d) = \mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$ and all $x \in \mathcal{X}$. However it is not true that $f(x) \cdot \nu(x) = 0$ for all $x \in M$. But the number of tangential points of $f \in \mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$ at $M$ increases with the dimension of $\mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$.

With the help of Lemma 3.9 we may prove the following result. Recall that $\mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d) \subset C(\mathbb{R}^d, \mathbb{R}^d)$.

**Lemma 3.10.** Suppose that $M$ is compact. The functions

$$(X, Y)_{L^2, M} := \int_M (X \cdot \nu)(Y \cdot \nu) \, ds, \quad (3.8)$$

$$(X, Y)_{H^1, M} := \int_M \nabla^T(X \cdot \nu) \cdot \nabla^T(Y \cdot \nu) + (X \cdot \nu)(Y \cdot \nu) \, ds, \quad (3.9)$$

define inner products on $\mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$. Hence $\mathcal{V}_M^M(\mathbb{R}^d, \mathbb{R}^d)$ equipped with (3.8) or (3.9) is a pre-Hilbert space.
Proof. It is also clear that the functions defined in \(3.8\) and \(3.9\) are bilinear and non-negative. It remains
to check that \((X, X) = 0\) if and only if \(X = 0\). If \(X = 0\), then it is obvious that \((X, X) = 0\). So it suffices to
show the other direction for \(3.8\). Suppose \(X \in \mathcal{V}^M(\mathbb{R}^d, \mathbb{R}^d)\) and

\[
(X, X)_{L_2,M} = \int_{\partial \Omega} (X \cdot \nu)^2 \, ds = 0.
\]

Then \(X \cdot \nu = 0\) on \(M\) and Lemma \(3.9\) shows that this implies \(X \in \mathcal{V}^M(\mathbb{R}^d, \mathbb{R}^d)\). Since \([\mathcal{H}(\mathbb{R}^d)]^d = \mathcal{V}^M(\mathbb{R}^d, \mathbb{R}^d)\) ⊕ \([\mathcal{V}^M(\mathbb{R}^d, \mathbb{R}^d)]\) we must have \(X = 0\).

The previous lemma shows that \((\mathcal{V}^M(\mathbb{R}^d, \mathbb{R}^d), (\cdot, \cdot))\) is a pre-Hilbert space with \((\cdot, \cdot)\) given by \(3.8\) or

3. Basis function of radial kernels

Let us now examine how "normal" the fields in \(\mathcal{V}^M(\mathbb{R}^d, \mathbb{R}^d)\) actually are. Recall that for a function \(f : \partial \Omega \to \mathbb{R}^d\) the tangential part is defined by \(f_\tau := f - (f \cdot \nu)\nu\), where \(\nu\) is the normal field along \(M\). In this
paragraph we specialise to the following class of kernels.

Assumption 3.11. Let \(\phi : \mathbb{R} \to \mathbb{R}\) be a \(C^k\)-function with \(k \geq 2\) and \(\text{supp}(\phi) \subset [-1, 1]\). Suppose \(k^\sigma(x, y) := \phi(x - y)\) is a reproducing kernel of class \(C^k\) that is bounded in \(C^k(\mathbb{R}^d)\). There is a constant \(c > 0\) so that for all \(\sigma > 0\),

\[
|\nabla_y k^\sigma(x, y)| \leq \frac{c}{\sigma} \quad \text{for all } x, y \in \mathbb{R}^d.
\]

A systematic study of radial kernels generated by compactly supported piecewise polynomial functions of
minimal degree may be found in [31] and [33, pp.119]; see also \([32, 34]\). For these kernels it is possible to
explicitly determine their native space, i.e., the Hilbert space they generate. For instance consider the kernel
from Example \(3.5\) (with \(\sigma = 1\)) \(k(x, y) := \phi(|x - y|)\) with \(\phi(r) := (1 - r)^\tau(4r + 1) \in C^2(\mathbb{R})\) and \(d \leq 3\).
Its native space can be shown (cf. \([33\] Theorem 10.35, p.160\)) to be equal to the classical Sobolev space \(\mathcal{H}(\mathbb{R}^d) = H^{d/2+3/2}(\mathbb{R}^d)\). So in dimension \(d = 2\) we obtain \(\mathcal{H}(\mathbb{R}^d) = H^{5/2}(\mathbb{R}^d)\).

Lemma 3.12. Let \(M \subset \mathbb{R}^d\) be a compact \(C^k\)-submanifold, \(k \geq 1\), of codimension one. Let \(v^\sigma_\nu\) be defined by a
kernel satisfying Assumption 3.11. For every \(x \in M\),

\[
\lim_{\sigma \to 0} \|(v^\sigma_\nu)|_{C(M, \mathbb{R}^d)} = 0.
\]

Suppose \(M\) is of class \(C^2\). Then there are constants \(c_1, c_2 > 0\), so that for \(x \in M\),

\[
\|\nabla^\tau (v^\sigma_\nu \cdot \nu)|_{C(M, \mathbb{R}^d)} \leq c_1 + \frac{c_2}{\sigma} \quad \text{for all } \sigma > 0.
\]

Proof. Since \(\nu\) is continuous on \(M\) and \(|\nu| = 1\) on \(M\), we find for every \(x \in M\) and every \(\epsilon > 0\) a number \(\delta > 0\)
so that \(|\nu(x) - \nu(y)| < \epsilon\) and \(|1 - \nu(x) \cdot \nu(y)| < \epsilon\) for all \(y \in M\) with \(|x - y| < \delta\). Define \(L := \max_{r \in \mathbb{R}} |\phi(r)|\),
then \(k^\sigma(x, y) \leq L\) for all \(x, y \in \mathbb{R}^d\) and all \(\sigma > 0\). Now for all \(y \in M\) with \(|x - y| < \delta\) we get the estimate

\[
\|v^\sigma_\nu(y)\|_\tau = \|k^\sigma(x, y)\nu(x) - \nu(x) \cdot (k^\sigma(x, y)\nu(y))\nu(y)\|
\leq \|k^\sigma(x, y)\| \|\nu(x) - \nu(y)\| + \|k^\sigma(x, y)\| |\nu(y)| \|1 - \nu(x) \cdot \nu(y)\|
\leq L \epsilon + \epsilon \|x - y\| \leq 2L^2 \epsilon.
\]

In view of \(\text{supp}(\phi) \subset [-1, 1]\) we have \(v^\sigma_\nu(y) = 0\) for all \(x, y \in M\) with \(|x - y| > \sigma\). As a consequence \(3.14\) is
valid for all \(y \in M\) when \(\sigma < \delta\) and thus for all \(\sigma < \delta\) we have \(\|(v^\sigma_\nu)|_{C(M, \mathbb{R}^d)} \leq L^2 \epsilon\). This shows that for
arbitrary \(\epsilon > 0\) we find \(\delta > 0\) so that \(\|(v^\sigma_\nu)|_{C(M, \mathbb{R}^d)} \leq L^2 \epsilon\) for all \(\sigma < \delta\) which shows \(3.12\).

Suppose now \(M\) is of class \(C^2\). By assumption \(\|\nabla^\tau k^\sigma(x, y)\| \leq \frac{c}{\sigma}\) for all \(x, y\) and \(\sigma > 0\). Therefore \(2.29\)
yields \(\nabla^\tau (v^\sigma_\nu \cdot \nu) = (\partial^\tau v^\sigma_\nu)^\tau \nu + (\partial^\tau \nu)^\tau v^\sigma_\nu = (\nu(x) \otimes \nabla_y)k^\sigma(x, y)\nu + (\partial^\tau \nu)^\tau v^\sigma_\nu\) and this shows \(\nabla^\tau (v^\sigma_\nu \cdot \nu)\) is bounded by \(c_1 + c_2/\sigma\) and finishes the prove.
3.5 Parallel transport

For every \( G \in \mathcal{F}(C^1_b) \), we define a mapping acting on \( v^G_M(y) = k(x,y)\nu(x), \ x \in M \) by

\[
T_{M,G(M)} : (x,)\nu(x) \mapsto k(\cdot,G(x)) \frac{\partial G(x)}{\partial G(x)} \nu(x).
\]

Since \( \nu(y) := \frac{\partial G^{-T} \nu}{\partial G^{-T} \nu} \circ G^{-1}(y) \) is the normal vector at \( G(x) \) to \( G(M) \) it is readily checked that \( T_{M,G(M)}(v^G_M) = v^G_{G(M)} \) (choosing the right orientation of the normal vector field). As a consequence \( T_{M,G(M)} \) can be interpreted as a sort of parallel transport when \( k(\cdot,\cdot) \) is a radial kernel as then the length of the the basis \( v^G_M \) at the point \( x \) is preserved, that is, \( |v^G_M(x)| = |T_{M,G(M)}(v^G_M(G(x)))| \). Notice that by linearity this parallel transport extends to \( T_{M,G(M)} : \hat{V}^M(R^d, R^d) \to V^{G(M)}(R^d, R^d) \). The next lemma shows that this transport is locally Lipschitz continuous.

Lemma 3.13. Assume \( k \) is a reproducing kernel in \( R^d \) of class \( C^2 \) that is bounded in \( C^2_0(R^d) \). Denote \( v^G_M(\cdot) = k(\cdot,\cdot)\nu(x), \ x \in M \), where \( \nu \) is the normal vector to \( M \) at \( x \). Suppose \( q \in (0,1) \) and define \( K := \sup_{x \in R^d} \|k(\cdot,\cdot)\|_{C^2(R^d)} \). For \( x \in M \) and every \( g \in C^1_0(R^d, R^d) \) with \( \|g\|_{C^1} < q \),

\[
\|v^G_M - v^{x+g(x)}_M\|_{C^1} \leq c\|g\|_{C^1},
\]  

(3.15)

where the constant is given by \( c := 2K(1+q)/(1-q) \).

Proof. Set \( G := \text{id} + g \) and let \( \nu \) be a normal field along \( M \). Since the kernel \( k \) is bounded in \( C^2_0(R^d) \) we get

\[
|k(x,z_1) - k(x,z_2)| \leq K|z_1 - z_2| \quad \text{and} \quad |\nabla_z k(x,z_1) - \nabla_z k(x,z_2)| \leq K|z_1 - z_2|
\]

(3.16)

for all \( x, z_1, z_2 \in R^d \). Since \( |q|_{C^1} \leq q < 1 \) it is readily checked that \( |(\partial G(x))^{-T} \nu(x)| \geq 1/(1+q) \) for all \( x \in R^d \). Thus for all \( x \in M \),

\[
|\nu(x) - \frac{\partial G(x)}{\partial G(x)} \nu(x)| \leq (1+q)||G(x)||^2 \|\nu(x) - \frac{\partial G(x)}{\partial G(x)} \nu(x)|| \leq (1+q)||G(x)|| \|\nu(x)|| - |\nu(x)|| + (1+q)||G(x)|| - |G(x)| - I| \leq 2q/(1-q)|I - G(x)|.
\]

(3.17)

Thus using this estimate we get for \( x \in M \) and \( z \in R^d \),

\[
|v^G_M(z) - v^{G(x)}_{G(M)}(z)| = |k(z,\nu(x)) - k(z,G(x))\frac{\partial G(x)}{\partial G(x)} \nu(x)|
\]

\[
\leq K|x - G(x)| + K(1+q)|\nu(x) - \frac{\partial G(x)}{\partial G(x)} \nu(x)|
\]

\[
\leq K|x - G(x)| + \frac{2K(1+q)}{1-q}|I - G(x)|
\]

\[
\leq 2K(1+q)/(1-q)(|g(x)| + |\nabla g(x)|) \leq c\|g\|_{C^1},
\]

(3.18)

where we used \( (1+q)/(1-q) \geq 1 \). As for the derivative notice that \( \partial_z v^G_M(z) = \nu(x) \otimes \nabla_z k(x,z) \) and \( \partial_z v^{G(x)}_{G(M)}(z) = \frac{\partial G(x)}{\partial G(x)} \otimes \nabla_z k(x,z) \) and hence for \( x \in M \) and \( z \in R^d \),

\[
|\partial_z v^G_M(z) - \partial_z v^{G(x)}_{G(M)}(z)| \leq |\nu(x) \otimes (\nabla_z k(x,z) - \nabla_z k(G(x),z))|
\]

\[
+ |\nu(x) - \frac{\partial G(x)}{\partial G(x)} \nu(x) \otimes \nabla_z k(G(x),z)|
\]

\[
\leq K|x - G(x)| + \frac{2K(1+q)}{1-q}|I - G(x)|
\]

\[
\leq 2K(1+q)/(1-q)(|g(x)| + |\nabla g(x)|) \leq c\|g\|_{C^1}.
\]

(3.19)

Taking the supremum over \( z \in R^d \) in (3.18) and (3.19) and summing both inequalities finishes the proof.
3.6 Invertibility of the second shape Hessian

We begin with a lemma.

**Lemma 3.14.** Let $M$ be a $C^k$-submanifold, $k \geq 2$, of $\mathbb{R}^d$ of codimension one with $|M| < \infty$. Denote by $\nu$ the normal field along $M$. Set $v^\tau(y) := k^\tau(x, y)\nu(x)$, where $k^\tau(x, y) = \phi(|x-y|)$ satisfies Assumption 3.11. Let $\tilde{g} \in L_p(M)$ where $p = (d-1)/(d-2)$ (in the planar case $d = 2$ we have $p = \infty$). Then for $x, y \in M$

$$\int_M |\tilde{g}| \|\nabla^\tau (v^x \cdot \nu)\| \, ds \to 0 \quad \text{as } \sigma \searrow 0. \tag{3.20}$$

**Proof.** Let $x \in M$. Thanks to Lemma 3.12 we find constants $c_1, c_2 > 0$ so that $\|\nabla^\tau (v^x \cdot \nu)\|_{C(M, \mathbb{R}^d)} \leq c_1 + \frac{c_2}{\sigma}$ for all $\sigma > 0$. Notice that for all sufficiently small $\sigma$ we have $|M \cap B_\sigma(x)| \leq \sigma \sigma^{-d}$ and thus by our choice $p = (d-1)/(d-2)$, $|M \cap B_\sigma(x)|^{\frac{1}{p+1}} \leq c\sigma$. Therefore using that $k$ is compactly supported and Hölder’s inequality yields

$$\int_M |\tilde{g}| \|\nabla^\tau (v^x \cdot \nu)\| \cdot (v^y) \| \, ds \leq \int_{M \cap B_\sigma(x)} |\tilde{g}| \|\nabla^\tau (v^x \cdot \nu)\| \cdot (v^y) \| \, ds$$

$$\leq \|\nabla^\tau (v^x \cdot \nu)\|_{C(M, \mathbb{R}^d)} \|v^y\|_{C(M, \mathbb{R}^d)} \|\tilde{g}\|_{L_p(M)} |M \cap B_\sigma(x)|^{\frac{1}{p+1}}$$

$$\leq c_1 + \frac{c_2}{\sigma} \|v^y\|_{C(M, \mathbb{R}^d)} \|\tilde{g}\|_{L_p(M)} \leq C \|v^y\|_{C(M, \mathbb{R}^d)} \|\tilde{g}\|_{L_p(M)}. \tag{3.21}$$

Now in view of Lemma 3.12 the right hand side of (3.21) tends to zero as $\sigma \searrow 0$. \qed

Let us now give sufficient conditions when the first and second shape Hessians are invertible.

**Lemma 3.15.** Let $J$ be a twice shape differentiable function and $\Omega$ a bounded domain of class $C^2$. Assume that there are constants $c_1, c_2$, so that

$$c_1 \|X \cdot \nu\|^2_{L^2(\partial \Omega)} \leq H^2_{\Omega, J}(X)(X) \quad \text{for all } X \in C^2_b(\mathbb{R}^d, \mathbb{R}^d) \tag{3.22}$$

and

$$H^2_{\Omega, J}(J)(X)(Y) \leq c_2 \|X\|_{C^2} \|Y\|_{C^2} \quad \text{for all } X, Y \in C^2_b(\mathbb{R}^d, \mathbb{R}^d). \tag{3.23}$$

Assume $DJ(\Omega)(X) = \int_{\partial \Omega} \tilde{g} X \cdot \nu \, ds$ with $\tilde{g} \in L_2(\partial \Omega)$. Let $v^x$ be as in the previous lemma. Then the matrix $H^2_X := (H^2_{\Omega, J}(v^x)(v^y))_{x, y \in X}$ is invertible and if $\sigma > 0$ is sufficiently small then also $H^2_X := (H^2_{\Omega, J}(v^x)(v^y))_{x, y \in X}$. In particular $H^2_X \simeq H^2_X$.

**Proof.** It directly follows from (3.22) that $H^2_X$ is positive semi-definite. Suppose $a \in \mathbb{R}^n$ so that $H^2_X a \cdot a = 0$. Then setting $v := \sum_{i=1}^n a_i v^x_i$, $x_i \in X$, yields $H^2_X a \cdot a = H^2_{\Omega, J}(v)(v)$ and we conclude from (3.22) that $\|v \cdot \nu\|^2_{L^2(\partial \Omega)} = 0$ and thus $v \cdot \nu = 0$ on $\partial \Omega$. Now Lemma 3.10 yields $v = 0$ and since $\{v^x_1, \ldots, v^x_n\}$ are linearly independent (see Lemma 3.8) we get $a = 0$. This shows that $H^2_X$ is positive definite. Define $g(v) := \int_{\partial \Omega} \tilde{g} v \, ds$. Recall the definition of the second shape Hessian

$$H^2_{\Omega, J}(X)(Y) = H^1_{\Omega, J}(X)(Y) + g(\nabla^\tau (v^x \cdot \nu) \cdot X \tau + \nabla^\tau (v^x \cdot \nu) \cdot Y \tau) \tag{3.24}$$

for all $X, Y \in C^2_b(\mathbb{R}^d, \mathbb{R}^d)$. From our assumption and Lemma 3.14 (applied to $M := \partial \Omega$), we obtain for $x, y \in \partial \Omega$,

$$|g(\nabla^\tau (v^x \cdot \nu) \cdot (v^y) \tau + \nabla^\tau (v^x \cdot \nu) \cdot (v^y) \tau)| \leq c \|v^y\|_{C(\partial \Omega, \mathbb{R}^d)} \tag{3.25}$$

and the right hand side tends to zero when $\sigma \searrow 0$. Thus $A_\sigma := (g(\nabla^\tau (v^x \cdot \nu) \cdot (v^y) \tau + \nabla^\tau (v^x \cdot \nu) \cdot (v^y) \tau))_{x, y \in X}$ satisfies $\|A_\sigma\| \to 0$ as $\sigma \to 0$. Since $H^2_X = H^2_X + A_\sigma$ we conclude that also $H^2_X$ must be invertible and positive definite. \qed

**Remark 3.16.** The previous lemma tells us that for our special basis $v^x$ from Definition 3.6 we do not need to distinguish the first and second Hessian provided $\sigma$ is sufficiently small. As a consequence we can work with the first Hessian which is easier to compute than the second Hessian.

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4 Newton’s method

This section is devoted to the convergence analysis of a Newton algorithm in the spirit of [7]. The Newton equation will be solved in the approximate normal space using the basis functions introduced in the previous section. We will proof the convergence of Newton’s method in the discrete setting, however, an analog in the finite dimensional setting should also hold under suitable conditions. Thanks to Lemma 3.15 it suffices to work with the first shape Hessian \( H_{\Omega}^{1} = \mathcal{D}^{2} J(\Omega) \) restricted to the space \( \mathcal{V}^{\partial \Omega}(\mathbb{R}^{d}, \mathbb{R}^{d}) \).

4.1 Setting and algorithm

Fix a bounded set \( \Omega \subset \mathbb{R}^{d} \) with \( C^{1} \)-boundary \( \partial \Omega \) (it does not need to be a domain). Suppose \( v_{\partial \Omega}^{i}, x \in \partial \Omega \) are defined via kernels satisfying Assumption 3.11. Let \( \mathcal{X} = \{x_{1}, \ldots, x_{n}\} \) be a finite number of points contained in \( \partial \Omega \). Assume that \( J \) is a twice differentiable shape function with first and second derivative \( DJ(\Omega) \) and \( \mathcal{D}^{2} J(\Omega) \), respectively. By assumption

\[
DJ(\Omega) : C_{b}^{1}(\mathbb{R}^{d}, \mathbb{R}^{d}) \to \mathbf{R}, \quad \mathcal{D}^{2} J(\Omega) : C_{b}^{1}(\mathbb{R}^{d}, \mathbb{R}^{d}) \times C_{b}^{1}(\mathbb{R}^{d}, \mathbb{R}^{d}) \to \mathbf{R}
\]  

are continuous. For a sequence \( (F_{k}) \) in \( \mathcal{F}(C_{b}^{1}) \), we will use the following abbreviations

\[
\mathcal{H}_{\mathcal{X}_{k}}(F_{k}) := (\mathcal{D}^{2} J(F_{k}(\Omega)))(v_{k}^{i}(v_{k}^{j}))_{i,j=1,\ldots,n}, \quad \mathcal{L}_{\mathcal{X}_{k}}(F_{k}) := (DJ(F_{k}(\Omega))(\partial v_{k}^{i} v_{k}^{j}))_{i,j=1,\ldots,n},
\]

where \( v_{k}^{i}(z) := v_{F_{k}(\partial \Omega)}^{i}(z) \) and \( \mathcal{X}_{k} = \{F_{k}(x_{1}), \ldots, F_{k}(x_{n})\} \). We identify the Euclidean space \( \mathbb{R}^{d} \) with the space \( \mathcal{V}_{\mathcal{X}_{k}}^{F_{k}(\partial \Omega)}(\mathbb{R}^{d}, \mathbb{R}^{d}) \) via

\[
P_{\mathcal{X}_{k}} : \mathbb{R}^{d} \to \mathcal{V}_{\mathcal{X}_{k}}^{F_{k}(\partial \Omega)}(\mathbb{R}^{d}, \mathbb{R}^{d}) : (x^{1}, \ldots, x^{n}) \mapsto \sum_{l=1}^{n} X_{l}^{1} v_{l}^{k}.
\]

Then the Newton iterations \( F_{k} \) are defined by

\[
\mathcal{H}_{\mathcal{X}_{k}}(F_{k}) X_{k} = -\mathcal{L}_{\mathcal{X}_{k}}(F_{k}), \quad F_{k} = (id + g_{k-1}) \circ F_{k-1}, \quad g_{k} = P_{\mathcal{X}_{k}}(X_{k}).
\]

The equation (4.2) is equivalent to: find \( \tilde{X}_{k} \in \mathcal{V}_{\mathcal{X}_{k}}^{\partial \Omega}(\mathbb{R}^{d}, \mathbb{R}^{d}) \)

\[
\mathcal{D}^{2} J(F_{k}(\Omega))(\tilde{X}_{k})(\varphi) = -DJ(F_{k}(\Omega))(\varphi) \quad \text{for all } \varphi \in \mathcal{V}_{\mathcal{X}_{k}}^{\partial \Omega}(\mathbb{R}^{d}, \mathbb{R}^{d}).
\]

Our main goal is to prove the convergence of the following algorithm.

**Data:** Let \( \gamma > 0 \) and \( n, N \in \mathbb{N} \) be given. Choose \( \Omega \subset \mathbb{R}^{d} \) and \( \mathcal{X}_{0} := \{x_{1}, \ldots, x_{n}\} \subset \Omega \). Let \( F_{0} := id \), initializations:

**while** \( k \leq N \) **do**

1. Compute \( X_{k} \in \mathbb{R}^{n} \) as solution of \( \mathcal{H}_{\mathcal{X}_{k}}(F_{k}) X_{k} = -\mathcal{L}_{\mathcal{X}_{k}}(F_{k}) \), and set \( g_{k} := P_{\mathcal{X}_{k}}(X_{k}) \).
2. Update \( F_{k+1} \leftarrow (id + g_{k}) \circ F_{k} \).
3. Update \( \mathcal{X}_{k+1} \leftarrow \{F_{k+1}(x_{1}), \ldots, F_{k+1}(x_{n})\} \).
4. Update \( \Omega_{k+1} \leftarrow F_{k+1}(\Omega_{k}) \).
5. Update \( v_{\partial \Omega_{k+1}}^{i}(x_{j}) \leftarrow v_{\partial \Omega_{k}}^{i}(x_{j}) \).

**if** \( J(F_{k}(\Omega)) - J(F_{k+1}(\Omega)) \geq \gamma (J(\Omega) - J(F_{k}(\Omega))) \) **then**

**end**

**Algorithm 1:** Newton algorithm

4.2 Convergence of Newton’s method

In order to prove convergence for the Newton algorithm we make the following assumption.
Assumption 4.1. Let $\Omega \subset \mathbb{R}^d$ and $q \in (0, 1)$. For every $\delta > 0$ and every $\gamma > 0$, there is a constant $C_1 > 0$, so that
\[
|DJ((id + g) \circ F(\Omega))(X) - DJ(F(\Omega))(X) - D^2J(F(\Omega))(X)(g)| \leq C_1\|g\|^2_c,
\]
for all $F \in \mathcal{C}^1_b$ with $d(id, F) < \delta$ and all $g \in C^1_b(\mathbb{R}^d, \mathbb{R}^d)$ with $\|g\|_{C^1} < q$ and all $X \in C^0_b(\mathbb{R}^d, \mathbb{R}^d)$ with $\|X\|_{C^1} \leq \gamma$.

Before we proof our main result we need the following lemma.

Lemma 4.2. Assume that $J$ is twice differentiable and also admits a second Euler derivative at all $\hat{\Omega} \in \mathcal{X}(\Omega)$. Denote by $(F_k)$ and $(g_k)$ the sequences defined in Algorithm 7. Suppose $(g_k)$ is such that $\|g_k\|_{C^1} < 1/2$ for all $k \geq 0$. Then there are constants $c_1, c_2, c_3 > 0$ independent of $(g_k)$, so that for all $k$,
\[
\begin{align*}
|L_{\chi_{k-1}}(F_{k-1}) - L_{\chi_k}(F_{k-1})| &\leq c_1\|DJ(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)}\|g_{k-1}\|_{C^1}, \\
|H_{\chi_{k-1}}(F_{k-1})X_{k-1} - H_{\chi_k}(F_{k-1})X_{k-1}| &\leq c_2\|D^2J(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)^2}\|g_{k-1}\|^2_{C^1}, \\
|\tilde{H}_{\chi_{k-1}}(F_{k-1})X_{k-1}| &\leq c_3\|DJ(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)}\|g_{k-1}\|_{C^1}.
\end{align*}
\]

Proof. In view of $F_k = (id + g_k) \circ F_{k-1}$ and the assumption $\|g_k\|_{C^1} < 1/2$ for all $k$, we get from Lemma 3.13 $\|v_{F_{k-1}(\partial \Omega)}^{k-1}(x) - v_{F_k(\partial \Omega)}^k(x)\|_{C^1} \leq 6K\|g_k\|_{C^1}$, where $K = \max_{x \in \mathbb{R}^d} \|k(x, \cdot)\|_{C^1}$ is independent of $k$. Hence we get component wise:
\[
\begin{align*}
|L_{\chi_{k-1}}(F_{k-1}) - L_{\chi_k}(F_{k-1})| &\leq \|DJ(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)}\|v_{F_{k-1}(\partial \Omega)}^{k-1}(x) - v_{F_k(\partial \Omega)}^k(x)\|_{C^1} \\
&\leq 3K\|DJ(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)}\|g_{k-1}\|_{C^1}.
\end{align*}
\]

In a similar fashion we find
\[
\begin{align*}
|H_{\chi_{k-1}}(F_{k-1})X_{k-1} - H_{\chi_k}(F_{k-1})X_{k-1}| &\leq \|D^2J(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)^2}\|v_{F_{k-1}(\partial \Omega)}^{k-1}(x) - v_{F_k(\partial \Omega)}^k(x)\|_{C^1} \\
&\leq 3K\|D^2J(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)^2}\|g_{k-1}\|^2_{C^1}.
\end{align*}
\]

Finally since $J$ is differentiable and $v^x$ bounded in $C^0_b(\mathbb{R}^d)$ we get for some $c > 0$ independent of $k$,
\[
\begin{align*}
|\tilde{H}_{\chi_{k-1}}(F_{k-1})X_{k-1}| &\leq \|DJ(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)}\|\partial v_{F_{k-1}(\partial \Omega)}^{k-1}(x)g_{k-1}\|_{C^1} \\
&\leq c\|DJ(F_{k-1}(\Omega))\|_{\mathcal{L}(C^1)}\|g_{k-1}\|_{C^1}.
\end{align*}
\]

Now (4.7) follows at once.

Now we are in a position to state our main theorem concerning the convergence of Newton’s method.

Theorem 4.3. Let $\Omega \subset \mathbb{R}^d$ be a bounded $C^1$-domain. Assume that $J$ satisfies Assumption 4.1 at $\Omega$ and the assumptions of Theorem 2.10 at all $\hat{\Omega} \in \mathcal{X}(\Omega)$. Denote by $(F_k)$ and $(g_k)$ the sequences defined in Algorithm 7. Assume that the inverse $H_{\chi_k}(F_k)^{-1}$ exists for all $k \geq 0$ and that there is $c > 0$, so that $\|H_{\chi_k}(F_k)^{-1}\| \leq c$ for $k \geq 0$. Suppose $\|g_k\|_{C^1} < 1/2$ for all $k \geq 0$ and assume that there is $c > 0$ so that $d(id, F_k) \leq c$ for all $k \geq 0$. Then there holds:

(i) There is a bounded series $\kappa_k$ of non-negative numbers, so that
\[
|X_{k+1}| \leq \kappa_k|X_k| \quad \text{for all } k \geq 0.
\]

Notice the sequence $(X_k)$ converges linearly to zero when $|X_0| < 1/\alpha$ where $\alpha := \sup_{k \geq 0} \kappa_k$.

(ii) If $\alpha\|g_0\|_{C^1} < 1$, then there is an element $F^* \in \mathcal{F}(C^1_b)$, so that $d(F^*, F_k) \to 0$ as $k \to \infty$ and we have an estimate
\[
d(F^*, F_k) \leq \frac{\alpha\|g_0\|_{C^1}^k}{1 - \alpha\|g_0\|_{C^1}} \quad \text{for all } k \geq 0.
\]
Moreover if
\[ F \mapsto \mathcal{D}^2 J(F(\Omega)) : \mathcal{F}(C^1_b) \to \mathcal{L}(C^1_b(\mathbb{R}^d, \mathbb{R}^d), \mathcal{L}(C^1_b(\mathbb{R}^d, \mathbb{R}^d), \mathbb{R})) \]
and
\[ F \mapsto DJ(F(\Omega)) : \mathcal{F}(C^1_b) \to \mathcal{L}(C^1_b(\mathbb{R}^d, \mathbb{R}^d), \mathbb{R}) \]
are continuous at \( F^* \in \mathcal{F}(C^1_b) \), then the element \( F^* := F^* - \text{id} \) is a root of \( L_X^* \), that is, \( L_X^*(F^*) = 0 \).

(iii) Assume the mappings \( (4.13), (4.14) \) are continuous at \( F^* \) and that Assumption 4.1 holds. Moreover, suppose that \( F^* \) is a stationary point for \( J \) on all of \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \) meaning that \( DJ(F^*(\Omega))(X) = 0 \) for all \( X \in C^1_b(\mathbb{R}^d, \mathbb{R}^d) \). Then the sequence \( (\kappa_k) \) from (i) converges to zero and thus \( (X_k) \) converges superlinearly to zero.

Proof. (i) We first show that \( (X_k) \) converges to zero. Inserting \( g = g_k, F = F_k \) and \( X = u^x, x \in X_k \) in (4.6), we obtain
\[ |X_k| = |L_{X_k}(F_k) - L_{X_k}(F_{k-1}) - H_{X_k}(F_{k-1})X_k - \bar{H}_{X_k}(F_{k-1})X_k| \leq C \|g_k\|^2 \]
with a constant \( C > 0 \) independent of \( k \) since \( \|g_k\| \leq 1/2 \) and \( d(F_k, \text{id}) \leq c \) for all \( k \geq 0 \) for some \( c > 0 \). Hence we get from the definition of the Newton iterations at \( k \) and \( k - 1 \) and the estimates proved in Lemma 4.2
\[ |X_k| = |L_{X_k}(F_k) - L_{X_k}(F_{k-1}) - H_{X_k}(F_{k-1})X_k - \bar{H}_{X_k}(F_{k-1})X_k| \leq C \|g_{k-1}\|^2 \]
\[ \leq C \|D^2 J(F_k(\Omega))(\Omega)\|_{L(C^1)} \|g_{k-1}\|_{C^1} \]
\[ \leq C \|D^2 J(F_k(\Omega))(\Omega)\|_{L(C^1)} \|g_{k-1}\|_{C^1} \]
\[ \leq \tilde{\kappa}_k \|g_{k-1}\|_{C^1} \leq \tilde{\kappa}_k \|P_{X_k}(g_{k-1})\|_{C^1} \leq \tilde{\kappa}_k \|X_{k-1}\| \]
with \( \kappa_k := C(\|g_{k-1}\|_{C^1} + \|DJ(F_k(\Omega))(\Omega)\|_{C^1} + \|D^2 J(F_k(\Omega))(\Omega)\|_{C^1} \|g_{k-1}\|_{C^1} \). Notice that we used \( \|P_{X_k}\| \leq c \) for all \( k \geq 0 \) for some constant \( c > 0 \). So from (4.16) we get \( |X_{k+1}| \leq \alpha \|X_{k}\| \). If \( |X_{0}| < 1/\alpha \) we obtain that \( X_{k+1} \to 0 \) as \( k \to \infty \) and the convergence is linear. Moreover since \( \|g_{k}\|_{C^1} = \|P_{X_k}(g_{k})\|_{C^1} \leq \|P_{X_k}\| \|X_{k}\| \) we also conclude \( g_k \to 0 \) in \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \).

(ii) Now we show that the sequence \( (F_k) \) is a Cauchy sequence in \( \mathcal{F}(C^1_b) \). Recall that \( F_m = (\text{id} + g_{m-1}) \circ \cdots \circ (\text{id} + g_0) \) for all \( m \geq 1 \) by definition. Hence using the triangle inequality and the right-invariance of \( d(\cdot, \cdot) \) gives
\[ d(F_m, F_{m+n+1}) = d((\text{id} + g_{m-1}) \circ \cdots \circ (\text{id} + g_0), (\text{id} + g_{m+n}) \circ \cdots \circ (\text{id} + g_{m-1}) \circ \cdots \circ (\text{id} + g_0)) \]
\[ = d((\text{id} + g_{m+n}) \circ \cdots \circ (\text{id} + g_{m})), \]
\[ \leq \sum_{l=m}^{n+m} d(\text{id}, \text{id} + g_l). \]
In view of Lemma 1.3 and estimate (4.11), we get
\[ \|F_k - F_{k+1}\| \leq \|g_k\|_{C^1} + \|g_k\|_{C^1} + 2 \|\partial g_k\|_{C^1} \|g_k\|_{C^1} \]
\[ \leq 2(1 + \alpha \|g_0\|_{C^1} + \|g_0\|_{C^1} + 1) \|g_k\|_{C^1} \]
\[ \leq 5 \alpha \|g_0\|_{C^1} \]

So using this result to further estimate (4.17) we find
\[ d(F_m, F_{m+n+1}) \leq \sum_{l=m}^{n+m} \alpha \|g_0\|_{C^1} \]
\[ \leq 5 \alpha \|g_0\|_{C^1} \]
\[ \leq 25 \alpha \|g_0\|_{C^1} \]
\[ \leq 25 \alpha \|g_0\|_{C^1} \]
and since \( \alpha \|g_0\|_{C^1} < 1 \) the geometric series converges and right hand side tends to zero when \( m, n \to 0 \). This shows that \( F_m \) is a Cauchy sequence in \( \mathcal{F}(C^1_b) \) and since this group is complete we find \( F^* \in \mathcal{F}(C^1_b) \), so that \( d(F_m, F^*) \to 0 \) as \( m \to \infty \). Additionally by using \( \sum_{i=0}^{n-1} q^i = (1 - q^n)/(1 - q) \) for \( |q| < 1 \) and setting \( q := \alpha \|g_0\|_{C^1} \) we obtain
\[
d(F_m, F_{m+n+1}) \leq 5 \sum_{i=m}^{n+m} q^i = 5q^m \frac{(1 - q^{n+1})}{1 - q}.
\]
Hence passing to the limit \( n \to \infty \) in (4.20) yields the apriori estimate (4.12). Suppose now assumptions (4.13), (4.14) are satisfied. Since \( F_n \to F^* \) in \( \mathcal{F}(C^1_b) \) Lemma 1.6 shows that \( F_k \circ (F^*)^{-1} - \text{id} \to 0 \) in \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \). Hence in view of Lemma 3.13 we obtain for all \( i = 1, \ldots, n \),
\[
\|v_{F_k(x_i)} - v_{F^*(x_i)}\|_{C^1} \leq \epsilon \|F_k \circ (F^*)^{-1} - \text{id}\|_{C^1} \to 0 \quad \text{as} \quad k \to \infty,
\]
where the constant \( \epsilon \) is independent of \( k \). Now employing (4.13), (4.14) and \( g_k \to 0 \) in \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \), we can pass to the limit in
\[
\mathcal{D}^2 J(F_k(\Omega))(g_k)(v_k) = -DJ(F_k(\Omega))(v_k)
\]
for \( i = 1, \ldots, n \). This shows that \( DJ(F^*(\Omega))(v_{F^*(x_i)}) = 0 \) for all \( x_i \in \mathcal{X} \). Note that this is equivalent to \( DJ(F^*(\Omega))(v) = 0 \) for all \( v \in V_{F^*(\partial \Omega)}(\mathbb{R}^d, \mathbb{R}^d) \).

(iii) Finally we observe that \( (X_k) \) converges indeed superlinearly thanks to \( \|DJ(F_k(\Omega))\|_{\mathcal{L}(C^1)} \to 0 \) as \( k \to \infty \) and the definition of \( \kappa_k \).

\[\square\]

Remark 4.4.
- Notice that according to item (iii) we only get superlinear convergence of \( (X_k) \) when the root \( F^* \) is a stationary point in \( C^1_b(\mathbb{R}^d, \mathbb{R}^d) \). In practice this cannot be expected and we are going to present some numerics in the last section.
- A significant difference between our approach and approaches on shape spaces such as [28] is that we only need estimates of the second derivative in the domain (cf. Assumption [1.4]). For PDE constrained shape optimisation problems this has the advantage that less regularity of the solution of the PDE is required and we can deal with less regular domains.
- In order to obtain linear convergence of our Newton method we may replace (4.1) by
\[
|DJ((\text{id} + g) \circ F(\Omega))(X) - DJ(F(\Omega))(X) - \mathcal{D}^2 J(F(\Omega))(X)(g)| \leq C_1 \|g\|_{C^1}.
\]
This is important when one wants to prove convergence of Newton-like methods such as the BFGS method which is, however, beyond the scope of the present work.

4.3 Checking the assumption for a simple example

The positive definiteness of the first and second shape Hessian \( J(\Omega) := \int_\Omega f \, dx \) with \( f \in C^{2,2}(\mathbb{R}^d, \mathbb{R}^d) \) was already discussed in Remark 2.22 and Lemma 3.13. Now we want to check Assumption 4.1 for a concrete example. Recall the first and second derivative:
\[
DJ(\Omega)(X) = \int_\Omega f \, \text{div}(X) + \nabla f : X \, dx.
\]
and
\[
\mathcal{D}^2 J(\Omega)(X)(Y) = \int_\Omega f \, \text{div}(X)(\nabla f \, \text{div}(Y) + \nabla \cdot Y) + X \cdot (\nabla f \, \text{div}(Y) + \nabla^2 f Y) - f \partial X : \partial Y^\top \, dx.
\]

Lemma 4.5. Suppose \( f \in C^{2,2}(\mathbb{R}^d) \) and \( X \in C^2_b(\mathbb{R}^d, \mathbb{R}^d) \). Fix \( q \in (0, 1) \). Then there are constants \( L_1, L_2, L_3 \), so that for all \( h \in C^2(\mathbb{R}^d, \mathbb{R}^d) \) with \( \|h\|_{C^1} < q \) we have
\[
|\partial (T^h)^{-1} - I| \leq L_1 |\partial h|,
\]
\[
|\text{div}(X) \circ T^h - \text{div}(X)| \leq \|X\|_{C^2} |h|,
\]
\[
|\nabla f \circ T^h - \nabla f| \leq L_2 |h|,
\]
\[
|\nabla^2 f \circ T^h - \nabla^2 f| \leq L_3 |h|,
\]
where \( T^h := \text{id} + h \). The constant \( L_1 \) depends on \( q \).
Lemma 4.6. The estimate holds for the shape function $J(\Omega) = \int_{\Omega} f \, dx$ provided $f \in C^2(\mathbb{R}^d)$ and $\Omega \subset \mathbb{R}^d$ is bounded and open.

Proof. For $X \in C^2_b(\mathbb{R}^d, \mathbb{R}^d)$ fix, we set $r(h) := DJ((\text{id} + h)(\Omega))(X)$, $h \in C^1_b(\mathbb{R}^d, \mathbb{R}^d)$. The mean value theorem yields $\zeta \in (0, 1)$ (depending on $h$), so that $r(h) = r(0) - \partial r(\zeta)(h)$. As a consequence

$$|r(h) - r(0) - \partial r(0)(h)| \leq |\partial r(0)(h) - \partial r(\zeta)(h)|$$

(4.30)

and hence it suffices to find an estimate for the right hand side. It is readily checked that (compare with Theorem 2.10)

$$\partial r(\zeta)(h) = \mathcal{D}^2 J((\text{id} + \zeta h)(\Omega))(X)(h \circ (\text{id} + \zeta h)^{-1}) + DJ((\text{id} + \zeta h)(\Omega))(\partial X(h \circ (\text{id} + \zeta h)^{-1})).$$

(4.31)

Let us set $T^h := \text{id} + th$. Then using $(\partial(T^h)^{-1}) \circ T^h = (\partial T^h)^{-1}$ and a change of variables shows

$$r_1(\zeta)(h) = \int_{\Omega} \det(\partial T^h) \left[ (f \circ T^h) \partial r(0)(h) + (\nabla f \circ T^h) \cdot \partial r(0)(h) \right] dx$$

(4.32)

and

$$r_2(\zeta)(h) = \int_{\Omega} \det(\partial T^h) \left[ \partial r(0)(h) \cdot (\nabla f \circ T^h) \right] dx.$$

(4.33)

Using Lemma 4.5 shows that $|r_2(\zeta)(h) - r_2(0)(h)| \leq c\|h\|_{C^1}$, and $|r_1(\zeta)(h) - r_2(0)(h)| \leq c\|h\|_{C^1}$ for some constants $c_1, c_2 > 0$. This finishes the proof.

5 Numerical aspects and applications

5.1 Problem formulation

In this section we want to present some numerical results for the shape function

$$J(\Omega) := \int_{\Omega} f \, dx,$$

where $f \in C^2(\mathbb{R}^2)$ is some given function and specified for our test below and $\Omega \subset \mathbb{R}^2$ is measurable and bounded. In general a global minimiser of the above shape function is $\Omega^* = \{ f < 0 \}$. Next we describe how we approximate the domain.

5.2 Domain approximation and adaptivity

Domain approximation The initial domain $\Omega \subset \mathbb{R}^2$ is assumed to be a polygonal set with boundary vertices $X = \{ x_1, \ldots, x_n \}$ that are homogeneously distributed. Moreover, we assume that $\Omega$ admits a triangulation on which the integrals are evaluated.

Choice of basis functions We use $\phi(r) := (1 - r)^4 (4r + 1)$ to construct our basis functions $v^\sigma(y) := \phi(|x - y|/\sigma)\nu(x)$, $\sigma > 0$ of $V^{\mathcal{D}\Omega}_X(\mathbb{R}^d, \mathbb{R}^d)$. How to choose parameter $\sigma$ in each iteration step is specified below.
Adaptivity of basis functions  In our proposed algorithms the set \( X_k \subset \partial \Omega_k \) always contained a constant number of points and we simply moved the points via \( \text{id} + g_k \). Since the shape stretches and bends and the support of the basis functions \( v^x \) is constant this is not a satisfying assumption. Indeed when the basis functions \( v^x \) go father away from each other the Hessian matrix becomes severely ill-conditioned as the conditions number explodes. Therefore we propose the adaptivity of the set \( X_k \). We propose the following: fix \( c > 0 \) and let the set \( X_k = \{ x_1, \ldots, x_n \} \) be computed. We define \( h_t := |x_{t+1} - x_t| \) and \( \hat{h}_k := \sum_{t=1}^k h_t \). Then an arc piece is defined by \( \gamma(t) := x_t + t \frac{x_{t+1} - x_t}{|x_{t+1} - x_t|} \) for \( t \in [0, h_t] \). By definition \( \gamma(0) = x_t \), \( \gamma(h_t) = x_{t+1} \) and \( |\gamma'(t)| = 1 \). Then we obtain an arc polygon by setting \( \gamma(s) := \gamma(s - \hat{h}_k) \quad \text{for} \ s \in [\hat{h}_k, \hat{h}_k + \hat{h}_k] \). (5.1)

By construction \( \gamma(\hat{h}_k) = x_k \) and \( |\gamma'(s)| = 1 \) for all \( s \). So \( \gamma \) is an arc length parameterized continuous polygonal curve going through the points \( x_t \). With this curve \( \gamma \) we replace the set \( X_k \) by \( \{ \gamma(s_0), \ldots, \gamma(s_N) \} \), where \( 0 = s_0 < \cdots < s_N = \hat{h}_n \) is a uniform partition of \( [0, \hat{h}_n] \). The number \( N \) is chosen so that \( |\gamma(\hat{h}_k) - \gamma(\hat{h}_{k+1})| = c \) has a prescribed length \( c \). The number \( N \) of course depends on the length \( L(\gamma) \) of the polygon \( \gamma \). In this way we can ensure that the distance between two points \( x_t \) in \( X_k \) is always constant. Of course this adjustment is only needed when the shape changes a lot which will usually be the case in the beginning of the optimisation process.

Normal vector approximation  Since \( \partial \Omega \) is a polygon the normal vector is defined everywhere except on the vertices \( x_t \). Let \( \gamma \) be the arc curve constructed in the previous paragraph so that \( \gamma(\hat{h}_k) = x_k \). We set \( \nu(s) := J\gamma'(s) \) on \( (\hat{h}_k, \hat{h}_{k+1}) \), where \( J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \) is a counter clockwise 2D rotation matrix. At the points \( \hat{h}_k \) the normal field is not continuous, however, we may define,

\[
\nu(x_k) := \lim_{t \searrow 0} \frac{\nu(\hat{h}_k + t) + \nu(\hat{h}_k - t)}{\nu(\hat{h}_k + t) + \nu(\hat{h}_k - t)}.
\]

(5.2)

It is readily checked that this approximation is consistent in the following sense. To be more precise let \( \Omega \) be a \( C^1 \)-domain and assume that \( \gamma : (-\epsilon, \epsilon) \rightarrow \mathbb{R}^2 \), \( \epsilon > 0 \), is an arc parametrized \( C^1 \) curve describing \( \partial \Omega \) around \( x \in \partial \Omega \). Set \( \nu_h^{-} := J(\gamma(0) - \gamma(-h))/|J(\gamma(0) - \gamma(-h))| \) and \( \nu_h^{+} := J(\gamma(h) - \gamma(0))/|J(\gamma(h) - \gamma(0))| \) . Then we check that

\[
\lim_{h \searrow 0} \frac{\nu_h^{+} + \nu_h^{-}}{|\nu_h^{+} + \nu_h^{-}|} = \lim_{h \searrow 0} \frac{J(\gamma(h) - \gamma(-h))}{|J(\gamma(h) - \gamma(-h))|} = \frac{J\gamma'(0)}{|\gamma'(0)|} = \nu(x).
\]

(5.3)

Notice that in contrast to our theoretical considerations in the previous sections the domain \( \Omega \) is now only piecewise smooth and globally Lipschitz, but not \( C^1 \). However, this does not influence the convergence analysis of the previous section as the reader may verify.

5.3 Numerical tests: gradient vs Newton

All implementations were carried out within the FEniCS Software package [15].
Newton methods We use three different Hessians, namely, (cf. \[2.39\], \[2.39\] and \[2.37\]),

\[
H_{1}^{1}(X)(Y) = \int_{\Omega} T_{1}(X) : \partial Y + T_{0}(X) \cdot Y \, dx,
\]

\[
H_{2}^{2}(X)(Y) = \int_{\Omega} (\nabla f \cdot \nu + \alpha f)(X) \cdot (Y \cdot \nu) \, ds,
\]

\[Hess J(r)|X| = \nabla f \cdot \nu(X \cdot \nu)\nu.
\]

For the Hessian Hess\(J(\Omega)|X|\) we directly solve the Newton system (as in \[28\]) and obtain the Newton direction \(g_{k} := -\int_{\partial \Omega_{k}} (\nabla f|_{\partial \Omega_{k}} \cdot \nu_{k})\nu_{k}\), where \(\nu_{k}\) is the outward pointing normal field along \(\partial \Omega_{k}\). The other two Hessians \(2.39\) and \(2.39\) are discretised by \(A_{1}^{k} := (H_{1}^{1}_{\partial \Omega_{k}}(v_{k}^{i})(v_{k}^{j}))_{i,j=1,...,n}, A_{2}^{k} := (H_{2}^{2}_{\partial \Omega_{k}}(v_{k}^{i})(v_{k}^{j}))_{i,j=1,...,n}\), where we used the abbreviation \(v_{k}^{i} := v_{\partial \Omega_{k}}^{F_{k}(x_{i})}, i = 1, \ldots, n\). Then in each Newton step we solve \(A_{1}^{k}X_{k} = -L_{X_{k}}^{k}\) respectively, where \(L_{X_{k}}^{k} := (DJ(\Omega_{k})(v_{k}^{i}))_{i=1,...,n} = (\int_{\Omega_{k}} \nabla f \cdot v_{k}^{i} + \text{div}(v_{k}^{i}f) \, dx)_{i=1,...,n}\).

Gradient methods For the gradient algorithm we employ three different gradients on \(V_{\partial \Omega}^{\Omega}(R^{d}, R^{d})\). The Euclidean gradient is defined by \(B_{1}^{d}X_{k} = L_{X_{k}}^{k}\), where \(B_{1}^{d} := I\) is the identity matrix. The \(H^{1}(\partial \Omega,R^{2})\)-gradient defined as the gradient with inner product \(3.9\) is defined as solution of \(B_{1}^{d}X_{k} = L_{k}\), where \((B_{1}^{d})_{ij} := \int_{\Omega_{k}} \nabla^{*}(v_{k}^{i} \cdot \nabla(v_{k}^{j}))(v_{k}^{i}) + (v_{k}^{i})^{T} \cdot (v_{k}^{j})^{T} \, ds, i,j = 1, \ldots, n\). The \(L_{2}(\partial \Omega, R^{2})\)-gradient is given by \(f_{\partial \Omega}(\nu_{k})\). In all three cases we use a standard gradient algorithm without line search; cf. \[8\] Algorithm 1).

Parameters In the following two tests we chose in each iteration step \(\sigma_{k} = \gamma d_{k}^{2}\), where \(d_{k}\) is the maximal distance between two neighboring points \(F_{k}(x_{i})\) and \(F_{k}(x_{i+1})\) and \(\gamma > 0\) is a fixed number. The chosen parameters \(\gamma\) and step size \(s\) for the gradient method are specified below. In all tests the initial shape is approximated with 200 points and adapted during the optimisation process.

In view of the compact support of the basis functions \(\nu\) we only need to assemble the elements \(H_{1}^{1}(v_{k}^{i})(v_{k}^{j})\) and \(H_{2}^{2}(v_{k}^{i})(v_{k}^{j})\) for \(|i-j| \leq 1\) (this depends on the choice of \(\sigma\)). Moreover the occurring integrals (e.g. \(\int_{\Omega_{k}} f \text{div}(v_{k}^{i}) \text{div}(v_{k}^{j}) \, dx\) are only integrated locally around the points \(x_{i}\). Accordingly the mesh is only refined around these regions as can be seen in Figure 4.

Test 1 In the first test we consider the shape function \(J(\Omega) = \int_{\Omega} f_{1} \, dx\), where

\[
f_{1}(x_{1}, x_{2}) := (b_{1}x_{1}^{2} + b_{2}x_{2}^{2} - r_{1})\]

(5.5)

We use the parameters \(b_{1} = 1, b_{2} = 15, r_{1} = 1\). Notice that \(\Omega^{*} = \{f_{1} < 0\}\) describes an ellipse and constitutes the global minimiser of \(J\). The shape evolution for the gradient and Newton algorithm described in the previous paragraphs are displayed in Figure 7.

The gradient methods are aborted either if the gradient is smaller than \(1e-8\) or the change of gradient is too small, but at least after 999 iterations when the change in the cost value is not significant anymore.

Test 2 The second second uses the shape function \(J(\Omega) = \int_{\Omega} f_{2} \, dx\), where

\[
f_{2}(x_{1}, x_{2}) := f_{1}(x_{1}, x_{2})g(x_{1}, x_{2}), \quad g(x_{1}, x_{2}) := ((x_{1} - a_{1})^{2} + (x_{2} - a_{2})^{2} - r_{2})\]

We use the parameters \(a_{1} = 0, a_{2} = 0.55\) and \(r_{2} = 0.1\). The function \(f_{1}\) is given by \(5.5\) with the same parameters as in test one. As before \(\Omega^{*} = \{f_{2} < 0\}\) is the global minimiser of \(J\). However, this domain cannot be approximated by our approach as it has a hole and is of the form \(\{f_{1} < 0\} \cup \{g < 0\} \setminus \{\{f_{1} < 0\} \Delta (g < 0)\}\), where \(\Delta\) denotes the symmetric difference. However, we may approximate \(\{f_{1} < 0\} \cup \{g < 0\}\) as it also is a stationary points for \(J\).

Discussion As expected the results for \(H_{1}^{1}(\Omega)\) and \(Hess J(\Omega)\) are very similar. The results using \(H_{1}^{1}(\Omega)\) are qualitatively different. Also we observe that the difference between the gradient and Newton method has a (visually) greater impact for more complicated shapes. From the convergence plots in Figure 5 we conclude that all Newton methods convergence at least linearly and all gradient methods only sublinearly.

The Newton method and gradient method using \(-f/|\nabla f| \cdot \nu\) and \(-f\) as descent direction, respectively, try to move the initial points \(\{x_{1}, \ldots, x_{n}\}\) to points \(x_{1}^{*}, \ldots, x_{n}^{*}\) so that \(f(x_{i}^{*}) = 0\) for \(i = 1, \ldots, n\). Unfortunately
Figure 4: Illustration of triangulation for test 2; depicted are triangulations of initial shape (left) and of optimal shape (right).

Table 1: Final values of $\|L_N^\Omega\|$ for gradient and Newton method using approximate normal basis

| method      | (test 2) $\|L_N^\Omega\|$ | iter. N | (test 1) $\|L_N^\Omega\|$ | iter. N |
|-------------|----------------------------|---------|----------------------------|---------|
| Newton $H^1_\Omega$ | 2.54595565351e-09 | 19 | 7.80002912199e-09 | 19 |
| Newton $H^2_\Omega$ | 1.9714045422e-08 | 19 | 5.47068417493e-13 | 16 |
| Euclidean gradient | 4.49575691501e-05 | 999 | 5.39350266559e-08 | 199 |
| $H^1$-gradient | 1.82774208947e-05 | 999 | 2.41232957281e-08 | 149 |

Table 2: Final values of $\|L_N^\Omega\|$ for $L^2$-gradient and Riemannian Newton method

due to our approximation of the domain this does not yield $\int_{\partial \Omega^*} f \, ds = 0$, where $\partial \Omega^*$ is the polygonal domain defined by the final control points $\{x_1^*, \ldots, x_n^*\}$. This can be seen in Table 2 where the maximum norm of $f$ over $X_k$ goes to zero but the $L^2$-norm squared on $\partial \Omega_k$ (which happens to be equal to $DJ(\Omega_k)(f/(\nabla f \cdot \nu_k))$) stays relatively large. However when we let the number of control points $n \to \infty$ also the $L^2$ norm of $f$ over $X_k$ will converge to zero.

In contrast the methods using the basis $v_k$ (Newton and gradient) guarantee that $DJ(\Omega_k)(v_k)$ converges to zero for all $i = 1, \ldots, n$ which implies $\int_{\partial \Omega^*} f(y)k(x_i^*, y)\nu(x_i^*)\nu(y) \, dx = 0$ for $i = 1, \ldots, n$. However since $f$ can change its sign this does not necessarily imply $f(x_i^*) = 0$ for $i = 1, \ldots, n$ at a stationary point $\Omega^*$. This explains why the Newton method using $H^1_\Omega$ (and also $H^2_\Omega$) only converges linearly in our tests. Indeed in order to show that $\kappa_k$, defined in Theorem 4.3, is a null sequence we must have $DJ(F_k(\Omega)) \to 0$ in the operator norm of $C^1_b(\mathbb{R}^d, \mathbb{R}^d)$. However this implies that $DJ(F(\Omega^*))(\varphi) = 0$ for all $\varphi \in C^1_b(\mathbb{R}^d, \mathbb{R}^d)$ and thus $f = 0$ on $\partial \Omega^*$ which is not true in general as explained before.

To summarise, our proposed Newton methods using $H^1_\Omega$ and $H^2_\Omega$ in conjunction with the approximate normal functions, despite linear convergence, have a significant advantage over gradient methods. In cases where the Hessian is not coercive or a second derivative is not available one should use a Newton-like method such as a BFGS method. However, this is beyond the scope of this paper and left for future research.

Table 2: Final values of $\|f\|_{L^2_{\partial \Omega_k}}^2$ and $\|f\|_{L^\infty(X_k)}$ for $L^2$-gradient and Riemannian Newton method
Figure 5: Comparison of convergence rates of Newton methods (top-right and bottom-left) and gradient methods (top-right and bottom-right); the irregularities in the convergence speed of the gradient method (top-left) come from a refinement of the control points at the boundary; similarly for the Newton methods (top-left) the number of control points in the first five steps changes drastically yielding the irregularities in the convergence speed at the beginning.
Figure 6: (a) Evolution of $\Omega_k$ for different methods; green: initial shape, red: final shape, dashed: intermediate shapes; (b) top left: Newton with $H_{\Omega_k,J}^1 (\gamma = 0.5)$; top center: Newton with $H_{\Omega_k,J}^2 (\gamma = 1.6)$; top right: Newton with Hess$J(\Omega_k)$; bottom left: gradient method Euclidean metric (step size $s = 1.8$ and $\gamma = 0.5$); bottom center: $H^1$-gradient (step size $s = 400$ and $\gamma = 0.5$); bottom right: $L_2$-gradient (step size $s = 0.02$)

Figure 7: (a) Evolution of $\Omega_k$ for different methods; green: initial shape, red: final shape, dashed: intermediate shapes; (b) top left: Newton with $H_{\Omega_k,J}^1 (\gamma = 0.5)$; top center: Newton with $H_{\Omega_k,J}^2 (\gamma = 1.6)$; top right: Newton with Hess$J(\Omega_k)$; bottom left: gradient method Euclidean metric (step size $s = 1.8$ and $\gamma = 0.5$); bottom center: $H^1$-gradient (step size $s = 300$ and $\gamma = 0.5$); bottom right: $L_2$-gradient (step size $s = 0.02$)
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