Newton's method for nonlinear mappings into vector bundles

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Abstract

We consider Newton's method for finding zeros of mappings from a manifold \mathcal{X} into a vector bundle \mathcal{E} . In this setting a connection on \mathcal{E} is required to render the Newton equation well defined, and a retraction on \mathcal{X} is needed to compute a Newton update. We discuss local convergence in terms of suitable differentiability concepts, using a Banach space variant of a Riemannian distance. We also carry over an affine covariant damping strategy to our setting. Finally, we discuss two simple applications of our approach, namely, finding fixed points of vector fields and stationary points of functionals.

Keywords: Newton's method, Banach manifolds, vector bundles

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1. Introduction

Newton's method is a central algorithm for the solution of nonlinear problems, but also, in its variants, a theoretical tool, e.g., in the proof of the implicit function theorem [21]. Most of the literature consider Newton's method for finding zeros F(x) = 0 for a differentiable mapping $F: X \to Y$, where X and Y are linear, normed, not necessarily finite dimensional spaces, in most cases Banach spaces. In this setting, a Newton step is defined straightforwardly as the solution $\delta x \in X$ of the linear operator equation and a simple additive update:

$$F'(x)\delta x + F(x) = 0$$
, $x_+ = x + \delta x$.

Extensions of Newton's method to problems $F: \mathcal{X} \to Y$, where \mathcal{X} is a Riemannian manifold and Y still a linear space with the help of so called retractions $R_x: T_x\mathcal{X} \to \mathcal{X}$, are relatively straightforward, replacing the simple update by $x_+ = R_x(\delta x)$. But also, Newton's method has been used to find stationary points of twice differentiable functions $f: \mathcal{X} \to \mathbb{R}$ [1], and finally to find zeros of vector fields $v \in \Gamma(\mathcal{X})$ on \mathcal{X} [2, 6]. However, much richer classes of problems are conceivable in a manifold setting, such as constrained optimization [3, 15, 22, 23], non-symmetric variational problems, problems of stationary action [16], or other saddle point problems, to name just a few.

Given this variety of settings, the following questions arise: What is an appropriate general mathematical framework for Newton's method for mappings between nonlinear spaces? What structure is actually needed to define, but also to implement and globalize Newton's method for such problems? It is the aim of this work to explore possible answers to these questions.

Specifically, we want to establish Newton's method for a mapping $F: \mathcal{X} \to \mathcal{E}$, where \mathcal{X} is a differentiable manifold and $p: \mathcal{E} \to \mathcal{M}$ is a vector bundle with fibres $E_y, y \in \mathcal{M}$. This formulation still allows the search for zeros, i.e. $F(x) = 0_{p(F(x))} \in E_{p(F(x))}$, and it covers many of the above mentioned settings. The derivative of F is a mapping $F'(x): T_x\mathcal{X} \to T_{F(x)}\mathcal{E}$, which means the Newton equation cannot be formulated in the usual way, since the codomains of F and F'(x), i.e., \mathcal{E} and $T_{F(x)}\mathcal{E}$, do not coincide. It is thus necessary to introduce some additional geometric structure. It turns out that we need a connection on \mathcal{E} , which induces for every $e \in \mathcal{E}$ a linear projection $Q_e: T_e\mathcal{E} \to E_{p(e)}$ onto the corresponding fibre. This allows us to formulate the Newton equation in a well defined way:

$$Q_{F(x)} \circ F'(x)\delta x + F(x) = 0_{p(F(x))}.$$

If $Q_{F(x)} \circ F'(x)$ is invertible, the Newton direction $\delta x \in T_x \mathcal{X}$ can be computed, and thus the Newton step via a retraction $x_+ = R_x(\delta x)$.

To observe convergence of Newton's method we need a metric $d: \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$ on \mathcal{X} . Since Newton's method in the linear setting is not restricted to Hilbert spaces and has important applications in Banach spaces (cf. e.g. [25] or [7]), we will introduce metrics similar to, but more general than Riemannian distances. Finally, to compare images of successive iterates on different fibres, e.g., $F(x_+)$ and F(x), vector back-transports of the form $V_y^{-1}: \mathcal{E} \to E_y$ are needed on \mathcal{E} (we call them back-transports, because they work in the opposite direction than classical vector transports).

After setting up this framework, we will establish basic local convergence results, based on minimal assumptions on the smoothness of F, using a geometric version of Newton differentiability. Besides giving a classical a-priori result, we also establish a theorem, which relates local convergence to a quantity that is purely defined in terms of the space of iterates \mathcal{X} , and which can be estimated a-posteriori. This opens the door to define an affine covariant damping strategy in the spirit of Deuflhard [9], which is based on following the so called Newton path. While carrying over this strategy from linear spaces to our nonlinear setting, we will observe that strict differentiability of F is required to make this strategy viable. In addition, it will turn out that the employed connection and the vector back-transport have to satisfy a consistency condition to ensure that useful steps are taken. Finally, we will illustrate our results for the two simplest applications, namely the search for fixed points of vector fields and stationary points of functions on \mathcal{X} .

2. Preliminaries

We consider a Banach manifold \mathcal{X} , i.e. a topological space \mathcal{X} and a collection of charts (U,ϕ) , where each chart $\phi:U\to\mathbb{X}$ maps an open subset U of \mathcal{X} homeomorphically into a real Banach space \mathbb{X} with norm $\|\cdot\|_{\mathbb{X}}$. Unless otherwise noted we will assume that the manifold is of class C^1 , which means that the transition mappings, i.e., $t_{ji}:=\phi_j\circ\phi_i^{-1}:\phi_i(U_i\cap U_j)\to\mathbb{X}$ for charts ϕ_i,ϕ_j , are local diffeomorphisms and thus, in particular, locally Lipschitz. Mappings $F:\mathcal{X}\to\mathcal{Y}$ between two Banach manifolds are called continuous, differentiable, locally Lipschitz, if their representations in charts, i.e. the composition with charts $\phi_{\mathcal{Y}}\circ F\circ\phi_{\mathcal{X}}^{-1}$, have the respective property. It can readily be shown that these properties are independent of the choice of charts. However, we cannot assign a local Lipschitz constant to a locally Lipschitz mapping, since this quantity is chart dependent.

For a manifold \mathcal{X} we define tangent spaces by using charts, see, e.g., [13, II §2]. Let $x \in \mathcal{X}$ and consider the set

$$\{(\phi, v) \mid \phi : U \to \mathbb{X} \text{ chart at } x \in \mathcal{X}, \ v \in \mathbb{X}\}.$$

The relation $(\phi_i, v_i) \sim (\phi_j, v_j)$: $\Leftrightarrow t'_{ji}(\phi_i(x))v_i = v_j$ defines an equivalence relation. The corresponding equivalence class is called a tangent vector v of \mathcal{X} at x. The set of these equivalence classes at a point $x \in \mathcal{X}$ is a vector space, called the tangent space $T_x\mathcal{X}$ of \mathcal{X} at x. Every differentiable map $F: \mathcal{X} \to \mathcal{M}$ between two C^1 -manifolds \mathcal{X} and \mathcal{M} induces a linear map $F'(x_0): T_{x_0}\mathcal{X} \to T_{F(x_0)}\mathcal{M}$, termed tangent map or derivative of F at $x_0 \in \mathcal{X}$ [13].

Vector Bundles. Consider a vector bundle $p: \mathcal{E} \to \mathcal{M}$. Its projection p is a smooth surjective map, which assigns to $e \in \mathcal{E}$ its base point y = p(e) in the base manifold \mathcal{M} [13, III §1]. The total space \mathcal{E} is a manifold with special structure: for each $y \in \mathcal{M}$ the preimage $E_y := p^{-1}(y)$ is a Banachable space (i.e. a complete topological vector space whose topology is induced by some norm, rendering E_y complete), called fibre over y. The zero element in E_y is denoted by 0_y . A mapping $v: \mathcal{M} \to \mathcal{E}$, such that p(v(y)) = y for all $y \in \mathcal{M}$ is called section of \mathcal{E} . The set of all sections is denoted by $\Gamma(\mathcal{E})$. The most prominent example for a vector bundle is the tangent bundle $\pi: T\mathcal{X} \to \mathcal{X}$ of a manifold \mathcal{X} with fibres $T_x\mathcal{X}$. A section of $T\mathcal{X}$ is called a vector field.

Vector bundles can be described via general local charts, but usually, local trivializations are used instead, which reflect their structure better. For a Banach space $(\mathbb{E}, \|\cdot\|_{\mathbb{E}})$ and an open set $U \subset \mathcal{M}$, a local trivialization is a diffeomorphism $\tau: p^{-1}(U) \to U \times \mathbb{E}$, such that $\tau_y := \tau|_{E_y} \in L(E_y, \mathbb{E})$ is a linear isomorphism. Thus, any element of $e \in \mathcal{E}$ can be represented as a pair $(y, e_\tau) \in \mathcal{M} \times \mathbb{E}$ with y = p(e) and e_τ depending on the trivialization. For two trivializations τ and $\tilde{\tau}$ around $y \in \mathcal{M}$ we can define smooth transition mappings $A: y \mapsto \tilde{\tau}_y \tau_y^{-1}$ with $A(y) \in L(\mathbb{E}, \mathbb{E})$, and obtain $e_{\tilde{\tau}} = A(y)e_{\tau}$. If $\phi: U \to \mathbb{M}$ is a chart of \mathcal{M} , then we can construct a vector bundle chart:

$$\Phi_{\mathcal{E}}: p^{-1}(U) \to \mathbb{M} \times \mathbb{E}, \quad e \mapsto (\phi(p(e)), \tau_{p(e)}e),$$

which retains the linear structure of the fibres. Vice versa, the second component of a vector bundle chart yields a local trivialization.

Remark 2.1. For the tangent bundle $\pi: T\mathcal{X} \to \mathcal{X}$ of a manifold \mathcal{X} we have trivializations and vector bundle charts in the following natural way:

Let (U, ϕ_i) be a chart of \mathcal{X} at x. Then every tangent vector $v \in T_x \mathcal{X}$ has a chart representation $v_i \in \mathbb{X}$, so $\tau_i(v) := v_i$ is a trivialization. Since tangent vectors transform by $t'_{ji}(\phi_i(x))v_i = v_j$ under change of charts, the transition mapping is given by $A(x) = t'_{ji}(\phi_i(x))$. A vector bundle chart for $T\mathcal{X}$ is then given by:

$$\Phi_{T\mathcal{X}}: \pi^{-1}(U) \to \mathbb{X} \times \mathbb{X}, \quad (x, v) \mapsto (\phi_i(x), v_i).$$

Similarly, each element $\delta e \in T_e \mathcal{E}$ can be represented in local trivializations as a pair of elements $(\delta y, \delta e_{\tau}) \in T_y \mathcal{M} \times \mathbb{E}$, where the tangential part $\delta y = p'(e) \delta e$ is given canonically. The representation δe_{τ} of the fibre part, however, depends crucially on the chosen trivialization, and so there is no natural splitting of δe into a tangential part and a fibre part. In fact, if $e_{\tilde{\tau}} = A(y)e_{\tau}$, then $\delta e_{\tilde{\tau}} = A(y)\delta e_{\tau} + (A'(y)\delta y)e_{\tau}$ by the product rule.

Fibrewise linear mappings. Consider two vector bundles $p_1: \mathcal{E}_1 \to \mathcal{M}_1, p_2: \mathcal{E}_2 \to \mathcal{M}_2$, and denote by $L(E_{1,y}, E_{2,z})$ the set of continuous linear mappings $E_{1,y} \to E_{2,z}$ for $y \in \mathcal{M}_1$ and $z \in \mathcal{M}_2$. Given a mapping $f: \mathcal{M}_1 \to \mathcal{M}_2$ we denote by $f^*\mathcal{E}_2$ the pullback bundle of \mathcal{E}_2 via f, i.e. $(f^*E_2)_y := E_{2,f(y)}$. Collecting all mappings in $L(E_{1,y}, E_{2,f(y)})$ for all $y \in \mathcal{M}_1$ in a set $\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2)$, we observe that $p_{\mathcal{L}}: \mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2) \to \mathcal{M}_1$ is a vector bundle itself with fibres $L(E_{1,y}, E_{2,f(y)})$. In trivializations an element H of $\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2)$ is represented by a pair (y, H_τ) where $y \in \mathcal{M}_1$ and $H_\tau \in L(\mathbb{E}_1, \mathbb{E}_2)$.

A fibrewise linear mapping, also called vector bundle morphism, see e.g., [13, III §1], is a section $S \in \Gamma(\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2))$, i.e., a mapping

$$S: \mathcal{M}_1 \to \mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2)$$
 with $p_{\mathcal{L}} \circ S = Id_{\mathcal{M}_1}$.

For example, if $F: \mathcal{X} \to \mathcal{M}$ is differentiable, then the derivative $S := F' \in \Gamma(\mathcal{L}(T\mathcal{X}, F^*T\mathcal{M}))$ is a fibrewise linear mapping, but also vector transports, defined below, are fibrewise linear mappings. S is called locally bounded, respectively differentiable, if its representation in local trivializations, i.e.

$$S_{\tau} := \tau_{\mathcal{E}_2} \circ S \circ \tau_{\mathcal{E}_1}^{-1} \tag{1}$$

has the same property. If S is differentiable, then its derivative is a section $S' \in \Gamma(T\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2))$ of the tangent bundle $p'_{\mathcal{L}}: T\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2) \to T\mathcal{M}_1$, i.e., a mapping

$$S': T\mathcal{M}_1 \to T\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2), \text{ such that } p'_{\mathcal{L}} \circ S' = Id_{T\mathcal{M}_1}.$$

From $S \in \Gamma(\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2))$ we can construct a mapping $\langle S \rangle \in C^1(\mathcal{E}_1, \mathcal{E}_2)$ as follows:

$$\langle S \rangle : \mathcal{E}_1 \to \mathcal{E}_2, \quad e \mapsto \langle S \rangle (e) := S(p_1(e))e.$$

Thus, we obtain a *natural inclusion* of the sections of the bundle of fibrewise linear mappings into the C^1 -mappings:

$$\varphi: \Gamma(\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2)) \to C^1(\mathcal{E}_1, \mathcal{E}_2), \quad S \mapsto \langle S \rangle.$$

Comparison of $S' \in \Gamma(T\mathcal{L}(\mathcal{E}_1, f^*\mathcal{E}_2))$ with $\langle S \rangle' \in \Gamma(\mathcal{L}(T\mathcal{E}_1, S^*T\mathcal{E}_2))$ in trivializations yields by the product rule

$$\langle S \rangle_{\tau}'(e)(\delta y, \delta e_{\tau}) = S_{\tau}(p_1(e))\delta e_{\tau} + (S_{\tau}'(p_1(e))\delta y)e_{\tau} \quad \forall (\delta y, \delta e_{\tau}) \in T_{p_1(e)}\mathcal{M}_1 \times \mathbb{E}_1. \tag{2}$$

Vector transports. Special fibrewise linear mappings, which will later be needed in our globalization strategy, are the so called *vector transports*.

Definition 2.2. For a vector bundle $p: \mathcal{E} \to \mathcal{M}$ and $y \in \mathcal{M}$ we define a vector transport as a section $V_y \in \Gamma(\mathcal{L}(\mathcal{M} \times E_y, \mathcal{E}))$, i.e.

$$V_y: \mathcal{M} \to \mathcal{L}(\mathcal{M} \times E_y, \mathcal{E}), \text{ with } p_{\mathcal{L}}(V_y(\hat{y})) = \hat{y} \ \forall \hat{y} \in \mathcal{M},$$

with the properties that $V_y(y) = Id_{E_y}$ and $V_y(\hat{y})$ is invertible for all $\hat{y} \in \mathcal{M}$. We define a vector back-transport as a section $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$, i.e.

$$V_y^{-1}: \mathcal{M} \to \mathcal{L}(\mathcal{E}, E_y), \text{ with } p_{\mathcal{L}}(V_y^{-1}(\hat{y})) = \hat{y} \ \forall \hat{y} \in \mathcal{M}$$

with the property that $V_u^{-1}(y) = Id_{E_u}$ and $V_u^{-1}(\hat{y})$ is invertible for all $\hat{y} \in \mathcal{M}$.

By restricting \mathcal{M} appropriately, vector transports can also be defined locally. Given a vector transport $V_y \in \Gamma(\mathcal{L}(\mathcal{M} \times E_y, \mathcal{E}))$, we can derive a vector back-transport $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$ by taking pointwise inverses $V_y^{-1}(\hat{y}) := (V_y(\hat{y}))^{-1}$, $\hat{y} \in \mathcal{M}$, and vice versa.

Connections on vector bundles. The concept of a connection of a vector bundle $p: \mathcal{E} \to \mathcal{M}$ is fundamental to differential geometry. It is an additional geometric structure imposed on \mathcal{E} that describes in an infinitesimal way, how neighboring fibres are related. The most prominent example is the Levi-Civita connection on $\mathcal{E} = T\mathcal{X}$ (see e.g. [13, VIII §4]) for a Riemannian manifold \mathcal{X} . Connections give rise to further concepts like the covariant derivative, curvature, geodesics, and parallel transports. They are described in the literature in various equivalent ways (cf. e.g. [13, IV §3 or X §4 or XIII]). For the purpose of our paper we choose a formulation that emphasizes the idea of a connection map $Q_e: T_e\mathcal{E} \to E_{p(e)}$, which then induces a splitting of $T_e\mathcal{E}$ into a vertical and a horizontal subspace.

It is well known that the kernel of $p': T\mathcal{E} \to T\mathcal{M}$ canonically defines the vertical subbundle $V\mathcal{E}$ of \mathcal{E} [13, IV §3]. Its fibres are closed linear subspaces, called the vertical subspaces $V_e := \ker p'(e) \subset T_e\mathcal{E}$. We can identify $E_{p(e)} \cong V_e$ canonically by the isomorphism $\kappa_e : E_{p(e)} \to V_e$, given by $w \mapsto \frac{d}{dt}(e+tw)|_{t=0}$. Elements of V_e are represented in trivializations by pairs of the form $(0_y, \delta e_\tau) \in T_y \mathcal{M} \times \mathbb{E}$.

Using this identification, we define a connection map $Q: T\mathcal{E} \to \mathcal{E}$ as a fibrewise projection onto \mathcal{E} . More precisely, $Q \in \Gamma(\mathcal{L}(T\mathcal{E}, p^*\mathcal{E}))$, i.e., for each $e \in \mathcal{E}$ we get a continuous linear map $Q_e \in L(T_e\mathcal{E}, E_{p(e)})$, such that $Q_e \kappa_e = Id_{E_{p(e)}}$. The kernels $H_e := \ker Q_e$ are called horizontal subspaces, collected in the horizontal subbundle $H\mathcal{E}$. While $V\mathcal{E}$ is given canonically, a choice of Q (or equivalently $H\mathcal{E}$), imposes additional geometric structure on \mathcal{E} .

Using the representations $(y, e_{\tau}) \in \mathcal{M} \times \mathbb{E}$ for $e \in \mathcal{E}$ and $(\delta y, \delta e_{\tau}) \in T_x \mathcal{M} \times \mathbb{E}$ for $\delta e \in T_e \mathcal{E}$, the representation for a linear connection map Q in trivializations can be written in the form

$$Q_e \delta e \sim Q_{e,\tau}(\delta y, \delta e_\tau) = \delta e_\tau - B_{u,\tau}(e_\tau) \delta y, \tag{3}$$

where $B_{y,\tau}: \mathbb{E} \to L(T_y\mathcal{M}, \mathbb{E})$ assigns a linear mapping $B_{y,\tau}(e_{\tau})$ to each $e_{\tau} \in \mathcal{E}$. Since $Q_{e,\tau}(0_y, \delta e_{\tau}) = \delta e_{\tau}$, we see that $Q_{e,\tau}$ indeed represents a projection onto V_y . To reflect the linearity of the fibres we want the connection to be *linear* (fibrewise with respect to e). To this end, we consider the fibrewise scaling $m_s: \mathcal{E} \to \mathcal{E}, e \mapsto se$ and require the condition $Q \circ m'_s = m_s \circ Q$ for all $s \in \mathbb{K}$, which reads in trivializations:

$$Q_{se,\tau}(\delta y, s\delta e_{\tau}) = sQ_{e,\tau}(\delta y, \delta e_{\tau}) \quad \forall s \in \mathbb{K}.$$

It can be shown that Q is linear, if and only if the mapping $e_{\tau} \to B_{y,\tau}(e_{\tau})$ is linear, or put differently, the mapping $(\delta y, e_{\tau}) \to B_{y,\tau}(e_{\tau})\delta y$ is bilinear. Alternatively, for a vector bundle chart Φ we have a representation $B_{y,\Phi}: \mathbb{M} \times \mathbb{E} \to \mathbb{E}$.

If $\mathcal{E} = T\mathcal{X}$ in classical Riemannian geometry, where Q is given by the Levi-Civita connection, the bilinear mapping $B_{x,\Phi}: \mathbb{X} \times \mathbb{X} \to \mathbb{X}$ is represented by Christoffel symbols, and it is symmetric, i.e. $B_{x,\Phi}(v_i)w_i = B_{x,\Phi}(w_i)v_i$, in natural tangent bundle charts.

Connections induced by vector back-transports. If no Levi-Civita connection is present or expensive to evaluate algorithmically, connections can be derived from differentiable vector back-transports, which are needed frequently for numerical purposes anyway:

Lemma 2.3. Let $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$ be a vector back-transport and $e \in E_y$, y = p(e). Then

$$Q_e := \langle V_y^{-1} \rangle'(e) : T_e \mathcal{E} \to E_y$$

defines a linear connection map at e, which is represented in trivializations by (3) with

$$B_{y,\tau}(e_{\tau})\delta y = -((V_{y,\tau}^{-1})'(y)\delta y)e_{\tau}. \tag{4}$$

If V_y^{-1} is defined via pointwise inverses of a vector transport $V_y \in \Gamma(\mathcal{M} \times E_y, \mathcal{E})$, then

$$B_{y,\tau}(e_{\tau})\delta y = (V'_{y,\tau}(y)\delta y)e_{\tau}. \tag{5}$$

Proof. By differentiation of $\langle V_y^{-1} \rangle : \mathcal{E} \to E_y$ we obtain that $\langle V_y^{-1} \rangle'(e) : T_e \mathcal{E} \to E_y$ is a continuous linear map. Using (2) and $V_y^{-1}(y) = Id_{E_y}$, the representation of $\langle V_y^{-1} \rangle' \in \Gamma(\mathcal{L}(T\mathcal{E}, E_y))$ in trivializations, where $V_{y,\tau}^{-1} : \mathcal{M} \to L(\mathbb{E}, \mathbb{E})$, reads

$$\langle V_y^{-1} \rangle_{\tau}'(e)(\delta y, \delta e_{\tau}) = \delta e_{\tau} + ((V_{y,\tau}^{-1})'(y)\delta y)e_{\tau} \quad \forall (\delta y, \delta e_{\tau}),$$

which is of the form (3), implying (4) and linearity. Let $\hat{e} \in E_y$. Since $\kappa_e(\hat{e}) \in V_e \cong E_y$ we get the representation $\kappa_e(\hat{e})_\tau \sim (0_y, \hat{\delta e}_\tau)$. Thus, we obtain $Q_e \kappa_e = Id_{E_y}$.

To show (5) we compute by the calculus rule for inverse matrices and $V_{y,\tau}^{-1}(y) = Id_{\mathbb{E}}$:

$$(V_{y,\tau}^{-1})'(y)\delta y = -V_{y,\tau}^{-1}(y)V_{y,\tau}'(y)\delta y V_{y,\tau}^{-1}(y) = -V_{y,\tau}'(y)\delta y.$$

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Definition 2.4. Let $e \in \mathcal{E}$ and y = p(e). We call a vector back-transport $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$ consistent with a connection map $Q: T\mathcal{E} \to \mathcal{E}$ at e, if $Q_e = \langle V_y^{-1} \rangle'(e)$.

3. Definition of Newton's method

Let $F: \mathcal{X} \to \mathcal{E}$ be a differentiable mapping between a Banach manifold \mathcal{X} and a vector bundle $p: \mathcal{E} \to \mathcal{M}$. By the composition

$$y := p \circ F : \mathcal{X} \to \mathcal{M}, \ y(x) := p(F(x)) \in \mathcal{M},$$

we can compute the base point $y(x) \in \mathcal{M}$ of $F(x) \in \mathcal{E}$ for given $x \in \mathcal{X}$. Consider the following root finding problem

$$F(x) = 0_{y(x)}.$$

In contrast to the classical case, the linear space $E_{y(x)}$ in which F(x) is evaluated now depends on x. Hence, iterative methods will have to deal with the situation that $E_{y(x)}$ changes during the iteration.

To derive Newton's method for this problem we need to define a suitable Newton direction $\delta x \in T_x \mathcal{X}$. The tangent map of F is a mapping $F': T\mathcal{X} \to T\mathcal{E}$. Since $F'(x)\delta x \in T_{F(x)}\mathcal{E}$ and $F(x) \in E_{y(x)}$, these two quantities cannot be added, and thus the classical Newton equation $F'(x)\delta x + F(x) = 0$ is not well defined.

A connection map $Q: T\mathcal{E} \to \mathcal{E}$ on \mathcal{E} allows us to resolve this issue. With its help we can define the following linear mapping at $x \in \mathcal{X}$, which maps into the correct space:

$$Q_{F(x)} \circ F'(x) : T_x \mathcal{X} \to E_{y(x)}.$$

Then the Newton equation is well defined as the following linear operator equation

$$Q_{F(x)} \circ F'(x)\delta x + F(x) = 0_{u(x)}.$$

If $Q_{F(x)} \circ F'(x)$ is invertible, then the Newton direction $\delta x \in T_x \mathcal{X}$ is given as the unique solution of this equation, and $\delta x = 0$ if and only if F(x) = 0.

The classical additive Newton update $x_+ = x + \delta x$ is also not well defined since $x \in \mathcal{X}$ and $\delta x \in T_x \mathcal{X}$ cannot be added. To obtain a new iterate, we have to map $\delta x \in T_x \mathcal{X}$ back to the manifold \mathcal{X} , which can be done by a *retraction*, a popular concept, used widely in numerical methods on manifolds [1, Chap. 4]:

Definition 3.1 (Retraction). A retraction on a manifold \mathcal{X} is a smooth mapping $R: T\mathcal{X} \to \mathcal{X}$, where $R_x: T_x\mathcal{X} \to \mathcal{X}$ for a fixed $x \in \mathcal{X}$ satisfies the following properties:

- (i) $R_x(0_x) = x$
- (ii) $R'_x(0_x) = Id_{T_x \mathcal{X}}$

Thus, after successfully computing the Newton direction we use a retraction to generate the $Newton\ step$

$$x_+ := R_x(\delta x).$$

The result is the following local algorithm:

Algorithm 1 Newton's method on vector bundles

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Require: x_0 (starting point) for k = 1,2,... do \delta x_k \leftarrow Q_{F(x_k)} \circ F'(x_k) \delta x_k + F(x_k) = 0_{y(x_k)} x_{k+1} = R_{x_k}(\delta x_k) end for
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4. Newton-Differentiability and Strict Differentiability

For the analysis of Newton's method we will carry over two differentiability concepts, which are known on linear spaces, but slightly non-standard in the context of manifolds. The first is the so called Newton-differentiability [17, 20, 25], a concept which is tailored for the analysis of local convergence of Newton's method, even for semismooth problems, the second one is strict differentiability [18, 21], a notion that is stronger than Fréchet differentiability, but weaker than continuous differentiability. As usual, we define these concepts by looking at the problem in local charts and showing invariance with respect to changes of charts.

Consider $f: \mathcal{X} \to \mathcal{Y}$ where \mathcal{X} and \mathcal{Y} are both C^1 Banach manifolds. Let (U, ϕ) be a chart of \mathcal{X} and (V, ψ) be a chart of \mathcal{Y} . For (U, ϕ) and (V, ψ) denote by Φ and Ψ the corresponding vector bundle charts of $T\mathcal{X}$ and $T\mathcal{Y}$ according to Remark 2.1. We define the pullback

$$f_{\phi,\psi} := \psi \circ f \circ \phi^{-1} : \phi(U) \to \mathbb{Y}.$$

Using this chart representation, we can define Newton-differentiability of f with respect to $f' \in \Gamma(\mathcal{L}(T\mathcal{X}, f^*T\mathcal{Y}))$ (which need not be the classical derivative) in the following way:

Definition 4.1 (Newton-differentiability of mappings between manifolds). Let $f: \mathcal{X} \to \mathcal{Y}$ be locally Lipschitz continuous and $f' \in \Gamma(\mathcal{L}(T\mathcal{X}, f^*T\mathcal{Y}))$ be locally bounded.

We call f Newton-differentiable at a point $x_0 \in \mathcal{X}$ with respect to f' if the chart representations of f and f' satisfy

$$\lim_{\xi \to \xi_0} \frac{\|f'_{\Phi,\Psi}(\xi)(\xi - \xi_0) - (f_{\phi,\psi}(\xi) - f_{\phi,\psi}(\xi_0))\|_{\mathbb{Y}}}{\|\xi - \xi_0\|_{\mathbb{X}}} = 0,$$

where $\xi_0 = \phi(x_0)$ and $\xi \in \phi(U)$. We call f' a Newton-derivative of f at x_0 .

Be aware that Newton-derivatives are not unique, that's why this definition refers to a given pair f, f'. As we will see in the following discussion, local Lipschitz continuity of f and local boundedness of f' are required to render Newton-differentiability independent of charts.

Analogously, we can define *strict differentiability* of $f: \mathcal{X} \to \mathcal{Y}$ in the following way:

Definition 4.2 (Strict differentiability of mappings between manifolds). Let $f: \mathcal{X} \to \mathcal{Y}$. f is called strictly differentiable at $x_0 \in \mathcal{X}$, if there is $f'(x_0) \in L(T_{x_0}\mathcal{X}, T_{f(x_0)}\mathcal{Y})$, such that the chart representations of f and f' satisfy the following condition:

For every $\varepsilon > 0$ there exists a neighborhood U of $\xi_0 = \phi(x_0)$ such that for $\xi, \eta \in U$

$$||f'_{\Phi,\Psi}(\xi_0)(\xi-\eta) - (f_{\phi,\psi}(\xi) - f_{\phi,\psi}(\eta))||_{\mathbb{Y}} < \varepsilon ||\xi-\eta||_{\mathbb{X}}.$$

The mapping $f'(x_0)$ is called strict derivative of f at x_0 .

In linear spaces it is well known, and also not hard to verify, that continuous differentiability implies Newton-differentiability, as well as strict differentiability. Since the chart representation of a C^1 -mapping $f: \mathcal{X} \to \mathcal{Y}$ is a C^1 -mapping between vector spaces, we can conclude, that f is also Newton-differentiable and strictly differentiable.

In linear spaces we have the following chain rule for the Newton-differentiability [10] and strict differentiability, which we will use to verify that our definition is independent of the used charts:

Lemma 4.3. Let \mathbb{X} , \mathbb{Y} and \mathbb{Z} be normed linear spaces. Consider $f: \mathbb{X} \to \mathbb{Y}$ and $g: \mathbb{Y} \to \mathbb{Z}$.

- (i) Let f and g be Newton-differentiable with respect to Newton-derivatives f' and g' in open sets V and U, respectively, with $U \subset \mathbb{X}$, $f(U) \subset V \subset \mathbb{Y}$. Assume that f is locally Lipschitz continuous and g' is locally bounded. Then $g \circ f : \mathbb{X} \to \mathbb{Z}$ is Newton-differentiable with respect to a Newton-derivative $g'(f(\cdot))f'(\cdot) : \mathbb{X} \to \mathbb{Z}$.
- (ii) Let f and g be strictly differentiable with strict derivative f' and g' in open sets V and U, respectively, with $U \subset \mathbb{X}$, $f(U) \subset V \subset \mathbb{Y}$. Then $g \circ f : \mathbb{X} \to \mathbb{Z}$ is strictly differentiable with strict derivative $g'(f(\cdot))f'(\cdot) : \mathbb{X} \to \mathbb{Z}$.

Proof. Let $x, y, x_0 \in U$. Consider the remainder term

$$||g'(f(x_0))f'(x_0)(x-y) - (g \circ f(x) - g \circ f(y))||_{\mathbb{Z}}$$

$$= ||g'(f(x_0))(f(x) - f(y)) - (g(f(x)) - g(f(y))) + R(x, y, x_0)||_{\mathbb{Z}}$$
(6)

where $R(x, y, x_0) := g'(f(x_0))f'(x_0)(x - y) - g'(f(x_0))(f(x) - f(y)).$

Since g' is locally bounded in the Newton-differentiable case and x_0 is fixed in the strict differentiable case, there exists a local constant C > 0 such that

$$||g'(f(x_0))||_{\mathbb{Y}\to\mathbb{Z}} \le C.$$

Thus, we obtain

$$||R(x, y, x_0)||_{\mathbb{Z}} = ||g'(f(x_0))[f'(x_0)(x - y) - (f(x) - f(y))]||_{\mathbb{Z}}$$

$$\leq C \cdot ||f'(x_0)(x - y) - (f(x) - f(y))||_{\mathbb{Y}}$$

Hence, we can estimate (6) by

$$||g'(f(x_0))f'(x_0)(x-y) - (g \circ f(x) - g \circ f(y))||_{\mathbb{Z}}$$

$$\leq ||g'(f(x_0))(f(x) - f(y)) - (g(f(x)) - g(f(y)))||_{\mathbb{Z}} + C \cdot ||f'(x_0)(x-y) - (f(x) - f(y))||_{\mathbb{Y}}.$$
(7)

Now consider the different cases:

(i): Set $x = x_0$. Let y be fixed. Newton-differentiability of f at x yields

$$||f'(x)(x-y) - (f(x) - f(y))||_{\mathbb{Y}} = o(||x-y||_{\mathbb{X}})$$

as $x \to y$. Since g is Newton-differentiable at $f(x) \in V$, we get that

$$\|g'(f(x))(f(x) - f(y)) - (g(f(x)) - g(f(y)))\|_{\mathbb{Z}} = o(\|f(x) - f(y)\|_{\mathbb{Y}}).$$

By local Lipschitz-continuity of f, we obtain that $||f(x) - f(y)||_{\mathbb{Y}} = \mathcal{O}(||x - y||_{\mathbb{X}})$ as $x \to y$. Using this in (7), we get for the remainder term

$$||g'(f(x))f'(x)(x-y) - (g \circ f(x) - g \circ f(y))||_{\mathbb{Z}} = o(||x-y||_{\mathbb{X}})$$

as $x \to y$, and thus Newton-differentiability of $g \circ f$ with respect to $g'(f(\cdot))f'(\cdot)$.

(ii): Let $\varepsilon > 0$ and $x_0 \in X$ be fixed. Using the strict differentiability of f at x_0 , there exists a neighborhood $W \subset U$ such that for $x, y \in W$:

$$||f'(x_0)(x-y) - (f(x) - f(y))||_{\mathbb{Y}} < \frac{\varepsilon}{2C} ||x-y||_{\mathbb{X}}.$$

Thus, (7) yields

$$||g'(f(x_0))f'(x_0)(x-y) - (g \circ f(x) - g \circ f(y))||_{\mathbb{Z}}$$

$$\leq ||g'(f(x_0))(f(x) - f(y)) - (g(f(x)) - g(f(y)))||_{\mathbb{Z}} + \frac{\varepsilon}{2}||x - y||_{\mathbb{X}}.$$

Using that $||f'(x_0)||_{\mathbb{X}\to\mathbb{Y}}$ is finite and f is strictly differentiable at x_0 , for every $\tilde{\varepsilon}>0$ there is a neighborhood such that

$$||f(x) - f(y)||_{\mathbb{Y}} \le ||f(x) - f(y) - f'(x_0)(x - y)||_{\mathbb{Y}} + ||f'(x_0)(x - y)||_{\mathbb{Y}}$$

$$< \tilde{\varepsilon} ||x - y||_{\mathbb{X}} + ||f'(x_0)||_{\mathbb{X} \to \mathbb{Y}} ||x - y||_{\mathbb{X}}$$

$$\le \tilde{C} ||x - y||_{\mathbb{X}}.$$
(8)

Since g is strictly differentiable at $f(x_0)$, we obtain by possibly shrinking W that

$$||g'(f(x_0))(f(x) - f(y)) - (g(f(x)) - g(f(y)))||_{\mathbb{Z}} < \frac{\varepsilon}{2\widetilde{C}} ||f(x) - f(y)||_{\mathbb{Y}}.$$

Using (8), we can in summary estimate the remainder term by

$$\|g'(f(x_0))f'(x)(x-y) - (g \circ f(x) - g \circ f(y))\|_{\mathbb{Z}} < \varepsilon \|x-y\|_{\mathbb{X}}$$

and thus $g \circ f$ is strictly differentiable with strict derivative $g'(f(\cdot))f'(\cdot)$.

Proposition 4.4. Newton-differentiability and strict differentiability of $f: \mathcal{X} \to \mathcal{Y}$ are independent of the choice of charts of \mathcal{X} and \mathcal{Y} .

Proof. Let ϕ_i and ψ_i be charts of \mathcal{X} and \mathcal{Y} such that f is Newton-, respectively strictly, differentiable at $x_0 \in \mathcal{X}$. Let ϕ_j be another chart of \mathcal{X} and ψ_j be another chart of \mathcal{Y} . Consider the mapping

$$\psi_j \circ f \circ \phi_j^{-1} = T_{ij}^{\mathcal{X}} \circ (\psi_i \circ f \circ \phi_i^{-1}) \circ T_{ji}^{\mathcal{Y}}.$$

 $T_{ji}^{\mathcal{Y}}$ and $T_{ij}^{\mathcal{X}}$ are continuously differentiable and thus Newton-differentiable, as well as strictly differentiable. By applying the chain rule twice, we obtain Newton- or strict differentiability of $\psi_j \circ f \circ \phi_j^{-1}$.

5. Local convergence of Newton's method

Similar to the case of linear spaces we will now study the local convergence of Newton's method. This will require some preparation. To formulate local superlinear convergence requires a metric on \mathcal{X} to measure the distance of iterates. In our general setting we are considering Banach manifolds which may not be endowed with a Riemannian metric. Thus, we will discuss a slightly more general way to define a metric on a manifold. Second, we will derive a geometric criterion on Newton-and strict differentiability. This will be especially useful later to connect our *a-priori* analysis of local convergence with some computable *a-posteriori* quantities, which are defined in the spirit of Deuflhard [9].

5.1. Local norms and a metric on manifolds

In Riemannian geometry, manifolds are equipped with a Riemannian metric, based on inner products on the tangent bundle [13, VII §6]. However, in the case of linear spaces, it is known that the convergence theory of Newton's method is not restricted to Hilbert spaces, but can be applied in general Banach spaces. Hence, we will present a slightly more general notion of a metric, replacing the usual inner products by general norms. In the infinite dimensional case, some care has to be taken, concerning continuity properties.

Definition 5.1. Consider a function $f: \mathcal{E} \to \mathbb{R}$. We call f fibrewise uniformly continuous around $D \subset E_y$, if for any local trivialization τ , the function

$$f_{\tau} := f \circ \tau^{-1} : \tau(p^{-1}(U)) \to \mathbb{R}$$

satisfies the following condition:

For all $\varepsilon > 0$ there exists a neighborhood $V \subset \mathcal{M}$ of y and $\delta > 0$, such that for all $(y, e_{\tau}) \in \tau(D)$ we have the estimate:

$$|f_{\tau}(y, e_{\tau}) - f_{\tau}(\xi, \eta_{\tau})| < \varepsilon \quad \forall (\xi, \eta_{\tau}) \in p^{-1}(U) : \xi \in V, \|\eta_{\tau} - e_{\tau}\|_{\mathbb{E}} < \delta.$$

It is not hard to show that this notion is independent of the choice of trivialization, taking into account that transition mappings are linear isomorphisms on \mathcal{E} .

Clearly, fibrewise uniform continuity is a stronger condition than continuity, since δ can only depend on y and not on e_{τ} . In particular, we conclude, setting $\eta_{\tau} = e_{\tau}$:

$$\sup_{e_{\tau} \in \tau(D)} |f_{\tau}(y, e_{\tau}) - f_{\tau}(\xi, e_{\tau})| < \varepsilon \quad \forall \xi \in V.$$
(9)

On a vector bundle $p: \mathcal{E} \to \mathcal{M}$ we can define a *continuous norm* as follows:

Definition 5.2. Consider a function $\|\cdot\|: \mathcal{E} \to [0, \infty[$ with the following properties:

- i) For each $y \in \mathcal{M}$ the restriction $\|\cdot\|_y$ to E_y is a norm on E_y which is equivalent to the $\|\cdot\|_{\mathbb{E}}$ norm that makes \mathbb{E} a Banach space. Thus, $(E_y, \|\cdot\|_y)$ is a Banach space. We denote by $\mathbb{S}_y \subset E_y$ the unit sphere with respect to $\|\cdot\|_y$.
- ii) For each $y \in \mathcal{M}$, $\|\cdot\|$ is fibrewise uniformly continuous around the unit sphere $\mathbb{S}_y \subset E_y$.

We call $\|\cdot\|$ a continuous norm on \mathcal{E} .

Our definition includes Riemannian metrics, as well as Finsler metrics, but is more general than those: no differentiability assumption is imposed, since this is not needed for our specific purpose. In particular, non-differentiable norms, such as 1-norms or ∞ -norms fit into our framework.

Lemma 5.3. Let $y \in \mathcal{M}$ and $\|\cdot\|: \mathcal{E} \to [0, \infty)$ be a continuous norm. Consider its representation $\|\cdot\|_{\tau}$ in a local trivialization around $y \in \mathcal{M}$. Then for every $1 > \varepsilon > 0$ there is a neighborhood V of y, such that

$$(1-\varepsilon)\|e_{\tau}\|_{\tau,y} \le \|e_{\tau}\|_{\tau,\xi} \le (1+\varepsilon)\|e_{\tau}\|_{\tau,y} \quad \forall \xi \in V, e_{\tau} \in \mathbb{E}.$$

Proof. Since $\|\lambda e_{\tau}\|_{\tau,y} = |\lambda| \|e_{\tau}\|_{\tau,y}$ we may assume $\|e_{\tau}\|_{\tau,y} = 1$. Now our result is a direct consequence of (9).

To define a metric on a manifold \mathcal{X} we will consider a continuous norm on the tangent bundle $T\mathcal{X}$. The following integral over a (piecewise) C^1 -curve $\alpha:[a,b]\to\mathcal{X}$ is well defined, because the integrand is (piecewise) continuous on [a,b]:

$$L(\alpha) := \int_a^b \|\alpha'(t)\|_{\alpha(t)} dt.$$

The value of this integral can be interpreted as the length of the curve α . The following derivations are analogous to the construction of a Riemannian distance (cf. e.g. [13, VII §6]), and generalize them from the case of a Hilbert space norm to the case of a Banach space norm.

To measure the "distance" between x and y on \mathcal{X} , we form the infimum over the lengths of all curves connecting x and y. If x and y cannot be connected, we set $d(x,y) = \infty$. According to this we define the map

$$d: \mathcal{X} \times \mathcal{X} \to \overline{\mathbb{R}} := \mathbb{R} \cup \{\infty\}$$

 $(x,y) \mapsto \inf\{L(\alpha) \mid \alpha : [a,b] \to \mathcal{X} \text{ piecewise } C^1\text{-curve s.t. } \alpha(a) = x, \alpha(b) = y\}.$

In the following we will always assume that \mathcal{X} is connected. Then the axioms of a metric follow readily. Symmetry d(x,y) = d(y,x) and non-negativity, $d(x,y) \geq 0$, are obvious from the definition. It is known from topology that on a connected manifold, two points can always be connected by a piecewise smooth curve [12], and thus $d(x,y) < \infty \ \forall x,y \in \mathcal{X}$. The triangle inequality follows straightforwardly from the fact that the length of curves adds up if they are concatenated. It thus remains to show positive definiteness of d, which is the only result that requires fibrewise uniform continuity.

To this end, we first prove some results which relates the mapping d to the local norms. Let (U,ϕ) be a local chart at $x_{\star} \in \mathcal{X}$ and $\Phi : \pi^{-1}(U) \to U \times \mathbb{X}$ be the corresponding natural vector bundle chart on the tangent bundle $\pi : T\mathcal{X} \to \mathcal{X}$. We define the *open ball with radius* r > 0 around 0 with respect to the local norm $\|\cdot\|_{x_{\star}}$ (with representation $\|\cdot\|_{\Phi,x_{\star}}$) as $rB_{x_{\star}} := \{v \in \mathbb{X} : \|v\|_{\Phi,x_{\star}} < r\}$.

Lemma 5.4. Let $x_{\star} \in \mathcal{X}$ and (U, ϕ) a local chart, such that w.l.o.g. $\phi(x_{\star}) = 0$. Let $x, y \in U$ with representatives x_{ϕ} and y_{ϕ} in the chart. Let $1 > \varepsilon > 0$. Then there exists a radius $r = r(\varepsilon) > 0$ such that for every C^1 -curve $\alpha : [a, b] \to \mathcal{X}$ connecting x and y the following holds:

- (a) If the image $\alpha_{\phi}: [a,b] \to \mathbb{X}$ lies in the open ball $rB_{x_{\star}}$, in particular x_{ϕ} , $y_{\phi} \in rB_{x_{\star}}$, then the following properties hold:
 - (i) $(1 \varepsilon) \| x_{\phi} y_{\phi} \|_{\Phi, x_{+}} \le L(\alpha)$
 - (ii) $d(x,y) \le (1+\varepsilon) \|x_{\phi} y_{\phi}\|_{\Phi,x_{\star}}$
- (b) If α_{ϕ} is leaving the ball $rB_{x_{\star}}$, i.e. $\alpha_{\phi}(a) = x_{\phi} \in rB_{x_{\star}}$ but $\alpha_{\phi} \not\subset rB_{x_{\star}}$, then it holds that

$$L(\alpha) \ge (1 - \varepsilon)(r - ||x_{\phi}||_{\Phi,x_{+}}).$$

Proof. Since $\|\cdot\|$ is a continuous norm on $T\mathcal{X}$, according to Lemma 5.3 for $1 > \varepsilon > 0$ there exists a neighborhood V of x_{\star} , such that

$$(1-\varepsilon)\|v\|_{\Phi,x_{+}} \leq \|v\|_{\Phi,\xi} \leq (1+\varepsilon)\|v\|_{\Phi,x_{+}} \ \forall \xi \in V, v \in \mathbb{X}.$$

The image of V in the chart contains a $\|\cdot\|_{\Phi,x_{\star}}$ -ball $rB_{x_{\star}}$ around $\phi(x_{\star})=0$ with radius $r=r(\varepsilon)>0$. Let $x,y\in U$ and $\alpha:[a,b]\to\mathcal{X}$ be a C^1 -curve connecting x and y.

(a) Assume that the image α_{ϕ} lies in $rB_{x_{\star}}$. Using that the curve integral in vector spaces is always greater than or equal to the distance of the end points, we can estimate the length of α by

$$(1 - \varepsilon) \|x_{\phi} - y_{\phi}\|_{\Phi, x_{\star}} \le (1 - \varepsilon) \int_{a}^{b} \|\alpha'_{\phi}(t)\|_{\Phi, x_{\star}} dt \stackrel{\alpha(t) \in V}{\le} \int_{a}^{b} \|\alpha'(t)\|_{\alpha(t)} dt$$
$$= L(\alpha) \le (1 + \varepsilon) \int_{a}^{b} \|\alpha'_{\phi}(t)\|_{\Phi, x_{\star}} dt.$$

Choosing the connecting line of x_{ϕ} and y_{ϕ} for α_{ϕ} this yields $d(x,y) \leq (1+\varepsilon) \|x_{\phi} - y_{\phi}\|_{\Phi,x_{\star}}$.

(b) If α_{ϕ} leaves the open ball $rB_{x_{\star}}$, there must be a first intersection point $s_{\phi} = \alpha_{\phi}(c)$, $c \in [a, b]$, with the sphere $r\mathbb{S}_{x_{\star}} \subset \mathbb{X}$ around 0. Let $\widetilde{\alpha}_{\phi}$ be the part of α_{ϕ} connecting x_{ϕ} and s_{ϕ} . Then by the norm equivalence and the inverse triangle inequality:

$$L(\widetilde{\alpha}) = \int_{a}^{c} \|\widetilde{\alpha}'(t)\|_{\widetilde{\alpha}(t)} dt \ge (1 - \varepsilon) \int_{a}^{c} \|\widetilde{\alpha}'_{\phi}(t)\|_{\Phi, x_{\star}} dt$$

$$\ge (1 - \varepsilon)(\|s_{\phi}\|_{\Phi, x_{\star}} - \|x_{\phi}\|_{\Phi, x_{\star}}) = (1 - \varepsilon)(r - \|x_{\phi}\|_{\Phi, x_{\star}}).$$

Thus, we get $L(\alpha) \geq (1 - \varepsilon)(r - ||x_{\phi}||_{\Phi, x_{\star}}).$

Proposition 5.5. Let $1 > \varepsilon > 0$. Then there is a neighborhood $W \subseteq U$ of x_{\star} such that

$$(1-\varepsilon) \cdot \|x_{\phi} - y_{\phi}\|_{\Phi, x_{\star}} \le d(x, y) \le (1+\varepsilon) \cdot \|x_{\phi} - y_{\phi}\|_{\Phi, x_{\star}} \ \forall x, y \in W,$$

where $x_{\phi}, y_{\phi} \in \mathbb{X}$ are representatives of x and y in the chart.

Proof. W.l.o.g. assume $\phi(x_{\star}) = 0$. By Lemma 5.4, we directly obtain

$$d(x,y) \le (1+\varepsilon) \|x_{\phi} - y_{\phi}\|_{\Phi,x_{\star}} \ \forall x,y \in \phi^{-1}(rB_{x_{\star}}),$$

where r > 0 is chosen sufficiently small. Now let α be an arbitrary curve connecting x and y. Lemma 5.4 yields

$$\alpha_{\phi} \subset rB_{x_{\star}} \Rightarrow L(\alpha) \ge (1 - \varepsilon) \|x_{\phi} - y_{\phi}\|_{\Phi, x_{\star}},$$

$$\alpha_{\phi} \not\subset rB_{x_{\star}} \Rightarrow L(\alpha) \ge (1 - \varepsilon) (r - \|x_{\phi}\|_{\Phi, x_{\star}}).$$

Thus, we obtain

$$d(x,y) \ge (1-\varepsilon) \cdot \min\{ \|x_{\phi} - y_{\phi}\|_{\Phi,x_{\star}}, r - \|x_{\phi}\|_{\Phi,x_{\star}} \}. \tag{10}$$

Choosing $W := \phi^{-1}(\frac{r}{3}B_{x_{\star}})$ yields $d(x,y) \geq (1-\varepsilon)\|x_{\phi} - y_{\phi}\|_{\Phi,x_{\star}}$ and thus our claim.

Corollary 5.6. Let \mathcal{X} be a connected C^1 Banach manifold with the Hausdorff property. Then d defines a metric on \mathcal{X} . Moreover, the induced topology coincides with the topology on \mathcal{X} induced by the atlas.

Proof. Let $x \neq y$. Let (U, ϕ) be a local chart at x such that w.l.o.g. $\phi(x) = x_{\phi} = 0$, and let $\Phi : \pi^{-1}(U) \to U \times \mathbb{X}$ be the natural vector bundle chart on the tangent bundle $\pi : T\mathcal{X} \to \mathcal{X}$. Since \mathcal{X} satisfies the Hausdorff property and $x \neq y$ holds, there is a $\|\cdot\|_{\Phi,x}$ -ball rB_x around 0 with radius r > 0 such that $y \notin \phi^{-1}(rB_x)$. Possibly decreasing r first, we obtain by (10)

$$d(x,y) \ge (1-\varepsilon) \cdot \min\{\|y_{\phi}\|_{\Phi,x}, r\} = (1-\varepsilon) \cdot r > 0.$$

Moreover, for $y \in \phi^{-1}(r\mathbb{S}_x)$ we obtain by Prop. 5.5

$$(1 - \varepsilon) \cdot ||y_{\phi}||_{\Phi, x} \le d(x, y) \le (1 + \varepsilon) \cdot ||y_{\phi}||_{\Phi, x}.$$

Since $\|\cdot\|_{\Phi,x}$ is equivalent to $\|\cdot\|_{\mathbb{X}}$, this implies that every \mathbb{X} -ball contains a d-ball and vice versa. Thus, the topology induced by d coincides with the topology induced by the atlas of \mathcal{X} .

Now consider a retraction $R: T\mathcal{X} \to \mathcal{X}$. For C^1 -retractions of this kind it is well known that the following property holds [1] by the inverse function theorem.

Proposition 5.7. Let $x_{\star} \in \mathcal{X}$ and let R be a C^1 -retraction. Then there exists a neighborhood $V \subseteq T\mathcal{X}$ of $(x_{\star}, 0) \in T\mathcal{X}$ such that $R : V \to R(V)$ is a diffeomorphism.

Finally, we can relate retractions, local norms and the metric on \mathcal{X} defined by the local norms.

Proposition 5.8. To $x_{\star} \in \mathcal{X}$ and $1 > \varepsilon > 0$ there exists a neighborhood V of x_{\star} such that for all $x, y, z \in V$ the following holds:

$$(1-\varepsilon)\|R_z^{-1}(x) - R_z^{-1}(y)\|_z \le d(x,y) \le (1+\varepsilon)\|R_z^{-1}(x) - R_z^{-1}(y)\|_z.$$

Proof. Choose a chart (U,ϕ) of \mathcal{X} at x_{\star} and denote by $\Phi:\pi^{-1}(U)\to U\times\mathbb{X}$ the natural vector bundle chart on the tangent bundle $\pi:T\mathcal{X}\to\mathcal{X}$. Let $x_{\star,\phi},\ x_{\phi},\ y_{\phi}$ and z_{ϕ} be representatives of x_{\star},x,y and z in the chart. Let R_{ϕ}^{-1} be the chart representation of R^{-1} . We show that

$$\lim_{x_{\phi}, y_{\phi}, z_{\phi} \to x_{\star, \phi}} \frac{\|R_{\phi}^{-1}(z_{\phi}, x_{\phi}) - R_{\phi}^{-1}(z_{\phi}, y_{\phi})\|_{\Phi, x_{\star}}}{\|x_{\phi} - y_{\phi}\|_{\Phi, x_{\star}}} = 1.$$

Since R^{-1} is continuously differentiable, R^{-1} is also strictly differentiable. Thus, by additionally using the properties of a retraction, there exists a neighborhood V, such that for arbitrary $\varepsilon > 0$ we obtain, denoting by $r_{R^{-1}}(x_{\phi}, y_{\phi})$ the remainder term of strict differentiability:

$$||R_{\phi}^{-1}(z_{\phi}, x_{\phi}) - R_{\phi}^{-1}(z_{\phi}, y_{\phi})||_{\mathbb{X}} = ||(R_{\phi}^{-1})'(x_{\star,\phi}, x_{\star,\phi})(x_{\phi} - y_{\phi}) + r_{R^{-1}}(x_{\phi}, y_{\phi})||_{\mathbb{X}}$$

$$= ||R'_{\phi}(R_{\phi}^{-1}(x_{\star,\phi}, x_{\star,\phi}))(x_{\phi} - y_{\phi}) + r_{R^{-1}}(x_{\phi}, y_{\phi})||_{\mathbb{X}}$$

$$= ||x_{\phi} - y_{\phi} + r_{R^{-1}}(x_{\phi}, y_{\phi})||_{\mathbb{X}}$$

$$\leq ||x_{\phi} - y_{\phi}||_{\mathbb{X}} + \varepsilon ||x_{\phi} - y_{\phi}||_{\mathbb{X}}.$$

Using that $\|\cdot\|_{\Phi,x_{\star}}$ is equivalent to $\|\cdot\|_{\mathbb{X}}$ and by possibly shrinking V, we obtain the desired assertion by Prop. 5.5.

5.2. Newton- and Strict Differentiability in Geometric Form

In order to analyse local convergence of Newton's method, we want to prove a result about a Newton- or strictly differentiable mapping $F: \mathcal{X} \to \mathcal{E}$ between a manifold \mathcal{X} and a vector bundle $p: \mathcal{E} \to \mathcal{M}$, which can be stated independently of the choice of charts.

In the following, we assume that the mapping

$$y = p \circ F : \mathcal{X} \to \mathcal{M}, \ y(x) := p(F(x)) \in \mathcal{M},$$

which computes the base point of $F(x) \in \mathcal{E}$ for any $x \in \mathcal{X}$, is locally Lipschitz continuous. We may use the linear map $V_y^{-1}(y_0) \in L(E_{y_0}, E_y)$ given by a vector back-transport $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$ to transport elements $F(x_0) \in E_{y_0}$ into the fibre E_y .

Proposition 5.9. Let $F: \mathcal{X} \to \mathcal{E}$. Let $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$ be a vector back-transport, $Q: T\mathcal{E} \to \mathcal{E}$ be a connection map and $R: T\mathcal{X} \to \mathcal{X}$ be a retraction.

(i) Let $F: \mathcal{X} \to \mathcal{E}$ be Newton-differentiable at a point $\xi \in \mathcal{X}$ with respect to a fibrewise linear mapping $F' \in \Gamma(\mathcal{L}(T\mathcal{X}, F^*T\mathcal{E}))$. If V_{ν}^{-1} is consistent with Q or $F(\xi) = 0$, then it holds

$$\lim_{x \to \xi} \frac{\|(Q_{F(x)} \circ F'(x))(R_x^{-1}(x) - R_x^{-1}(\xi)) - (F(x) - V_{y(x)}^{-1}(y(\xi))F(\xi))\|_{E_{y(x)}}}{d_{\mathcal{X}}(x,\xi)} = 0.$$

(ii) Let F be strictly differentiable at $a \in \mathcal{X}$. If V_y^{-1} is consistent with Q or F(a) = 0 then for every $\varepsilon > 0$ there exists a neighborhood W of a such that for all $x, \xi \in W$ it holds

$$\|(Q_{F(a)} \circ F'(a))(R_a^{-1}(x) - R_a^{-1}(\xi)) - (V_{y(a)}^{-1}(y(x))F(x) - V_{y(a)}^{-1}(y(\xi))F(\xi))\|_{E_{y(a)}}$$

$$< \varepsilon \|R_a^{-1}(x) - R_a^{-1}(\xi)\|_a.$$

Proof. Choose a chart ϕ of \mathcal{X} and a vector bundle chart η of the vector bundle \mathcal{E} . In the following, we use ϕ or η as an index to denote the chart representation of elements of \mathcal{X} or \mathcal{E} , respectively. We begin by discussing the numerators in (i) and (ii) in a unified way. Then for the proof of (i) we will fix ξ and consider the case x = a and $x \to \xi$. For the proof of (ii) we will fix a and consider a and a

Let $R_{a,\phi}^{-1}$ be a representation of the inverse retraction in charts. Since R_a^{-1} is a C^1 -mapping and using $(R_a^{-1})'(a) = Id_{T_a\mathcal{X}}$, we obtain

$$R_{a,\phi}^{-1}(x_{\phi}) - R_{a,\phi}^{-1}(\xi_{\phi}) = (R_{a,\phi}^{-1})'(a_{\phi})(x_{\phi} - \xi_{\phi}) + r_R = (x_{\phi} - \xi_{\phi}) + r_R$$

where r_R is a remainder term. Setting $\delta x_{\phi} = x_{\phi} - \xi_{\phi}$ and $\delta y_{\eta} := y(x)_{\eta} - y(\xi)_{\eta} \in \mathbb{M}$, we obtain the chart representation of

$$(Q_{F(a)} \circ F'(a))(R_a^{-1}(x) - R_a^{-1}(\xi))$$

by

$$(F_{\eta})'(a_{\phi})(\delta x_{\phi} + r_R) - B_{y(a),\eta}(F_{\eta}(a_{\phi}))\delta y_{\eta}. \tag{11}$$

Next, we consider the representation of

$$V_{y(a)}^{-1}(y(x))F(x)-V_{y(a)}^{-1}(y(\xi))F(\xi),$$

which is of the form

$$V_{u(a),\eta}^{-1}(y(x)_{\eta})F_{\eta}(x_{\phi}) - V_{u(a),\eta}^{-1}(y(\xi)_{\eta})F_{\eta}(\xi_{\phi}). \tag{12}$$

Using the differentiability of the mapping $V_{y,\eta}^{-1}:\mathbb{M}\to L(\mathbb{E},\mathbb{E})$, we can write:

$$V_{y(a),\eta}^{-1}(y(x)_{\eta}) - V_{y(a),\eta}^{-1}(y(\xi)_{\eta}) = (V_{y(a),\eta}^{-1})'(y(a)_{\eta})\delta y_{\eta} + r_{V}.$$

Inserting this into (12) we obtain by linearity of $V_u^{-1}(y)$

$$((V_{y(a),\eta}^{-1})'(y(a)_{\eta})\delta y_{\eta})F_{\eta}(\xi_{\phi}) + V_{y(a),\eta}^{-1}(y(x)_{\eta})(F_{\eta}(x_{\phi}) - F_{\eta}(\xi_{\phi})) + r_{V}F_{\eta}(\xi_{\phi}). \tag{13}$$

Writing the difference $F_{\eta}(x_{\phi}) - F_{\eta}(\xi_{\phi})$ as

$$F_{\eta}(x_{\phi}) - F_{\eta}(\xi_{\phi}) = (F_{\eta})'(a_{\phi})\delta x_{\phi} + r_F.$$

and subtracting (13) from (11) we finally obtain the following representation of the numerators of (i) and (ii) in charts:

$$(Id_{E_{y(a)}} - V_{y(a),\eta}^{-1}(y(x)_{\eta}))(F_{\eta})'(a_{\phi})\delta x_{\phi}$$

$$- B_{y(a),\eta}(F_{\eta}(a_{\phi}))\delta y_{\eta} - ((V_{y(a),\eta}^{-1})'(y(a)_{\eta})\delta y_{\eta})F_{\eta}(\xi_{\phi})$$

$$+ (F_{\eta})'(a_{\phi})r_{R} - V_{y(a),\eta}^{-1}(y(x)_{\eta})r_{F} - r_{V}F_{\eta}(\xi_{\phi}).$$

Now consider the different cases.

(i): Set a = x and let F be Newton-differentiable at ξ . Since $V_y^{-1}(y) = Id_{E_y}$ for $y \in \mathcal{M}$ and x = a our representation reduces to

$$-B_{y(x),\eta}(F_{\eta}(x_{\phi}))\delta y_{\eta} - ((V_{y(x),\eta}^{-1})'(y(x)_{\eta})\delta y_{\eta})F_{\eta}(\xi_{\phi}) + (F_{\eta})'(x_{\phi})r_{R} - r_{F} - r_{V}F_{\eta}(\xi_{\phi}).$$

Since R_x^{-1} is continuously differentiable, it is also Newton-differentiable and thus the remainder term r_R is of order $o(\|x_\phi - \xi_\phi\|_{\mathbb{X}})$ as $x_\phi \to \xi_\phi$. Since F is Newton-differentiable with respect to F', $(F_\eta)'(x_\phi)$ is locally bounded. Thus, the remainder term $(F_\eta)'(x_\phi)r_R$ is still of order $o(\|x_\phi - \xi_\phi\|_{\mathbb{X}})$ as $x_\phi \to \xi_\phi$. Since F is Newton-differentiable r_F is also of order $o(\|x_\phi - \xi_\phi\|_{\mathbb{X}})$ as $x_\phi \to \xi_\phi$. The remainder term r_V depends on $y(x)_\eta$ and $y(\xi)_\eta$ and is of order $o(\|y(x)_\eta - y(\xi)_\eta\|_{\mathbb{M}})$. Since the mapping y is locally Lipschitz continuous, $r_V F_\eta(\xi_\phi)$ is of order $o(\|x_\phi - \xi_\phi\|_{\mathbb{X}})$ as $x_\phi \to \xi_\phi$.

Thus, we have to discuss the remaining two terms

$$-B_{y(x),\eta}(F_{\eta}(x_{\phi}))\delta y_{\eta} - ((V_{y(x),\eta}^{-1})'(y(x)_{\eta})\delta y_{\eta})F_{\eta}(\xi_{\phi}). \tag{14}$$

Using the bilinearity of $B_{y(x),\eta}$ we can write (14) as

$$-B_{y(x),\eta}(F_{\eta}(x_{\phi}) - F_{\eta}(\xi_{\phi}))\delta y_{\eta} - \left[B_{y(x),\eta}(F(\xi_{\phi}))\delta y_{\eta} + ((V_{y(x),\eta}^{-1})'(y(x)_{\eta})\delta y_{\eta})(F_{\eta}(\xi_{\phi}))\right]$$

Since F is Newton-differentiable and $x \mapsto B_{y(x),\eta}$ is locally bounded, the first term is of order $\mathcal{O}(\|x_{\phi} - \xi_{\phi}\| \|\delta y_{\eta}\|)$, and thus, by Lipschitz continuity of y, of order $o(\|x_{\phi} - \xi_{\phi}\|)$. If V_{y}^{-1} is consistent with the connection map Q, i.e. $B_{y(x),\eta} = -(V_{y(x),\eta}^{-1})'(y(x)_{\eta})$, or $F(\xi) = 0$ the second term in braces vanishes. Thus, the numerator of (i) is of order $o(\|x_{\phi} - \xi_{\phi}\|_{\mathbb{X}})$ as $x_{\phi} \to \xi_{\phi}$. Finally, using Prop. 5.5 to estimate $d_{\mathcal{X}}(x,\xi)$, we obtain the desired result.

(ii): Let F be strictly differentiable at $a \in \mathcal{X}$. Let $x, \xi \in \mathcal{X}$. If V_y^{-1} is consistent with the connection map Q we have

$$B_{y(a),\eta}(F_{\eta}(a_{\phi}))\delta y_{\eta} = -((V_{y(a),\eta}^{-1})'(y(a)_{\eta})\delta y_{\eta})F_{\eta}(a_{\phi}).$$

Otherwise, we assume that F(a) = 0. In both cases our representation reads (the sign in the second line depends on these cases):

$$(Id_{E_{y(a)}} - V_{y(a),\eta}^{-1}(y(x)_{\eta}))(F_{\eta})'(a_{\phi})\delta x_{\phi}$$

$$\pm ((V_{y(a),\eta}^{-1})'(y(a)_{\eta})\delta y_{\eta})(F_{\eta}(a_{\phi}) - F_{\eta}(\xi_{\phi}))$$

$$+ (F_{\eta})'(a_{\phi})r_{R} - V_{y(a),\eta}^{-1}(y(x)_{\eta})r_{F} - F_{\eta}(\xi_{\phi})r_{V}.$$

Since $(F_{\eta})'(a_{\phi})$ is fixed, we obtain that $(F_{\eta})'(a_{\phi})\delta x_{\phi}$ is of order $\mathcal{O}(\|x_{\phi}-\xi_{\phi}\|_{\mathbb{X}})$. Using that $V_{y(a),\eta}^{-1}(y(x)_{\eta}) \to Id_{E_{y(a)}}$ for $y(x) \to y(a)$, and $x \mapsto y(x)$ is continuous, we get that $Id_{E_{y(a)}} - V_{y(a),\eta}^{-1}(y(x)_{\eta})$ is of order $\omega(\|x_{\phi}-a_{\phi}\|_{\mathbb{X}})$ as $x \to a$. Thus, the first line vanishes for $x, \xi \to a$.

By strict differentiability, we have that $F_{\eta}(a_{\phi}) - F_{\eta}(\xi_{\phi})$ is of order $\omega(\|\xi_{\phi} - a_{\phi}\|_{\mathbb{X}})$ as $\xi \to a$. The mapping y is locally Lipschitz continuous, and thus δy_{η} is of order $\mathcal{O}(\|x_{\phi} - \xi_{\phi}\|_{\mathbb{X}})$. In addition $(V_{y(a),\eta}^{-1})'(y(a)_{\eta})$ is bilinear. Thus, the second line also vanishes for $x, \xi \to a$.

The mappings R_a^{-1} and V_y^{-1} are continuously differentiable and thus strictly differentiable. Using in addition that $(F_\eta)'(a_\phi)$ is constant, $V_{y(a),\eta}^{-1}(y(x)_\eta)$ is locally bounded and F is strictly differentiable, all the terms in the third line vanish for $x, \xi \to a$. By using Prop. 5.5 and Prop. 5.8 this finally yields the desired result (ii).

5.3. Local superlinear convergence

In this section we want to prove the local superlinear convergence of Newton's method. In the spirit of Deuflhard [9], our proof will not rely on quantities, which may allow a qualitative *a-priori* convergence result, but rather on quantities for which good *a-posteriori* algorithmic estimates are accessible. This will be the basis of an affine covariant damping strategy, elaborated below. Nevertheless, we will also show some results which allow an a-priori analysis.

Let $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$ be a vector back-transport. Let $Q: T\mathcal{E} \to \mathcal{E}$ be a connection map and $R: T\mathcal{X} \to \mathcal{X}$ be a retraction. For a fixed $x \in \mathcal{X}$ we can locally perform pullbacks

$$R_x^{-1}: \mathcal{X} \to T_x \mathcal{M}$$

 $\hat{x} \mapsto \hat{\mathbf{x}} := R_x^{-1}(\hat{x})$

Since R is a retraction, we obtain $\mathbf{x} = R_x^{-1}(x) = 0_x$. For the Newton method, defined in Section 3, we consider the following affine-covariant quantity at $x \neq z \in \mathcal{X}$

$$\theta_z(x) := \frac{\left\| (Q_{F(x)} \circ F'(x))^{-1} \left[(Q_{F(x)} \circ F'(x))(\mathbf{x} - \mathbf{z}) - (F(x) - V_{y(x)}^{-1}(y(z))F(z)) \right] \right\|_x}{\|\mathbf{x} - \mathbf{z}\|_x}$$

The use of this quantity gives us a very simple result on local superlinear convergence of Newton's method, which serves two purposes. First, it will be the basis for an a-priori result for Newton-differentiable mappings, second, it yields an algorithmic idea to monitor local convergence.

Proposition 5.10. Let \mathcal{X} be a manifold and $p: \mathcal{E} \to \mathcal{M}$ a vector bundle. Consider a mapping $F: \mathcal{X} \to \mathcal{E}$ and a section $F' \in \Gamma(\mathcal{L}(T\mathcal{X}, F^*T\mathcal{E}))$. Let $Q: T\mathcal{E} \to \mathcal{E}$ be a connection map and $R: T\mathcal{X} \to \mathcal{X}$ be a retraction. Let $x_{\star} \in \mathcal{X}$ be a zero of F and assume that all Newton steps x_k are well defined. Assume that

$$\lim_{x \to x_+} \theta_{x_\star}(x) = 0. \tag{15}$$

Then Newton's method converges locally to x_{\star} with a superlinear rate, i.e.

$$d_{\mathcal{X}}(x_{\star}, x_{k+1}) \leq \theta_{x_{\star}}(x_k) d_{\mathcal{X}}(x_{\star}, x_k).$$

Proof. Let $x \in \mathcal{X}$. Set $x_+ := R_x(\delta x)$, where $\delta x \in T_x \mathcal{X}$ is the Newton direction at x. Using the pullback $\mathbf{x}_+ = R_x^{-1}(x_+) = \delta x$ and $F(x_*) = 0$ we get the following equation in the tangent space $T_x \mathcal{X}$:

$$\|\mathbf{x}_{+} - \mathbf{x}_{\star}\|_{x} = \|(Q_{F(x)} \circ F'(x))^{-1}[(Q_{F(x)} \circ F'(x))(\mathbf{x} - \mathbf{x}_{\star}) - (F(x) - V_{u(x)}^{-1}(y(x_{\star}))F(x_{\star}))]\|_{x}.$$

By definition of $\theta_{x_*}(x)$ it follows

$$\|\mathbf{x}_{+} - \mathbf{x}_{\star}\|_{x} = \theta_{x_{\star}}(x) \cdot \|\mathbf{x} - \mathbf{x}_{\star}\|_{x}. \tag{16}$$

Consider a neighborhood V of x_{\star} , where Prop. 5.8 holds for some $1 > \varepsilon > 0$. Since $\lim_{x \to x_{\star}} \theta_{x_{\star}}(x) = 0$, we find a metric ball $r\mathcal{B}_{x_{\star}} = \{x \in \mathcal{X} : d_{\mathcal{X}}(x, x_{\star}) < r\} \subset V$ of radius r > 0, such that

$$\theta_{x_{\star}}(x) \leq \frac{1}{2} \frac{1-\varepsilon}{1+\varepsilon} \ \forall x \in r\mathcal{B}_{x_{\star}}.$$

Now choose a starting point $x_0 \in r\mathcal{B}_{x_{\star}}$ and consider the sequence of Newton steps given by $x_{k+1} := x_{k,+}$ for $k \geq 0$. Assuming for induction that $x_k \in 2^{-k}r\mathcal{B}_{x_{\star}}$, we obtain by using (16):

$$d_{\mathcal{X}}(x_{k+1}, x_{\star}) \le \theta_{x_{\star}}(x_k) \frac{1+\varepsilon}{1-\varepsilon} d_{\mathcal{X}}(x_k, x_{\star}) < r2^{-(k+1)}.$$

Thus, all Newton steps remain in $r\mathcal{B}_{x_{\star}}$ and $x_k \to x_{\star}$. This implies $\theta_{x_{\star}}(x_k) \to 0$ for $k \to \infty$ and thus superlinear convergence.

We now also want to give conditions for local superlinear convergence which can be used for a-priori analysis. With the help of a local norm on \mathcal{X} and a fibrewise norm on \mathcal{E} we can define a norm of a linear operator $A: E_y \to T_x \mathcal{X}$:

$$||A||_{E_y \to T_x \mathcal{X}} := \sup_{||e||_{E_x} < 1} ||Ae||_{T_x \mathcal{X}}.$$

Proposition 5.11. Let $F: \mathcal{X} \to \mathcal{E}$ be Newton-differentiable at $x_{\star} \in \mathcal{X}$ with respect to a Newton derivative $F' \in \Gamma(\mathcal{L}(T\mathcal{X}, F^*T\mathcal{E}))$, where $F(x_{\star}) = 0$. Assume that for $x \in \mathcal{X}$ the operator norm of $(Q_{F(x)} \circ F'(x))^{-1}$ is uniformly bounded, i.e. there exists $\beta < \infty$ such that

$$||(Q_{F(x)} \circ F'(x))^{-1}||_{E_y \to T_x \mathcal{X}} \le \beta.$$

Then Newton's method converges locally to x_{\star} at a superlinear rate.

Proof. Let $\varepsilon \in (0,1)$. Using that the operator norm of $(Q_{F(x)} \circ F'(x))^{-1}$ is bounded and applying Prop. 5.8, we can estimate $\theta_{x_{\star}}(x)$ in a neighborhood V of x_{\star} as follows:

$$\theta_{x_{\star}}(x) \leq \beta \cdot (1+\varepsilon) \cdot \frac{\|(Q_{F(x)} \circ F'(x))(R_x^{-1}(x) - R_x^{-1}(x_{\star})) - (F(x) - V_y^{-1}(y_{\star})F(x_{\star}))\|_{E_y}}{d_{\mathcal{X}}(x, x_{\star})}.$$

Since $F(x_{\star}) = 0$ and F is Newton-differentiable at x_{\star} , we can apply Prop. 5.9 (i) and obtain $\lim_{x \to x_{\star}} \theta_{x_{\star}}(x) = 0$.

5.4. Monitoring local convergence

Let us now define a computable quantity to monitor local convergence. For this, we set $x = x_k$, $y := y(x_k) = p(F(x_k))$, $y_* := y(x_*) = p(F(x_*))$ and consider the affine-covariant quantity $\theta_{x_*}(x)$ that we have seen in the proof of the local convergence:

$$\theta_{x_{\star}}(x) = \frac{\|(Q_{F(x)} \circ F'(x))^{-1} \left[(Q_{F(x)} \circ F'(x))(\mathbf{x} - \mathbf{x}_{\star}) - (F(x) - V_y^{-1}(y_{\star})F(x_{\star})) \right] \|_{x}}{\|\mathbf{x} - \mathbf{x}_{\star}\|_{x}}.$$

Since the target point x_{\star} is not available, we replace x_{\star} by the next iterate $x_{+} := x_{k+1}$, correspondingly the pullback \mathbf{x}_{\star} by $\mathbf{x}_{+} = \delta x \in T_{x} \mathcal{X}$, and y_{\star} by $y_{+} = p(F(x_{+}))$. By using $\mathbf{x} = 0_{x}$ and the definition of the k-th Newton direction $\delta x = \mathbf{x}_{+} - \mathbf{x}$, we obtain:

$$\theta_{x_{+}}(x) = \frac{\|(Q_{F(x)} \circ F'(x))^{-1} \left[(Q_{F(x)} \circ F'(x))(\mathbf{x} - \mathbf{x}_{+}) - (F(x) - V_{y}^{-1}(y_{+})F(x_{+})) \right] \|_{x}}{\|\mathbf{x} - \mathbf{x}_{+}\|_{x}}$$

$$= \frac{\|(Q_{F(x)} \circ F'(x))^{-1}V_{y}^{-1}(y_{+})F(x_{+})\|_{x}}{\|\mathbf{x} - \mathbf{x}_{+}\|_{x}}$$

Hence, we can calculate $\theta_{x_+}(x)$ at the computational cost of the next simplified Newton direction $\overline{\delta x_+}$ for our original problem with starting point $x_0 = x_k = x$. Namely, this is the solution $\overline{\delta x_+} \in T_x \mathcal{X}$ of the equation

$$Q_{F(x)} \circ F'(x) \overline{\delta x_{+}} + V_{y}^{-1}(y_{+}) F(x_{+}) = 0_{y}.$$
(17)

Note, that a vector back-transport is needed here since $Q_{F(x)} \circ F'(x) \overline{\delta x_+}$ and $F(x_+)$ do not lie in the same fibre. Thus, we can rewrite $\theta_{x_+}(x)$ as

$$\theta_{x_+}(x) = \frac{\|\overline{\delta x_+}\|_x}{\|\delta x\|_x}.$$
(18)

Lemma 5.12. Let F be Newton-differentiable at x_{\star} with respect to a Newton derivative F', where $F(x_{\star}) = 0$. Assume that the operator norm of $(Q_{F(x)} \circ F'(x))^{-1}$ is uniformly bounded by $\beta < \infty$. Then it holds:

$$\lim_{x \to x_+} \theta_{x_+}(x) = 0.$$

Proof. Using that the operator norm of $(Q_{F(x)} \circ F'(x))^{-1}$ is bounded and applying Prop. 5.8, we can estimate $\theta_{x_{\perp}}(x)$ as follows:

$$\theta_{x_+}(x) \le C \cdot \frac{\|(Q_{F(x)} \circ F'(x))(R_x^{-1}(x) - R_x^{-1}(x_+)) - (F(x) - V_y^{-1}(y_+)F(x_+))\|_{E_y}}{d_{\mathcal{X}}(x, x_+)}.$$

Consider the numerator of $\theta_{x\perp}(x)$.

$$\begin{split} &\|(Q_{F(x)}\circ F'(x))(R_x^{-1}(x)-R_x^{-1}(x_+))-(F(x)-V_y^{-1}(y_+)F(x_+))\|_{E_y} \\ &\leq \|(Q_{F(x)}\circ F'(x))(R_x^{-1}(x)-R_x^{-1}(x_\star))-(F(x)-V_y^{-1}(y_\star)F(x_\star))\|_{E_y} \\ &+\|(Q_{F(x)}\circ F'(x))(R_x^{-1}(x_\star)-R_x^{-1}(x_+))-(V_y^{-1}(y_\star)F(x_\star)-V_y^{-1}(y_+)F(x_+))\|_{E_y} \end{split}$$

Since F is Newton-differentiable at x_{\star} and $F(x_{\star}) = 0$, we can apply by Prop. 5.9 (i) and obtain

$$\|(Q_{F(x)} \circ F'(x))(R_x^{-1}(x) - R_x^{-1}(x_\star)) - (F(x) - V_y^{-1}(y_\star)F(x_\star))\|_{E_y} = o(d_{\mathcal{X}}(x, x_\star)). \tag{19}$$

Since V_y^{-1} is differentiable, F', F and V_y^{-1} are locally bounded and F and y are locally Lipschitz continuous, we can estimate the second summand analogously to the proof of Prop. 5.9 by

$$\|(Q_{F(x)} \circ F'(x))(R_x^{-1}(x_\star) - R_x^{-1}(x_+)) - (V_y^{-1}(y_\star)F(x_\star) - V_y^{-1}(y_+)F(x_+))\|_{E_y} \le \widetilde{C}d_{\mathcal{X}}(x_\star, x_+). \tag{20}$$

Since Newton's method converges superlinearly, we obtain $d_{\mathcal{X}}(x_{\star}, x_{+}) = o(d_{\mathcal{X}}(x, x_{\star}))$ as $x \to x_{\star}$. Thus, combining (19) and (20), the numerator is of order $o(d_{\mathcal{X}}(x, x_{\star}))$ as $x \to x_{\star}$. Estimating the denominator of $\theta_{x_{+}}(x)$ by $d_{\mathcal{X}}(x, x_{+}) \geq |d_{\mathcal{X}}(x, x_{\star}) - d_{\mathcal{X}}(x_{\star}, x_{+})|$, we obtain the desired result. \square

6. An Affine Covariant Damping Strategy

In the following we want to develop a method that can also deal with initial values $x_0 \in \mathcal{X}$ that are not sufficiently close to the solution. Especially in Newton's method applied in optimization on Riemannian manifolds some strategies including BFGS, Levenberg-Marquardt and trust region methods were introduced, see e.g. [4, 8, 24]. In a linear setting it is well-known that damped Newton methods are one way to globalize the convergence of Newton's method ([4, 8, 11, 13, 19]). Here, the step size of the Newton direction is scaled by a factor $\lambda \in (0, 1]$. Bortoli et. al. provided a damped Newton's method to solve the problem of finding singularities of vector fields defined on Riemannian manifolds in [5, 6], where A damping factor λ is chosen by a linear line search together with a merit function.

We will also use a damping strategy to globalize our method. The choice of the damping factor is more geometrically motivated here and follows an affine covariant strategy in the spirit of Deuflhard [9]. Since we will not use any Riemannian metric, our way of globalization also works for non-Riemannian manifolds. To prepare the choice of our damping factor, we first define a so called *Newton path*. Our strategy will then be to follow this path by suitably scaling down the Newton directions until the local convergence area of Newton's method is reached.

6.1. Newton path

First, we define an algebraic Newton path, a generalization of the Newton path in linear spaces [9, Sec. 3.1.4]. Denote by x(0) the starting point of the path. For $\lambda \in [0,1]$ and $x(\lambda) \in \mathcal{X}$ we denote by $y(\lambda) := p(F(x(\lambda)))$ the base point of $F(x(\lambda))$ on the base manifold \mathcal{M} of \mathcal{E} . Consider a vector back-transport $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$. We consider the Newton path problem, which is based on the idea of scaling down the residual by a factor of $1 - \lambda$:

$$\langle V_{y(0)}^{-1} \rangle (F(x(\lambda))) = (1 - \lambda)F(x(0)), \ \lambda \in [0, 1].$$
 (21)

In contrast to the case of linear spaces, a vector back-transport is needed here since $F(x(\lambda))$ and F(x(0)) do not lie in the same fibre. The vector back-transport allows us to formulate the Newton path problem in the fixed fibre $E_{y(0)}$, i.e. on a linear space. We call $x(\lambda)$ the algebraic Newton path starting at x(0).

Remark 6.1. For a mapping $g : \mathbb{X} \to \mathbb{Y}$ between linear spaces \mathbb{X} and \mathbb{Y} the Newton path is often defined as the solution of the ordinary differential equation [9, Eq. (3.24)]:

$$\frac{dx_d(\lambda)}{d\lambda} = -g'(x_d(\lambda))^{-1}g(x_d(0)).$$

We may also generalize this idea and define the differential Newton path as the trajectory of the differential equation

$$Q_{F(x_d(\lambda))} \circ F'(x_d(\lambda))x_d'(\lambda) + F(x_d(\lambda)) = 0.$$
(22)

In contrast to the case of linear spaces the algebraic and the differential Newton path do not coincide in general.

Proposition 6.2. Assume that $F: \mathcal{X} \to \mathcal{E}$ is strictly differentiable at x(0) and

$$\|(\langle V_{y(0)}^{-1}\rangle'(F(x(0)))F'(x(0)))^{-1}\|_{E_{y(0)}\to T_{x(0)}\mathcal{X}}$$

is finite. Then for sufficiently small λ there exists a solution $x(\lambda)$ of the Newton path problem (21) and the simplified Newton method locally converges to this solution with a linear rate.

Proof. Application of the implicit function theorem [26], which also holds for strictly differentiable mappings (cf. e.g. [21, Chap. 25]), on

$$g(\lambda, x) := \langle V_{u(0)}^{-1} \rangle (F(x)) - (1 - \lambda) F(x(0))$$

yields the existence of $x(\lambda)$ for sufficiently small λ and convergence of the simplified Newton steps towards $x(\lambda)$.

Remark 6.3. Repeated application of Proposition 6.2, using a homotopy technique yields a piecewise algebraic Newton path that either ends in a solution x_* , at a point, where the linearization $\langle V_{y(0)}^{-1} \rangle'(F(x(0)))F'(x(0))$ is singular, or at the boundary of the domain of definition of F (cf. the discussion in [9, Sec. 3.1.4]).

By using the chain rule, we obtain the following expression for the computation of simplified Newton directions $\delta x^{\lambda} \in T_x \mathcal{X}$ at an initial guess $x \in \mathcal{X}$:

$$\langle V_{y(0)}^{-1} \rangle'(F(x(0)))F'(x(0))\overline{\delta x^{\lambda}} + \langle V_{y(0)}^{-1} \rangle(F(x)) - (1-\lambda)F(x(0)) = 0.$$

Using $V_{y(0)}^{-1}(y(0)) = Id_{E_{y(0)}}$, we calculate the first (simplified) Newton direction δx^{λ} for the Newton path problem as a solution of the following equation:

$$\langle V_{y(0)}^{-1} \rangle'(F(x(0)))F'(x(0))\delta x^{\lambda} + \underbrace{F(x(0)) - (1 - \lambda)F(x(0))}_{=\lambda F(x(0))} = 0.$$
(23)

Lemma 6.4. Let $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$ be consistent with a linear connection map $Q: T\mathcal{E} \to \mathcal{E}$. Then the damped Newton direction $\lambda \delta x$ at x of the original problem conicides with the first Newton direction of the Newton path problem and is tangent to the algebraic and to the differential Newton path starting at x(0) = x. In particular, we obtain

$$\lambda \delta x = \delta x^{\lambda} = \lambda x'(0) = \lambda x'_{d}(0). \tag{24}$$

Proof. Consider the Newton path problem (21). Implicit differentiation at x(0) with respect to λ yields the tangent x'(0) by

$$\langle V_{u(0)}^{-1} \rangle' (F(x(0))) F'(x(0)) x'(0) + F(x(0)) = 0.$$

The first (simplified) Newton direction δx^{λ} for the Newton path problem with fixed λ at the current starting point x(0) = x can be computed by (23):

$$\langle V_{u(0)}^{-1} \rangle' (F(x(0))) F'(x(0)) \delta x^{\lambda} + \lambda F(x(0)) = 0.$$

Thus, the Newton direction δx^{λ} for the Newton path problem is tangent to the algebraic Newton path.

Using the linearity of the connection map Q, we can compute the damped Newton direction $\lambda \delta x$ for our original problem at x(0) by

$$Q_{F(x(0))} \circ F'(x(0))(\lambda \delta x) + \lambda F(x(0)) = 0.$$

Comparison with (22) yields $\lambda \delta x = x_d'(0)$. Using the consistency of V_y^{-1} and Q at e = F(x(0)), i.e. $Q_{F(x(0))} = \langle V_{y(0)}^{-1} \rangle'(F(x(0)))$, this finally yields

$$\delta x^{\lambda} = \lambda \delta x$$

In particular, the Newton direction δx is tangent to the Newton path at x(0).

6.2. Computation of Damping Factors

Lemma 6.4 shows that if we choose the vector back-transport and the connection map consistent, the first Newton direction for the Newton path problem coincides with the Newton direction for the original problem scaled by a damping factor $\lambda \in [0,1]$. If we successively choose the current iterate $x = x_k$ for the starting point x(0) of the Newton path, we obtain a damped Newton method. More precisely, for a previously computed Newton direction and a damping factor λ we compute the Newton step

$$x_{+} = R_{x}(\lambda \delta x).$$

For the choice of the damping factor we again consider our Newton path problem (21). The idea is to choose λ sufficiently small such that the simplified Newton method for solving (21) with starting point x(0) = x is likely to converge to the target point $x(\lambda)$ on the Newton path. To monitor the local convergence, we use the estimator $\theta_{x_+}(x)$ at the current iterate x for $\theta_{x(\lambda)}(x)$. According to (18) and using (24), we have to compute

$$\theta_{x_{+}}(x) = \theta_{R_{x}(\lambda \delta x)}(x) = \frac{\|\overline{\delta x_{+}^{\lambda}}\|_{x}}{\|\lambda \delta x\|_{x}}.$$

Thus, we need the next simplified Newton direction $\overline{\delta x_{+}^{\lambda}}$ for the Newton path problem (21) at initial guess x. This direction is given by the solution of the equation

$$\langle V_{y(x)}^{-1} \rangle'(F(x))F'(x)\overline{\delta x_+^{\lambda}} + V_{y(x)}^{-1}(y(x_+))F(x_+) - (1-\lambda)F(x) = 0.$$

These calculations are repeated with decreasing damping factor until $\theta_{x_+}(x) < \Theta_{acc}$ for some acceptable contraction Θ_{acc} holds. To achieve this, the damping factor λ is readjusted iteratively in the following way. If $\theta_{x_+}(x) \geq \Theta_{acc}$, choose $\lambda_+ \in (0,1]$ such that for user defined parameters $0 < \Theta_{des} < \Theta_{acc}$ the inequality $\frac{\lambda_+}{\lambda} \cdot \theta_{x_+}(x) \leq \Theta_{des}$ holds, i.e. we compute the next damping factor

$$\lambda_{+} := \min \left(1, \frac{\lambda \Theta_{des}}{\theta_{x_{+}}(x)} \right).$$

We summarise the results in an algorithm, which is a modification of [9, Alg. NLEQ-ERR]:

Algorithm 2 Affine covariant damped Newton's method

```
Require: x, \lambda (initial guesses); \lambda_{fail}, TOL, \Theta_{des} < \Theta_{acc} (parameters)
           solve \delta x \leftarrow (Q_{F(x)} \circ F'(x))\delta x + F(x) = 0
  2:
           repeat
  3:
               compute x_{+} = R_{x}(\lambda \delta x)

solve \delta x_{+}^{\lambda} \leftarrow \langle V_{y(x)}^{-1} \rangle'(F(x))F'(x)\delta x_{+}^{\lambda} + V_{y(x)}^{-1}(y(x_{+}))F(x_{+}) - (1-\lambda)F(x) = 0
  4:
               compute \theta_{x_{+}}(x) = \frac{\|\delta x_{+}^{\lambda}\|_{x}}{\|\lambda \delta x\|_{x}}
              update \lambda \leftarrow \min\left(1, \frac{\lambda \Theta_{des}}{\theta_{x_{+}}(x)}\right)
  7:
  8:
                    terminate: "Newton's method failed"
  9:
               end if
10:
            until \theta_{x_+}(x) \leq \Theta_{acc}
11:
           update x \leftarrow x_+
12:
           if \lambda = 1 and \theta_{x_+}(x) \leq \frac{1}{4} and \|\delta x\|_x \leq TOL then terminate: "Desired Accuracy reached", x_{out} = x_+
13:
14:
15:
16: until maximum number of iterations is reached
```

Proposition 6.5. Let F be strictly differentiable at x and V_y^{-1} be consistent with Q. Then there exists $\hat{\lambda} > 0$ such that

$$\forall \lambda \leq \widehat{\lambda} : \theta_{R_x(\lambda \delta x)}(x) \leq \Theta_{acc},$$

and thus the inner loop terminates after finitely many iterations.

Proof. If $\theta_{R_x(\lambda \delta x)}(x) > \Theta_{acc}$, we obtain

$$\lambda_{+} \leq \frac{\lambda \Theta_{des}}{\theta_{R_{x}(\lambda \delta x)}(x)} \leq \frac{\Theta_{des}}{\Theta_{acc}} \lambda.$$

Since $\Theta_{des} < \Theta_{acc}$, this yields $\lambda_+ < C \cdot \lambda$ with C < 1. Now choose $\hat{\lambda} > 0$ sufficiently small such that the Newton path with starting point x(0) = x exists (Prop. 6.2). Since

$$\theta_{R_x(\lambda\delta x)}(x) = \frac{\|\overline{\delta x_+^{\lambda}}\|_x}{\|\delta x^{\lambda}\|_x}.$$

measures the ratio between the first and second simplified Newton step for the Newton path problem and the simplified Newton method converges locally to $x(\lambda)$, we obtain

$$\theta_{R_x(\lambda\delta x)}(x) \le \Theta_{acc} \ \forall \lambda \le \widehat{\lambda}.$$

Remark 6.6. By the choice of $\Theta_{des} \in]0,1[$ it is possible to adjust how aggressive the step size strategy acts. If $\Theta_{des} \approx 0$, then Newton's method follows the Newton path very closely and takes short steps. If $\Theta_{des} \approx 1$, then larger steps will be taken, but the methods might perform less robustly for highly nonlinear problems. The choices $\Theta_{des} = 0.5$ and $\Theta_{acc} = 1.1\Theta_{des}$ work well in practice.

7. Applications

In this section we discuss the two simplest applications of Newton's method on vector bundles. First, the tangent bundle of a Banach manifold \mathcal{X} is considered. Like in [6, 2], Newton's method is then used to find fixed points of vector fields $\nu \in \Gamma(T\mathcal{X})$. Second, considering the *cotangent bundle* $T^*\mathcal{X}$, Newton's method can also be applied in optimization on manifolds and to find stationary points of *covector fields*.

If \mathcal{X} is a Riemannian manifold, in both applications the *Levi-Civita connection* (see e.g. [13]) is often used to compute the Newton direction. This connection induces the parallel transport along geodesics and the exponential map. Computing these classical parallel transports can be computationally very expensive. Thus, instead of starting with a connection and deriving a vector transport from it, we take the opposite route. We start with a computationally tractable vector back-transport $V_y^{-1} \in \Gamma(\mathcal{L}(\mathcal{E}, E_y))$, and derive a consistent connection Q by differentiation. Consistency is needed to apply our globalization strategy. Since retractions are anyway used in algorithms, we will discuss how vector transports on $T\mathcal{X}$ and $T^*\mathcal{X}$ can be derived from retractions.

7.1. Fixed points of vector fields

Consider the tangent bundle $\pi: T\mathcal{X} \to \mathcal{X}$ of a Banach manifold \mathcal{X} and a vector field $\nu \in \Gamma(T\mathcal{X})$, i.e. $\nu: \mathcal{X} \to T\mathcal{X}$ with $\pi(\nu(x)) = x \ \forall x \in \mathcal{X}$. Our aim is to apply Newton's method on $\nu: \mathcal{X} \to T\mathcal{X}$ to compute a zero $x \in \mathcal{X}$ of the vector field, i.e. a point $x \in \mathcal{X}$ such that

$$\nu(x) = 0_x \in T_x \mathcal{X}.$$

The computation of the Newton direction requires a connection map $Q: T(T\mathcal{X}) \to T\mathcal{X}$, which we define with the help of a vector back-transport $V_x^{-1} \in \Gamma(\mathcal{L}(T\mathcal{X}, T_x\mathcal{X}))$. As seen before in Lemma 2.3, differentiating $\langle V_x^{-1} \rangle \in C^1(T\mathcal{X}, T_x\mathcal{X})$, leads to the consistent connection map at $\nu(x) \in T\mathcal{X}$ with $\pi(\nu(x)) = x$:

$$Q_{\nu(x)} := \langle V_x^{-1} \rangle'(\nu(x)) : T_{\nu(x)}(T\mathcal{X}) \to T_x \mathcal{X}.$$

Vector back-transports derived from retractions. From a numerical point of view, a natural way to generate vector transports on the tangent bundle $\pi: T\mathcal{X} \to \mathcal{X}$ is by differentiating retractions $R: T\mathcal{X} \to \mathcal{X}$, which are anyway required to define the Newton step.

Keeping $x \in \mathcal{X}$ fixed, the derivative of R_x at a point $v \in T_x \mathcal{X}$ is a linear mapping

$$R'_x(v): T_x\mathcal{X} \to T_{R_x(v)}\mathcal{X}.$$

Since $R_x(0_x) = x$ and $R'_x(0_x) = Id_{T_x\mathcal{X}}$ holds, we can also view this as a section

$$V_x \in \Gamma(\mathcal{L}(\mathcal{X} \times T_x \mathcal{X}, T\mathcal{X})) \text{ by } V_x(\xi) := R'_x(R_x^{-1}(\xi)),$$
 (25)

i.e. a vector transport. Using $(R_x^{-1})'(x) = Id_{T_x\mathcal{X}}$ we compute in trivializations $(V'_{x,\tau}(x)\delta x)v_{\tau} = R''_{x,\tau}(0_x)(\delta x, v_{\tau})$, or in short:

$$V'_{x,\tau}(x) = R''_{x,\tau}(0_x) \in L(T_x \mathcal{X}, L(\mathbb{X}, \mathbb{X})).$$

The corresponding vector back-transport is defined by the inverse of the derivative of the retraction, i.e. we compute:

$$V_x^{-1}(\xi) := R_x'(R_x^{-1}(\xi))^{-1} : T_{\xi}\mathcal{X} \to T_x\mathcal{X},$$

Remark 7.1. In the Newton iteration we use $\xi = x_+ = R_x(\delta x)$, and thus $R_x^{-1}(\xi) = \delta x$. Hence, $V_x^{-1}(\xi) = R_x'(\delta x)$, and the inverse retraction is not needed for the evaluation of the vector backtransport.

Lemma 2.3 allows us to define a connection via the natural inclusion:

$$Q_v = \langle V_x^{-1} \rangle'(v) : T_v(T\mathcal{X}) \to T_x \mathcal{X}.$$

By (5) we get $R''_{x,\tau}(0_x)(\delta x, v_\tau) = B_{x,\tau}(v_\tau)\delta x$ and thus for $\delta v \sim (\delta x, \delta v_\tau)$:

$$Q_v \delta v \sim Q_{v,\tau}(\delta x, \delta v_\tau) = \delta v_\tau - R_{x,\tau}''(0_x)(\delta x, v_\tau). \tag{26}$$

Embedded submanifolds. If \mathcal{X} is an embedded submanifold of a Hilbert space H we can use the embedding $E_H: T\mathcal{X} \to H$ with $E_H(\xi): T_{\xi}\mathcal{X} \to H$ and the orthogonal projection $P(x): H \to T_x\mathcal{X}$ on the tangent space to define a vector back-transport locally by

$$V_x^{-1}(\xi) := P(x)E_H(\xi) \in L(T_{\xi}\mathcal{X}, T_x\mathcal{X})$$

Consider a vector field $\nu: \mathcal{X} \to T\mathcal{X}$. By our natural inclusion φ , we obtain the C^1 -mapping $\langle V_x^{-1} \rangle : T\mathcal{X} \to T_x\mathcal{X}$ with $\langle V_x^{-1} \rangle (\nu)(\xi) = P(x)(E_H\nu)(\xi)$. Differentiating this with respect to ξ at $\xi = x$, we obtain

$$Q_{\nu(x)}\nu'(x)\delta x = \langle V_x^{-1}\rangle'(\nu(x))\nu'(x)\delta x = P(x)(E_H\nu)'(x)\delta x \in T_x\mathcal{X},$$

which defines the consistent connection map $Q_{\nu(x)} = \langle V_x^{-1} \rangle'(\nu(x))$. The covariant derivative $Q \circ \nu'$ of a vector field ν w.r.t. the connection map Q can therefore be determined by projecting the euclidean directional derivatives onto $T\mathcal{X}$ by the orthogonal projection. The connection which belongs to this covariant derivative is sometimes called tangential connection. It actually defines the Levi-Civita connection on $T\mathcal{X}$, see e.g. [14, Chap. 5].

7.2. Variational problems on manifolds

Consider a twice differentiable function $f: \mathcal{X} \to \mathbb{R}$, defined on a Banach manifold \mathcal{X} . In order to find a critical point, we want to apply Newton's method on the *cotangent bundle* $T^*\mathcal{X}$ to compute a zero of the *covector field* $f': \mathcal{X} \to T^*\mathcal{X}$, i.e. a point $x \in \mathcal{X}$ such that

$$f'(x) = 0_x^* \in T_x \mathcal{X}^*.$$

Thus, we need a dual connection map $Q_{f'(x)}^*: T_{f'(x)}(T^*\mathcal{X}) \to T_x^*\mathcal{X}$ on the dual bundle $T^*\mathcal{X}$. Again, such a connection map can be derived from a vector transport. We will first discuss dual connection maps in general and come back to the cotangent bundle afterwards.

Dual vector bundles and dual connections. Let $p: \mathcal{E} \to \mathcal{M}$ be a vector bundle. The *dual bundle* $p^*: \mathcal{E}^* \to \mathcal{M}$ is defined as a vector bundle with fibres via $(p^*)^{-1}(y) = E_y^*$, i.e. the dual space of E_y . We can view this as a special case $\mathcal{E}^* = \mathcal{L}(\mathcal{E}, \mathcal{M} \times \mathbb{R})$. For example the dual bundle of the tangent bundle $T\mathcal{X}$ is the cotangent bundle $T^*\mathcal{X}$.

We denote the dual pairing for $\ell \in \Gamma(\mathcal{E}^*)$ and $e \in \Gamma(\mathcal{E})$ by $\ell(e) : \mathcal{M} \to \mathbb{R}$. Its derivative at a point $y \in \mathcal{M}$ is given by $\ell(e)'(y) : T_y \mathcal{M} \to \mathbb{R}$. If \mathcal{E} admits a connection map it is possible to define a dual connection map on the dual bundle \mathcal{E}^* as follows [14, Chap. 4].

Definition 7.2. Let Q be a connection map on the vector bundle $p: \mathcal{E} \to \mathcal{M}$. The dual connection map $Q^*: T\mathcal{E}^* \to \mathcal{E}^*$ on the dual vector bundle $p^*: \mathcal{E}^* \to \mathcal{M}$ is defined by

$$((Q^* \circ \ell')(y)\delta y)(e) := \ell(e)'(y)\delta y - \ell((Q \circ e')(y)\delta y) \ \forall e \in \Gamma(\mathcal{E}), \ \forall \delta y \in T_y \mathcal{M}$$

In trivializations the connection map Q is represented as in (3) by

$$Q_e \delta e \sim Q_{e,\tau}(\delta y, \delta e_\tau) = \delta e_\tau - B_{y,\tau}(e_\tau) \delta y \in \mathbb{E}.$$
 (27)

Using this, and the representation of $\ell'(y)\delta y$ by $(\delta y, \delta \ell_{\tau})$ and $e'(y)\delta y$ by $(\delta y, \delta e_{\tau})$ we obtain by the product rule and cancellation of the term $\ell_{\tau}(\delta e_{\tau})(y)\delta y$:

$$((Q_{\ell,\tau}^* \circ \ell_{\tau}')(y)\delta y)(e_{\tau}(y)) = \ell_{\tau}(e_{\tau})'(y) - \ell_{\tau}(y)(\delta e_{\tau} - B_{y,\tau}(e_{\tau}(y))\delta y) = \delta \ell_{\tau}(e_{\tau}(y)) + \ell_{\tau}(y)(B_{y,\tau}(e_{\tau}(y))\delta y).$$

Thus, $(Q^* \circ \ell')(y)\delta y)(e)$ does not depend on $e'_{\tau}(y)$, but on $e_{\tau}(y)$ only, so indeed $(Q^* \circ \ell')(y)\delta y \in E^*_y$ with the representation

$$Q_{\ell}^* \delta \ell \sim Q_{\ell,\tau}^* (\delta y, \delta \ell_{\tau}) = \delta \ell_{\tau}(\cdot) + \ell \circ B_{y,\tau}(\cdot) \delta y \in \mathbb{E}^*.$$
 (28)

Comparison of (27) and (28) shows that if the dual connection map Q^* corresponds to a connection map Q on \mathcal{E} the bilinear form $B_{y,\tau}$ is used in both representations.

Now consider a vector transport $V_y \in \Gamma(\mathcal{L}(\mathcal{M} \times \mathcal{E}, E_y))$. We can define a covector back-transport $V_y^* \in \Gamma(\mathcal{L}(\mathcal{E}^*, E_y^*))$, which acts as a vector back-transport on the dual bundle by using pointwise adjoints $V_y^*(\hat{y}) := (V_y(\hat{y}))^* \in L(E_{\hat{y}}^*, E_y^*)$, i.e.

$$V_y^*(\hat{y})\ell := \ell \circ V_y(\hat{y}) \quad \forall \ell \in E_{\hat{y}}^*.$$

We can define a connection map on \mathcal{E}^* via the covector back-transport by setting

$$Q_{\ell}^* := \langle V_{\eta}^* \rangle'(\ell) : T_{\ell} \mathcal{E}^* \to E_{\eta}^*, \ y = p^*(\ell). \tag{29}$$

Lemma 7.3. The choice (29) defines the dual connection map on \mathcal{E}^* corresponding to the connection map $Q_e = \langle V_y^{-1} \rangle'(e)$ at e with $y = p(e) = p^*(\ell)$ on \mathcal{E} derived from the vector transport V_y .

Proof. Let $\ell \in \Gamma(\mathcal{E}^*)$, $e \in \Gamma(\mathcal{E})$, and $\delta y \in T_y \mathcal{M}$. In trivializations, if $\ell(y)$ is represented by $(y, \ell_\tau(y))$ and $\ell'(y)\delta y$ by $(\delta y, \delta \ell_\tau)$, we obtain by using $\langle V_y^* \rangle(\ell) = \ell \circ V_y(p^*(\ell))$ and (2):

$$\langle V_y^* \rangle'(\ell(y))\ell'(y)\delta y \sim \delta \ell_\tau + \ell \circ V_{y,\tau}'(y)\delta y.$$

Since $B_{y,\tau}(e_{\tau}(y))\delta y = -((V_{y,\tau}^{-1})'(y)\delta y)e_{\tau}(y) = (V_{y,\tau}'(y)\delta y)e_{\tau}(y)$ by (4) and (5), we obtain the desired result.

Remark 7.4. Classically, connections are closely related to covariant derivatives:

$$\nabla_{\delta y} e(y) := Q \circ e'(y) \delta y \text{ for } y \in \mathcal{M}, e \in \Gamma(\mathcal{E}), \delta y \in \Gamma(T\mathcal{M}),$$

in which case Definition 7.2 yields a product rule:

$$\ell(e)'(y)\delta y = \nabla_{\delta y}^* \ell(y)(e) + \ell(\nabla_{\delta y} e(y)).$$

On Riemannian manifolds the Levi-Civita connection is widely used on TM. In this case, dual connections can also be defined with the help of a Riesz isomorphism $\mathcal{R}: TM \to T^*M$:

$$\nabla_{\delta y}^* \ell := \mathcal{R}(\nabla_{\delta y} \mathcal{R}^{-1}(\ell)).$$

However, this expression is often expensive to evaluate numerically.

Covector back-transports via retractions. Consider the cotangent bundle $\pi^*: T^*\mathcal{X} \to \mathcal{X}$. Since the cotangent bundle is the dual vector bundle to the tangent bundle it admits a corresponding dual connection map. In order to define the dual connection map which fits to the connection map on $T\mathcal{X}$ induced by the retraction, we first define the covector back-transport corresponding to $V_x \in \Gamma(\mathcal{X} \times T_x\mathcal{X}, T\mathcal{X})$ given by (25). For $v^* \in T_{\mathcal{E}}^*\mathcal{X}$ we set

$$V_x^*(\xi)(v^*) := v^* \circ R_x'(R_x^{-1}(\xi)) = R_x'(R_x^{-1}(\xi))^*(v^*) \in T_x^* \mathcal{X}.$$

Thus, we obtain a linear mapping

$$V_x^*(\xi) = R_x'(R_x^{-1}(\xi))^* : T_{\varepsilon}^* \mathcal{X} \to T_x^* \mathcal{X},$$

which defines a covector back-transport $V_x^* \in \Gamma(\mathcal{L}(T^*\mathcal{X}, T_x^*\mathcal{X}))$ on the cotangent bundle.

By using the natural inclusion φ and differentiating $\langle V_x^* \rangle$, we obtain the dual connection map at $v^* \in T^* \mathcal{X}$ with $x = \pi^*(v^*) \in \mathcal{X}$:

$$Q_{v^*}^* := \langle V_x^* \rangle'(v^*) : T_{v^*}(T^*\mathcal{X}) \to T_x^*\mathcal{X}.$$

Combining (26) and (28) we obtain in trivializations

$$Q_{v^*}^* \delta v^* \sim Q_{v^* \tau}^* (\delta x, \delta v_{\tau}^*) = \delta v_{\tau}^* + v_{\tau}^* \circ R_{r \tau}''(0_x) (\delta x, \cdot). \tag{30}$$

Embedded submanifolds. Consider an embedded submanifold \mathcal{X} of a Hilbert space H. We can use the embedding $E_H: T\mathcal{X} \to H$ with $E_H(x): T_x\mathcal{X} \to H$ and the orthogonal projection $P(\xi): H \to T_{\xi}\mathcal{X}$ on the tangent space to define a vector transport locally by

$$V_x(\xi) := P(\xi)E_H(x) \in L(T_x\mathcal{X}, T_{\xi}\mathcal{X}).$$

A covector back-transport is then given by taking pointwise adjoints $V_x^*(\xi) := (V_x(\xi))^*$, i.e.

$$V_x^*(\xi)\ell = \ell \circ V_x(\xi) = \ell \circ P(\xi) \circ E_H(x) \quad \forall \ell \in T_{\varepsilon}^* \mathcal{X}.$$

Consider a covector field $\ell_H : \mathcal{X} \to H^*$ and its restriction $\ell \in T^*\mathcal{X}$, given by $\ell(\xi) := \ell_H(\xi) \circ E_H(\xi)$. Differentiating $\langle V_x^* \rangle(\ell)(\xi) = \ell_H(\xi) \circ E_H(\xi) \circ V_x(\xi)$ with respect to ξ at $\xi = x$ yields

$$\langle V_x^* \rangle'(\ell(x))\ell'(x)\delta x = \ell'_H(x)\delta x + \ell_H(x)(E_H \circ V_x)'(x)\delta x$$

= $\ell'_H(x)\delta x + \ell_H(x)(E_H \circ P)'(x)E_H(x)\delta x$,

or, suppressing the embeddings notationally:

$$Q_{\ell(x)}^* \ell'(x) \delta x = \langle V_x^* \rangle'(\ell(x)) \ell'(x) \delta x = \ell'_H(x) \delta x + \ell_H(x) P'(x) \delta x \in T_x^* \mathcal{X}. \tag{31}$$

Vice versa, if $\ell \in T^*\mathcal{X}$ is given, we may extend ℓ to $\ell_H : \mathcal{X} \to H^*$, for example by specifying $\ell_H(x)$ on $T_x\mathcal{X}^{\perp}$. Then by its intrinsic definition $Q_{\ell(x)}^*\ell'(x)\delta x$ is independent of the extension, and thus also (31) is independent of the extension.

If \mathcal{X} is given by a constraint of the form $\mathcal{X} = \{x \in H : c(x) = 0\}$, where $c : H \to R$ is a differentiable mapping between Hilbert spaces, such that $c'(x) : H \to R$ is surjective, then we can find a Lagrangian multiplier $\lambda(x) \in R^*$, such that $(\ell_H(x) + \lambda(x)c'(x))w = 0$ for all $w \in T_x\mathcal{X}^{\perp}$. Using $\ker c'(x) = T_x\mathcal{X}$ this relation can be written as

$$0 = (\ell_H(x) + \lambda(x)c'(x))(Id_H - P(x))v = \ell_H(x)(Id_H - P(x))v + \lambda(x)c'(x)v \quad \forall v \in H.$$

Differentiation with respect to x in direction $\delta x \in T_x \mathcal{X}$ yields

$$0 = (\ell'_H(x)\delta x(Id_H - P(x)) - \ell_H(x)P'(x)\delta x + \lambda'(x)\delta x c'(x) + \lambda(x)c''(x)\delta x)v \quad \forall v \in H$$

and thus, testing with $v \in T_x \mathcal{X}$, so that $(Id_H - P(x))v = 0$ and c'(x)v = 0, we get:

$$\lambda(x)c''(x)(\delta x, v) = \ell_H(x)P'(x)\delta x v \quad \forall v \in T_x \mathcal{X}.$$

Hence, (31) reads in this case:

$$Q_{\ell(x)}^* \ell'(x) \delta x = \ell'_H(x) \delta x + \lambda(x) c''(x) \delta x \in T_x^* \mathcal{X}. \tag{32}$$

Newton's method and optimization. Given a dual connection map $Q_{f'(x)}^*: T_{f'(x)}(T^*\mathcal{X}) \to T_x^*\mathcal{X}$, we can determine the Newton direction $\delta x \in T_x\mathcal{X}$ to find a zero of the covector field $f': \mathcal{X} \to T^*\mathcal{X}$ by solving the following equation in $T_x^*\mathcal{X}$:

$$Q_{f'(x)}^* \circ f''(x)\delta x + f'(x) = 0_x^*. \tag{33}$$

Since this is an equation in a dual space, δx has to fulfill

$$(Q_{f'(x)}^* \circ f''(x)\delta x)v + f'(x)v = 0 \quad \forall v \in T_x \mathcal{X}.$$

Alternatively, we can use a second order model of the pullback $f \circ R_x : T_x \mathcal{X} \to \mathbb{R}$ of f at x with respect to the same retraction:

$$(f \circ R_x)(0_x + \delta x) = f(x) + (f \circ R_x)'(0_x)\delta x + \frac{1}{2}(f \circ R_x)''(0_x)(\delta x, \delta x) + o(\|\delta x\|_x^2).$$

If $(f \circ R_x)''(0_x)$ is positive definite, then a Newton-SQP direction can be computed by

$$\min_{\delta x \in T_x \mathcal{X}} (f \circ R_x)'(0_x) \delta x + \frac{1}{2} (f \circ R_x)''(0_x) (\delta x, \delta x) \quad \Leftrightarrow \quad (f \circ R_x)''(0_x) \delta x + (f \circ R_x)'(0_x) = 0_x^*. \tag{34}$$

Proposition 7.5. Let $x \in \mathcal{X}$. Let $Q^* : T(T^*\mathcal{X}) \to T^*\mathcal{X}$ be a dual connection map derived from a retraction $R_x : T_x\mathcal{X} \to \mathcal{X}$. Then

$$(f \circ R_x)'(0_x) = f'(x),$$

 $(f \circ R_x)''(0_x) = Q_{f'(x)}^* \circ f''(x).$

Thus, the Newton direction computed by (33) coincides with the Newton-SQP direction computed by (34) if $(f \circ R_x)''(0_x)$ is positive definite.

Proof. Let $v \in T_x \mathcal{X}$. Using that R_x is a retraction, we obtain:

$$(f \circ R_x)'(0_x)v = f'(R_x(0_x))R'_x(0_x)v = f'(x)v.$$

Next, we have for $\delta x \in T_x \mathcal{X}$

$$(f \circ R_x)''(0_x)(\delta x, v) = \frac{d}{d\xi} (f'(R_x(\xi))R'_x(\xi)\delta x)|_{\xi=0_x} v.$$

Consider the trivializations $\tau_{TX}: TX \to X \times \mathbb{X}$ and $\tau_x: X \times T_xX \to X \times \mathbb{X}$. Using (1), we compute for $\xi \in T_xX$:

$$f'_{\tau}(R_x(\xi))R'_{\tau,\tau}(\xi)\delta x \circ \tau_x = (f'(R_x(\xi)) \circ \tau_{T\mathcal{X}}^{-1}) \circ (\tau_{T\mathcal{X}} \circ R'_{\tau}(\xi)\delta x \circ \tau_x^{-1}) \circ \tau_x = f'(R_x(\xi))R'_{\tau}(\xi)\delta x.$$

On the one hand, computing the derivative at $\xi = 0_x$ yields, with $(R'_{x,\tau}(0_x) \circ \tau_x)(v) = \tau_x(v) = v_\tau$ for $v \in T_x \mathcal{X}$:

$$\frac{d}{d\xi} \left(f_{\tau}'(R_x(\xi)) R_{x,\tau}'(\xi) \delta x \circ \tau_x \right) |_{\xi=0_x} v = f_{\tau}''(x) (\delta x, v_{\tau}) + f_{\tau}'(x) R_{x,\tau}''(0_x) (\delta x, v_{\tau}).$$

On the other hand, in trivializations we get with (30), using $v^* = f'(x)$ and $\delta v^* \sim (\delta x, f''_{\tau}(x)\delta x)$:

$$(Q_{f'(x)}^* \circ f''(x)\delta x)v = f_{\tau}''(x)(\delta x, v_{\tau}) + f_{\tau}'(x) \circ R_{x,\tau}''(0_x)(\delta x, v_{\tau}).$$

This yields

$$(f \circ R_x)''(0_x)\delta x = Q_{f'(x)}^* \circ f''(x)\delta x$$
 in $T_x^* \mathcal{X}$.

Since δx is an arbitrary tangent vector it holds that

$$(f \circ R_x)''(0_x) = Q_{f'(x)}^* \circ f''(x).$$

Thus, the Newton equation (33) and the optimality constraint (34) coincide.

Remark 7.6. Our affine covariant damping strategy is well suited to find stationary points of f. If the computation of a local minimizer of f is desired, different strategies from nonlinear optimization should be employed, such as linesearch or trust-region methods, that enforce descent in f during the iteration.

If \mathcal{X} is embedded into a Hilbert space H, $f_H: H \to \mathbb{R}$ and $f = f_H|_{\mathcal{X}}$, we may consider the constrained problem

$$\min_{x \in \mathcal{X}} f(x) \quad \Leftrightarrow \quad \min_{x \in H} f_H(x) \text{ subject to } x \in \mathcal{X}.$$

A stationary point is then given as $x \in \mathcal{X}$, such that $f'(x)v = f'_H(x)v = 0$ for all $v \in T_x\mathcal{X}$. Then in view of (31) we obtain for the connection, induced by the orthogonal projection:

$$Q_{f'(x)}^* f''(x)\delta x = f_H''(x)\delta x + f_H'(x)P'(x)\delta x.$$

In the case $\mathcal{X} = \{x \in H : c(x) = 0\}$ this relation becomes

$$Q_{f'(x)}^* f''(x) \delta x = f_H''(x) \delta x + \lambda(x) c''(x) \delta x.$$

where $(f'_H(x) + \lambda(x)c'(x))v = 0$ for all $v \in T_x \mathcal{X}$ due to (32). Hence, in this case we retain the well known Lagrange-Newton step, used in constrained optimization.

8. Conclusion and future research

In our study of Newton's method for a mapping $F: \mathcal{X} \to \mathcal{E}$ from a manifold into a vector bundle we have found a number of structural insights. The most basic distinction from the classical case is the need for a connection on \mathcal{E} to render the Newton equation well defined. Together with a geometric version of Newton differentiability this already allows a local convergence theory of Newton's method. A Banach type version of a Riemannian metric can be used as a flexible framework to formulate superlinear convergence.

For the development of further algorithmic strategies, like monitoring local convergence or globalization, vector back-transports are required. They make it possible to compare residuals from different fibres and to compute simplified Newton steps. We propose an affine covariant globalization scheme, which works purely with quantities that can be computed in terms of the domain \mathcal{X} . In the global regime, where residuals are not small, it is necessary that the employed connection is consistent with the vector back-transport in order to guarantee that the Newton direction is tangential to the algebraic Newton path. If \mathcal{E} is the tangent bundle $T\mathcal{X}$ or the cotangent bundle $T^*\mathcal{X}$, then vector back-transports and connections can be derived from retractions on \mathcal{X} by differentiation. In this way an algorithmic quantity on \mathcal{X} , a retraction, induces some geometric structure on \mathcal{X} , namely a connection.

Our general approach can be used to tackle various classes of problems numerically, posed on manifolds of finite and infinite dimension and thus opens the door for future research. Possible applications are the simulation and optimal control of geometric variational problems and differential equations, problems of stationary action, or shape optimization. Depending on the structure of the problem, alternative globalization schemes can be devised, for example, residual based schemes or descent methods from nonlinear optimization.

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