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# Energy functionals for manifold-valued mappings and their properties 

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#### Abstract

This technical report is merely an extended version of the appendix of [8] with complete proofs, which had to be omitted due to space restrictions. This technical report requires a basic knowledge of differential geometry. However, apart from that requirement the technical report is self-contained.


## 1 Overview

In Section 2 we start with a review of material contained in [1] about the pull-back connection and present an appropriate generalization of Green's theorem. In Section 3 we provide a general principle how to define energies for manifold-valued mappings, in particular we define the Eells energy which is the natural generalization of the Thin-Plate Spline energy to manifold-valued mappings. A variational approach in Section 4 provides necessary conditions for the minimizer of the Eells energy. Most importantly we can derive natural boundary conditions for the Eells energy. After a discussion of basic properties of the harmonic and Eells energy in Section 5 we discuss the extrinsic representation of the Eells energy and the boundary conditions given that the output manifold is an isometric submanifold of a $p$-dimensional Euclidean space.

Notation: Throughout the article we will use the following notation. $M$ is always the input manifold, $N$ the target manifold and $\phi: M \rightarrow N$ is the mapping from input to target manifold. The dimensions of $M$ and $N$ are $m$ and $n$, and $x$ and $y$ are coordinates in $M$ and $N$. Moreover we will use the abstract index notation, that is the tensor type is indicated by the position of "abstract" indices. They should not be mixed up with the indices for the components. A two-times covariant tensor $h$ is written as $h_{a b}$ and the coordinate representation would be $h_{a b}=h_{\mu \nu} d x_{a}^{\mu} \otimes d x_{b}^{\nu}$. In general, we use Greek letters for components ( $\alpha, \beta, \gamma$ for components of $M$ and $\mu, \nu, \rho$ for components in $N$ ) and Latin ones for abstract indices ( $a, b, c$ for indices in $M$ and $r, s, t$ in $N$ ) indicating the tensor character of the expression. We abbreviate the coordinate vector at $p, \frac{\partial^{a}}{\partial x^{\mu}} \in T_{p} M$, as $\partial_{\mu}^{a}$.

## 2 The pull-back connection, its curvature, and Green's theorem

This section is a review of basic ingredients of connections and curvature of vector bundles. Except the extension of the Green's theorem the material can be found in [1].

Let $M$ be a smooth, connected, orientable Riemannian manifold. Let $V$ be a smooth vector bundle over $M$ of finite rank with base projection $\pi: V \rightarrow M$. We denote by $C(V)$ the vector space of smooth sections of $V$, i.e. of smooth maps $\sigma: M \rightarrow V$ such that $\pi \circ \sigma=\mathbb{1}_{M}$. Let $V$ and $W$ be two vector bundles over $M$, then we denote by

- $V^{*}$ is the dual bundle of $V$,
- $V \oplus W$ is the direct sum of $V$ and $W$,
- $V \otimes W$ is the tensor product of $V$ and $W$,
- $\otimes^{p} V$ the $p$-the tensor power of $V$,
- $\wedge^{p} V$ the $p$-the exterior power of $V$ (completely antisymmetric),
- $\odot^{p} V$ the $p$-the tensor power of $V$ (completely symmetric).

A very important concept for manifold-valued mappings is the pull-back bundle $\phi^{-1} W$
Definition 1 If $\phi: M \rightarrow N$ and $W$ is a vector bundle over $N$, we denote by $\phi^{-1} W$ the pull-back bundle, whose fibre over $x \in M$ is $W_{\phi(x)}$, the fibre of $W$ over $\phi(x)$.

Next we define the Riemannian metric and the connection on vector bundles.
Definition 2 A Riemannian metric on a vector bundle $V$ is a section a in $C\left(V^{*} \odot V^{*}\right)$, which induces on each fibre a positive definite inner product. Let $\sigma, \rho \in C(V)$, then we use $\langle\sigma, \rho\rangle:=a(\sigma, \rho)$.

Similar to the case of the tangent bundle one can introduce the musical isomorphisms to define maps $V \rightarrow V^{*}$ and $V^{*} \rightarrow V$. One can also define a Riemannian metric on the pull-back bundle. Let $\phi: M \rightarrow N$ and $W$ be a vector bundle over $N$ with metric $b$. We can identify $\sigma, \rho \in\left(\phi^{-1} W\right)_{x}$ with $\sigma, \rho \in W_{\phi(x)}$ and thereby define $\langle\sigma, \rho\rangle_{b}$.
Definition 3 A linear connection on a vector bundle $V$ over $M$ is a bilinear map $\nabla$ on spaces of sections,

$$
\nabla: C(T M) \times C(V) \rightarrow C(V)
$$

written $\nabla:(X, \sigma) \mapsto \nabla_{X} \sigma, X \in C(T M), \sigma \in C(V)$, such that for $f \in C(M)$ we have

- $\nabla_{f X} \sigma=f \nabla_{X} \sigma$,
- $\nabla_{X}(f \sigma)=X(f) \sigma+f \nabla_{X} \sigma$.

Since $\nabla$ is linear in its first argument we also write in abstract index notation $X^{a} \nabla_{a} \sigma_{b_{1}, \ldots, b_{r}}^{t_{1}, \ldots, t_{s}}$ for a $(s, r)$ vector bundle $V$.

Definition 4 Let ${ }^{V} \nabla$ and ${ }^{W} \nabla$ be connections on $V$ and $W$.

1. The dual connection on $V^{*}$ is defined by

$$
\begin{equation*}
\theta \in C\left(V^{*}\right), \sigma \in C(V) ; \quad\left(\nabla_{X} \theta\right)(\sigma)=X(\theta(\sigma))-\theta\left(\nabla_{X} \sigma\right) . \tag{1}
\end{equation*}
$$

2. The direct sum connection on $V \oplus W$ is defined as,

$$
\begin{equation*}
\sigma \in C(V), \lambda \in C(W) ; \quad \nabla_{X}(\sigma \oplus \lambda)={ }^{V} \nabla_{X} \sigma \oplus{ }^{W} \nabla_{X} \lambda \tag{2}
\end{equation*}
$$

3. The tensor product connection on $V \otimes W$ is defined as,

$$
\begin{equation*}
\sigma \in C(V), \lambda \in C(W) ; \quad \nabla_{X}(\sigma \otimes \lambda)={ }^{V} \nabla_{X} \sigma \otimes \lambda+\sigma \otimes{ }^{W} \nabla_{X} \lambda \tag{3}
\end{equation*}
$$

The following definition of the pull-back connection is the central key to the definition of energy functionals for manifold-valued mappings.
Definition 5 For a smooth map $\phi: M \rightarrow N$ and a vector bundle $W$ over $N$ with connection ${ }^{W} \nabla$, we define the pull-back or induced connection on $\phi^{-1} W$ as the connection $\nabla^{\prime}$ on $\phi^{-1} W$ such that for each $x \in M, X \in T_{x} M$ and $\lambda \in C(W)$, we have

$$
\nabla_{X}^{\prime}\left(\phi^{*} \lambda\right)=\phi^{*}\left({ }^{W} \nabla_{d \phi(X)} \lambda\right)
$$

where $d \phi: T_{x} M \rightarrow T_{\phi(x)} N$ is the push-forward or differential of $\phi$ and $\phi^{*} \lambda=\lambda \circ \phi \in C\left(\phi^{-1} W\right)$. In abstract index notation

$$
\nabla_{a}^{\prime} \lambda(\phi(x))=\left.d \phi_{a}^{r}{ }^{W} \nabla_{r} \lambda\right|_{\phi(x)}
$$

This definition which formally only applies to elements $\phi^{*} \lambda \in \phi^{-1} W$ derived from $\lambda \in C(W)$ can be uniquely extended to all elements of $\phi^{-1} W$ using the defining properties of a connection [1].

Definition 6 A Riemannian structure on a bundle $V$ is a pair $(\nabla, a)$, where $a$ is a Riemannian metric, $\nabla$ is a connection and $\nabla a=0$, where $\nabla a$ is defined using the tensor product connection in Eq. (3).
The condition $\nabla a=0$ means that for all $X \in C(T M), \sigma, \omega \in C(V)$ we have

$$
X\langle\sigma, \omega\rangle=\left\langle\nabla_{X} \sigma, \omega\right\rangle+\left\langle\sigma, \nabla_{X} \omega\right\rangle,
$$

i.e. the connection is compatible with the inner product. It is straightforward to check that if $\left({ }^{V} \nabla, a\right)$ and $\left({ }^{W} \nabla, b\right)$ are Riemannian structures on $V$ and $W$ respectively, then the direct sum, the tensor product and the pull-back -connection are again Riemannian structures.

Definition 7 The curvature tensor of a connection is the map $R: C(T M) \wedge C(T M) \otimes C(V) \rightarrow C(V)$ defined by

$$
\begin{equation*}
R(X, Y) \sigma=\nabla_{X} \nabla_{Y} \sigma-\nabla_{Y} \nabla_{X} \sigma-\nabla_{[X, Y]} \sigma=-R(Y, X) \sigma \tag{4}
\end{equation*}
$$

Lemma 1 Let $R^{V}$ and $R^{W}$ be the curvature tensors of $V$ and $W$. Then it holds,

- for $V^{*},(R(X, Y) \theta)(\sigma)=-\theta(R(X, Y) \sigma)$ for all $X, Y \in C(T M)$ and $\theta \in C\left(V^{*}\right)$ and $\sigma \in C(V)$,
- for $V \oplus W, R(X, Y)(\sigma \oplus \lambda)=R^{V}(X, Y) \sigma \oplus R^{W}(X, Y) \lambda$ where $\lambda \in C(W)$,
- for $V \otimes W, R(X, Y)(\sigma \otimes \lambda)=R^{V}(X, Y) \sigma \otimes \lambda+\sigma \otimes R^{W}(X, Y) \lambda$,
- for $\phi^{-1} W, R_{x}(X, Y) \rho(x)=R_{\phi(x)}^{W}(d \phi(X), d \phi(Y)) \rho(x)$ where $\rho \in C\left(\phi^{-1} W\right)$.

In the following we only consider connections derived from the Levi-Civita connections on tangent bundles on $M$ and $N$. In particular, for the smooth map $\phi: M \rightarrow N$ we repeatedly consider on $\phi^{-1} T N$ the pull-back connection $\nabla^{\prime}$ of the Levi-Civita connection on $N$.

Let the metric on $M$ be $g$, the metric on $N$ be $h$. Furthermore, let ${ }^{M} \nabla$ and ${ }^{N} \nabla$ be the Levi-Civita connections for the tangent bundles of $M$ and $N$. For a mixed tensor $T_{a}^{r} \in T^{*} M \otimes \phi^{-1} T N$ we apply the tensor product connection by using ${ }^{M} \nabla$ for $T^{*} M$ and $\nabla^{\prime}$ for $\phi^{-1} T N$. By some abuse of notation we use the same symbol $\nabla^{\prime}$ for all tensor product connections on $\otimes^{k} T M \otimes^{l} T^{*} M \otimes \phi^{-1} T N$, and also refer to it as the pull-back connection for all these bundles. The following recipe for a covariant derivative of the mixed tensor $T$ can be generalized in a straightforward manner.

$$
\begin{aligned}
\nabla_{b}^{\prime} T_{a}^{r} & =\nabla_{b}^{\prime}\left(T_{\alpha}^{\mu} d x_{a}^{\alpha} \otimes \partial_{\mu}^{r}\right) \\
& :=\left({ }^{M} \nabla_{b} T_{\alpha}^{\mu}\right) d x_{a}^{\alpha} \otimes \partial_{\mu}^{r}+T_{\alpha}^{\mu}\left({ }^{M} \nabla_{b} d x_{a}^{\alpha}\right) \otimes \partial_{\mu}^{r}+T_{\alpha}^{\mu} d x_{a}^{\alpha} \otimes\left(\nabla_{b}^{\prime} \partial_{\mu}^{r}\right) .
\end{aligned}
$$

As an example consider the differential $d \phi_{a}^{r}: T_{x} M \rightarrow T_{\phi(x)} N$,

$$
d \phi_{a}^{r}(x)=\left.\left.\frac{\partial \phi^{\mu}}{\partial x^{\alpha}} d x_{a}^{\alpha}\right|_{x} \otimes \frac{\partial^{r}}{\partial y^{\mu}}\right|_{\phi(x)}=\left.\left.{ }^{M} \nabla_{a} \phi^{\mu}\right|_{x} \otimes \frac{\partial^{r}}{\partial y^{\mu}}\right|_{\phi(x)}
$$

With the Christoffel symbols ${ }^{M} \Gamma_{\beta \alpha}^{\gamma}$ and ${ }^{N} \Gamma_{\nu \rho}^{\mu}$ for the connections on $M$ and $N$ the coordinate expression of $\nabla_{b}^{\prime} d \phi_{a}^{r}$ is

$$
\begin{align*}
\nabla_{b}^{\prime} d \phi_{a}^{r} & ={ }^{M} \nabla_{b}{ }^{M} \nabla_{a} \phi^{\mu} \otimes \frac{\partial^{r}}{\partial y^{\mu}}+{ }^{M} \nabla_{a} \phi^{\mu} \otimes \nabla_{b}^{\prime} \frac{\partial^{r}}{\partial y^{\mu}}  \tag{5}\\
& =\left[\frac{\partial^{2} \phi^{\mu}}{\partial x^{\beta} \partial x^{\alpha}}+\frac{\partial \phi^{\mu}}{\partial x^{\gamma}}{ }^{M} \Gamma_{\beta \alpha}^{\gamma}+\frac{\partial \phi^{\rho}}{\partial x^{\alpha}} \frac{\partial \phi^{\nu}}{\partial x^{\beta}}{ }^{N} \Gamma_{\nu \rho}^{\mu}\right] d x_{b}^{\beta} \otimes d x_{a}^{\alpha} \otimes \frac{\partial^{r}}{\partial y^{\mu}} \tag{6}
\end{align*}
$$

One can read off that $\nabla_{b}^{\prime} d \phi_{a}^{r}=\nabla_{a}^{\prime} d \phi_{b}^{r}$, because the Levi-Civita connections on $M$ and $N$ are symmetric implying that ${ }^{M} \Gamma_{\beta \alpha}^{\gamma}={ }^{M} \Gamma_{\alpha \beta}^{\gamma}$ and ${ }^{N} \Gamma_{\nu \rho}^{\mu}={ }^{N} \Gamma_{\rho \nu}^{\mu}$. With this in mind, we can show a small lemma which will be useful later on.
Lemma 2 Let $\phi: M \rightarrow N$ and $X, Y \in C(T M)$, then we have

$$
\nabla_{X}^{\prime}(d \phi(Y))-\nabla_{Y}^{\prime}(d \phi(X))=d \phi([X, Y])
$$

where $[X, Y]$ is the Lie-bracket.
Proof: It is

$$
\begin{aligned}
X^{b} \nabla_{b}^{\prime}\left(d \phi_{a}^{r} Y^{a}\right)-Y^{b} \nabla_{b}^{\prime}\left(d \phi_{a}^{r} X^{a}\right)= & d \phi_{a}^{r}\left(X^{b}{ }^{M} \nabla_{b} Y^{a}-Y^{b}{ }^{M} \nabla_{b} X^{a}\right) \\
& +X^{b} Y^{a}\left[\nabla_{b}^{\prime} d \phi_{a}^{r}-\nabla_{a}^{\prime} d \phi_{b}^{r}\right] \\
= & d \phi_{a}^{r}[X, Y]^{a}
\end{aligned}
$$

where we have used in the first equality the definition of the pull-back connection for tensor product spaces and in the second equality the definition of the Lie bracket together with $\nabla_{b}^{\prime} d \phi_{a}^{r}=\nabla_{a}^{\prime} d \phi_{b}^{r}$.

In the following we will provide a generalization of Green's theorem to the case of the pull-back connection. This extension will be very helpful later on when we derive the variation of the Eells energy.
Lemma 3 Let $\sigma \in \otimes^{p} T M$ and $\lambda \in \otimes^{p+1} T M$, then

$$
\int_{M}\langle\nabla \sigma, \lambda\rangle=\int_{\partial M}\langle N \otimes \sigma, \lambda\rangle-\int_{M}\left\langle\sigma, \operatorname{trace}_{g} \nabla \lambda\right\rangle
$$

where $N$ is the covector associated to the normal vector at $\partial M$ and the trace is taken with respect to the first two indices of $\lambda$. In abstract index notation

$$
\begin{aligned}
& \int_{M} g^{a c_{0}} g^{b_{1} c_{1}} \ldots g^{b_{p} c_{p}} \nabla_{a} \sigma_{b_{1} \ldots b_{p}} \lambda_{c_{0} \ldots c_{p}} \\
& =\int_{\partial M} g^{a c_{0}} g^{b_{1} c_{1}} \ldots g^{b_{p} c_{p}} N_{a} \sigma_{b_{1} \ldots b_{p}} \lambda_{c_{0} \ldots c_{p}} \\
& -\int_{M} g^{a s_{1}} g^{a c_{0}} g^{b_{1} c_{1}} \ldots g^{b_{p} c_{p}} \sigma_{b_{1} \ldots b_{p}} \nabla_{a} \lambda_{c_{0} \ldots c_{p}}
\end{aligned}
$$

Furthermore we have the following extension. Let $T \in C\left(\otimes^{p+1} T^{*} M \otimes \phi^{-1} T N\right)$ and $S \in C\left(\otimes^{p} T^{*} M \otimes \phi^{-1} T N\right)$ , then with $\nabla^{\prime}$ being the pull-back connection, we have

$$
\int_{M}\left\langle T, \nabla^{\prime} S\right\rangle=\int_{\partial M}\langle T, N \otimes S\rangle-\int_{M}\left\langle\operatorname{trace}_{g} \nabla^{\prime} T, S\right\rangle,
$$

where $N$ is the covector associated to the normal vector at $\partial M$ and the trace is taken with respect to the first two indices. In abstract index notation the expression can be written as,

$$
\begin{aligned}
& \int_{M} g^{a c_{0}} g^{b_{1} c_{1}} \ldots g^{b_{p} c_{p}} h_{r s} T_{c_{0} \ldots c_{p}}^{r} \nabla_{a}^{\prime} S_{b_{1} \ldots b_{p}}^{s} \\
& =\int_{\partial M} g^{a c_{0}} g^{b_{1} c_{1}} \ldots g^{b_{p} c_{p}} h_{r s} T_{c_{0} \ldots c_{p}}^{r} N_{a} S_{b_{1} \ldots b_{p}}^{S} \\
& -\int_{M} g^{a c_{0}} g^{b_{1} c_{1}} \ldots g^{b_{p} c_{p}} h_{r s} \nabla_{a}^{\prime} T_{c_{0} \ldots c_{p}}^{r} S_{b_{1} \ldots b_{p}}^{s}
\end{aligned}
$$

Proof: The first result is a standard result in differential geometry, see [4]. We show the second one for $T \in$ $C\left(T^{*} M \otimes \phi^{-1} T N\right)$ and $S \in C\left(\phi^{-1} T N\right)$ using explicit coordinates. The extension to higher tensor powers in $T^{*} M$ is then a straightforward calculation. We write the part of the covariant derivative associated to the pull-back connection explicitly,

$$
\begin{equation*}
\int_{M} g^{a b} h_{r s} T_{b}^{r} \nabla_{a}^{\prime} S^{s}=\int_{M} g^{a b} h_{\mu \nu} T_{b}^{\mu}\left[{ }^{M} \nabla_{a} S^{\nu}+S^{\rho}{ }^{N} \Gamma_{\rho \omega}^{\nu} \nabla_{a} \phi^{\omega}\right] \tag{7}
\end{equation*}
$$

where ${ }^{N} \Gamma_{\rho \omega}^{\nu}$ are the Christoffel-symbols of $N$. We have

$$
\begin{aligned}
\int_{M} g^{a b} h_{\mu \nu} T_{b}^{\mu M} \nabla_{a} S^{\nu}= & \int_{M} g^{a b{ }^{M}} \nabla_{a}\left(h_{\mu \nu} T_{b}^{\mu} S^{\nu}\right)-\int_{M} g^{a b}\left({ }^{M} \nabla_{a} h_{\mu \nu}\right) T_{b}^{\mu} S^{\nu} \\
& -\int_{M} g^{a b} h_{\mu \nu}\left({ }^{M} \nabla_{a} T_{b}^{\mu}\right) S^{\nu} \\
= & \int_{\partial M} N^{b} h_{r s} T_{b}^{r} S^{s}-\int_{M} g^{a b} \frac{\partial h_{\mu \nu}}{\partial y^{\rho}}{ }^{M} \nabla_{a} \phi^{\rho} T_{b}^{\mu} S^{\nu} \\
& -\int_{M} g^{a b} h_{\mu \nu} S^{\nu}{ }^{M} \nabla_{a} T_{b}^{\mu}
\end{aligned}
$$

With $\frac{\partial h_{\mu \nu}}{\partial y^{\rho}}=h_{\nu \omega}{ }^{N} \Gamma_{\rho \mu}^{\omega}+h_{\mu \omega}{ }^{N} \Gamma_{\rho \nu}^{\omega}$ we get,

$$
\int_{M} g^{a b} \frac{\partial h_{\mu \nu}}{\partial y^{\rho}}{ }^{M} \nabla_{a} \phi^{\rho} T_{b}^{\mu} S^{\nu}=\int_{M} g^{a b}\left[h_{\nu \omega}{ }^{N} \Gamma_{\rho \mu}^{\omega}+h_{\mu \omega}{ }^{N} \Gamma_{\rho \nu}^{\omega}\right]^{M} \nabla_{a} \phi^{\rho} T_{b}^{\mu} S^{\nu}
$$

Plugging the expression for $\int_{M} g^{a b} h_{\mu \nu} T_{b}^{\mu}{ }^{M} \nabla_{a} S^{\nu}$ into Equation (7) we get,

$$
\begin{aligned}
\int_{M} g^{a b} h_{r s} T_{b}^{r} \nabla_{a}^{\prime} S^{s} & =\int_{\partial M} N^{b} h_{r s} T_{b}^{r} S^{s}-\int_{M} g^{a b} h_{\mu \nu} S^{\nu}\left[{ }^{M} \nabla_{a} T_{b}^{\mu}+T_{b}^{\omega}{ }^{N} \Gamma_{\omega \alpha}^{\mu}{ }^{M} \nabla_{a} \phi^{\alpha}\right] \\
& =\int_{\partial M} N^{b} h_{r s} T_{b}^{r} S^{s}-\int_{M} g^{a b} h_{r s} S^{s} \nabla_{a}^{\prime} T_{b}^{r}
\end{aligned}
$$

## 3 Energy functionals for mappings between Riemannian manifolds

Given pairs $\left(X_{i}, Y_{i}\right)$ with $X_{i} \in M$ and $Y_{i} \in N$ we would like to learn a mapping $\phi: M \rightarrow N$. This learning problem reduces to standard multivariate regression if $M$ and $N$ are both Euclidean spaces $\mathbb{R}^{m}$ and $\mathbb{R}^{n}$ and to regression on a manifold if at least $N$ is Euclidean. The goal is to develop a regularization functional which is independent of the parametrization of $M$ and $N$ and respects the intrinsic geometry of both manifolds.

One could argue that by mapping both $m$-and $n$-dimensional manifolds $M$ and $N$ into Euclidean spaces we arrive again at the standard multivariate problem. However, in general there exists no isometric mapping from a $m$-dimensional Riemannian manifold into $\mathbb{R}^{m}$. For $M=S^{2}$ this assertion has been formulated in the famous Theorema Egregium of Gauss, which states that there exists no isometric mapping from the 2 -sphere into $\mathbb{R}^{2}$. In the general setting a reduction of the manifold learning problem to the multivariate problem is therefore not possible if one wants to use the given geometry of the manifolds. The second requirement of invariance against changes of the parametrization can be achieved by using the (mathematical) language of differential geometry.

The differential $d \phi_{a}^{r}$ measures the change of the output $\phi(x) \in N$ as one varies $x$ in the input manifold $M$. This object can be used to define the most simple differential energy, the so called harmonic energy.
Definition 8 The harmonic energy $S_{\text {harmonic }}(\phi)$ of a mapping $\phi: M \rightarrow N$ is defined as

$$
\begin{align*}
S_{\text {harmonic }}(\phi) & =\int_{M}\|d \phi\|_{T_{x}^{*} M \otimes T_{\phi(x)} N}^{2} d V(x) \\
& =\int_{M} g^{\alpha \beta}(x) h_{\mu \nu}(\phi(x)) \frac{\partial \phi^{\mu}}{\partial x^{\alpha}} \frac{\partial \phi^{\nu}}{\partial x^{\beta}} d V(x), \tag{8}
\end{align*}
$$

where $d V=\sqrt{\operatorname{det} g} d x$ is the natural volume element of $M$.
For standard multivariate regression, that is $M=\mathbb{R}^{m}$ and $N=\mathbb{R}$, the harmonic energy reduces to

$$
S_{\text {harmonic }}(\phi)=\int_{\mathbb{R}^{m}}\|\nabla \phi\|^{2} d x
$$

For $m=1$, this is just the energy functional of linear splines, and it is well-known that using this energy functional for interpolation/approximation leads to piecewise linear solutions. For curves on manifolds, that means $M=[a, b]$ and $N$ a manifold we get

$$
S_{\text {harmonic }}(\phi)=\int_{a}^{b}\|\dot{\phi}\|^{2} d t
$$

where $\dot{\phi}(t)=\frac{d \phi}{d t}(t)$. It is well-known that minimizing this energy (for fixed start and end points) leads to a geodesic. Using the harmonic energy for interpolation and approximation of curves on manifolds one gets piecewise geodesic solutions with non-differentiable knots at data point locations, see [5].

Since we are generally interested in solutions which have higher smoothness, we will use higher order derivatives in the regularizer. In the Euclidean case this is typically done e.g. using the thin-plate spline energy $\int_{\mathbb{R}^{m}}\|H f\|_{F} d x$, where $H f$ is the Hessian of $f$ at $x$ and $\|\cdot\|_{F}$ the Frobenius norm. For the generalization of this
type to the case of mappings between manifolds we have to define covariant derivatives of the differential $d \phi_{a}^{r}$. The problem is here that $d \phi$ "lives" in the cotangent and tangent space, $T_{x}^{*} M$ and $T_{\phi(x)} N$, of two different manifolds. Thus we cannot simply use the connection ${ }^{M} \nabla$ of $M$. The solution is to use the pull-back connection defined in the last section, which yields a notion of the derivative of a vector field on $N$ with respect to a variation in $M$, where $M$ and $N$ are connected via $\phi$. In order to build a general regularization functional for mappings between Riemannian manifolds we therefore just take covariant derivatives of the differential $d \phi_{a}^{r}$ using the pull-back connection. The $m$-th order covariant derivative will yield the tensor field $\nabla_{b_{1}}^{\prime} \ldots \nabla_{b_{m}}^{\prime} d \phi_{a}^{r} \in \otimes^{m+1} T^{*} M \otimes \phi^{-1} T N$. It can be easily checked that it is invariant with respect to parametrization. In order to obtain a real-valued regularization functional we just have to define an operation $\otimes^{m+1} T^{*} M \otimes \phi^{-1} T N \rightarrow \mathbb{R}_{+}$.

We illustrate this for $m=1$. For the tensor field $\nabla_{b}^{\prime} d \phi_{a}^{r}$ we can either first take the trace in $b$ and $a$ and then use the inner product in $T_{\phi(x)} N$, which yields the biharmonic energy [6].
Definition 9 The biharmonic energy $S_{\text {biharmonic }}(\phi)$ is defined as

$$
\begin{align*}
S_{\text {biharmonic }}(\phi) & =\int_{M}\left\|g^{b a} \nabla_{b}^{\prime} d \phi_{a}^{r}\right\|_{T_{\phi(x)} N}^{2} d V(x) \\
& =\int_{M} g^{b a} g^{c d} h_{r s} \nabla_{b}^{\prime} d \phi_{a}^{r} \nabla_{c}^{\prime} d \phi_{d}^{s} d V(x) \tag{9}
\end{align*}
$$

Another possibility is to take the inner product in the tensor product $T^{*} M \otimes T^{*} M \otimes \phi^{-1} T N$.
Definition 10 The Eells energy $S_{\text {Eells }}(\phi)$ is defined as

$$
\begin{align*}
S_{\mathrm{Eells}}(\phi)= & \int_{M}\left\|\nabla_{b}^{\prime} d \phi_{a}^{r}\right\|_{T_{x}^{*} M \otimes T_{x}^{*} M \otimes T_{\phi(x)} N}^{2} d V(x) \\
& =\int_{M} g^{a c} g^{b d} h_{r s} \nabla_{b}^{\prime} d \phi_{a}^{r} \nabla_{d}^{\prime} d \phi_{c}^{s} d V(x) \tag{10}
\end{align*}
$$

This energy functional has to our knowledge not been studied in differential geometry or elsewhere. We have named it after James Eells, who pioneered the study of harmonic maps between Riemannian manifolds [2] and recently passed away. The Eells energy reduces to the thin-plate spline energy in the Euclidean case. If $M$ and $N$ are Euclidean we obtain

$$
S_{\mathrm{Eells}}(\phi)=\int_{M} g^{\alpha \beta} g^{\gamma \delta} h_{\mu \nu} \frac{\partial^{2} \Phi^{\mu}}{\partial x^{\alpha} \partial x^{\gamma}} \frac{\partial^{2} \Phi^{\nu}}{\partial x^{\beta} \partial x^{\delta}} d V(x)
$$

where $g$ and $h$ are the Riemannian metrics corresponding to Euclidean space. This is the parametrization independent form of the Thin-Plate spline energy. In Cartesian coordinates we have $g^{\alpha \beta}=\delta^{\alpha \beta}$ and $h_{\mu \nu}=\delta_{\mu \nu}$ and the Eells energy reduces to the standard form of the Thin-Plate spline energy:

$$
S_{\mathrm{Eells}}(\phi)=\sum_{\mu=1}^{n} \int_{M} \sum_{\alpha, \gamma=1}^{m}\left(\frac{\partial^{2} \Phi^{\mu}}{\partial x^{\alpha} \partial x^{\gamma}}\right)^{2} d x
$$

## 4 Variation of the Eells energy and the derivation of boundary conditions

In the following, we show that using the extension of Green's Theorem and the commutator formula derived below one can derive in a relatively straightforward way the extremal equation of the different energy functionals for a variation $\phi(t, x)$, where $t \in(-\varepsilon, \varepsilon)$. A direct calculation in coordinates would be extremely tedious. The extremal equation for the variation provides us with necessary conditions for a minima of the Eells energy. We will use this to define natural boundary conditions which guarantee that the boundary terms in the extremal equation vanish.

We denote by $T(M \times(-\varepsilon, \varepsilon))$ the tangent space of the product manifold $M \times(-\varepsilon, \varepsilon)$. Note that $T(M \times(-\varepsilon, \varepsilon))$ is isomorphic to $T M \oplus T(-\varepsilon, \varepsilon)$. The product metric is given as $g=g_{T M} \oplus g_{T(-\varepsilon, \varepsilon)}$ and is block-diagonal in any local coordinate system. This implies that also all other structures on the product manifold like Christoffel-symbols or curvature tensor have this block-diagonal structure.
Lemma 4 Let $\phi(t, x):(-\varepsilon, \varepsilon) \times M \rightarrow N$ be a variation of the mapping $\phi=\phi(0, x)$. Let $\nabla^{\prime}$ be the pull-back connection on $T^{*}(M \times(-\varepsilon, \varepsilon)) \otimes \phi^{-1} T N$, then

$$
\begin{equation*}
\nabla_{b}^{\prime}\left(d \phi_{a}^{r} \frac{\partial^{a}}{\partial_{t}}\right)=\nabla_{b}^{\prime} \frac{\partial \phi^{r}}{\partial t}=\frac{\partial^{a}}{\partial t} \nabla_{a}^{\prime} d \phi_{b}^{r} \tag{11}
\end{equation*}
$$

Moreover, we have

$$
\begin{equation*}
\frac{\partial^{c}}{\partial t} \nabla_{c}^{\prime} \nabla_{a}^{\prime} d \phi_{b}^{r}=\nabla_{a}^{\prime} \nabla_{b}^{\prime} \frac{\partial \phi^{r}}{\partial t}+R_{s u v}^{N}{ }^{r} d \phi_{a}^{s} \frac{\partial \phi^{u}}{\partial t} d \phi_{b}^{v} \tag{12}
\end{equation*}
$$

Proof: Since $\frac{\partial}{\partial_{t}}$ and $\frac{\partial}{\partial_{x_{i}}}$ are coordinate vectors, we have $\left[\frac{\partial}{\partial_{t}}, \frac{\partial}{\partial_{x_{i}}}\right]=0$. Moreover, the tensor product of the pull-back connection of $\phi^{-1} T N$ and $T^{*}(M \times(-\varepsilon, \varepsilon))$ is compatible with the Riemannian structure on $T^{*}(M \times$ $(-\varepsilon, \varepsilon)) \otimes \phi_{t}^{-1} T N$ (note that $T^{*}(M \times(-\varepsilon, \varepsilon)) \simeq T^{*} M \oplus T(-\varepsilon, \varepsilon)$ so that the metric is block-diagonal). We use the result of Lemma 2 with $Y^{a}=\frac{\partial^{a}}{\partial t} \in T(M \times(-\varepsilon, \varepsilon))$,

$$
X^{b} \nabla_{b}^{\prime}\left(d \phi_{a}^{r} \frac{\partial^{a}}{\partial t}\right)-\frac{\partial^{a}}{\partial t} \nabla_{a}^{\prime}\left(d \phi_{b}^{r} X^{b}\right)=0
$$

With $\frac{\partial^{b}}{\partial t} \nabla_{b}^{\prime}\left(d \phi_{a}^{r} X^{a}\right)=X^{a} \frac{\partial^{b}}{\partial t} \nabla_{b}^{\prime} d \phi_{c}^{r}+d \phi_{c}^{r} \frac{\partial^{b}}{\partial t} \nabla_{b}^{\prime} X^{a}$ and $\frac{\partial^{a}}{\partial t} \nabla_{a}^{\prime} X^{b}=0\left(X^{b}\right.$ is a vector field on $M$ and does not change with $t$ ) we obtain

$$
\begin{equation*}
\nabla_{b}^{\prime}\left(d \phi_{a}^{r} \frac{\partial^{a}}{\partial_{t}}\right)=\nabla_{b}^{\prime} \frac{\partial \phi^{r}}{\partial t}=\frac{\partial^{a}}{\partial t} \nabla_{b}^{\prime} d \phi_{a}^{r}=\frac{\partial^{a}}{\partial t} \nabla_{a}^{\prime} d \phi_{b}^{r} \tag{13}
\end{equation*}
$$

where the last equality follows by the symmetry of $\nabla_{d}^{\prime} d \phi_{c}^{r}$. Taking the derivative of Equation 13 we get

$$
\nabla_{a}^{\prime} \nabla_{b}^{\prime} \frac{\partial \phi^{r}}{\partial t}=\left(\nabla_{a}^{\prime} \frac{\partial^{c}}{\partial t}\right) \nabla_{c}^{\prime} d \phi_{b}^{r}+\frac{\partial^{c}}{\partial t} \nabla_{a}^{\prime} \nabla_{c}^{\prime} d \phi_{b}^{r}=\frac{\partial^{c}}{\partial t} \nabla_{a}^{\prime} \nabla_{c}^{\prime} d \phi_{b}^{r}
$$

where we have used that $\left.\left(\nabla_{a}^{\prime} \frac{\partial^{c}}{\partial t}\right)\right|_{T M}=0$. We will now exchange the order of the derivatives in front of $d \phi_{b}^{r}$ using the definition of the curvature tensor for objects of type $T^{*}(M \times(-\varepsilon, \varepsilon)) \otimes \phi^{-1} T N$,

$$
\frac{\partial^{c}}{\partial t} \nabla_{a}^{\prime} \nabla_{c}^{\prime} d \phi_{b}^{r}=\frac{\partial^{c}}{\partial t} \nabla_{c}^{\prime} \nabla_{a}^{\prime} d \phi_{b}^{r}+\frac{\partial^{c}}{\partial t} R_{a c b}^{M} d \phi_{d}^{r}-\frac{\partial^{c}}{\partial t} R_{s u v}^{N}{ }^{r} d \phi_{a}^{s} d \phi_{c}^{u} d \phi_{b}^{v}
$$

where we have used that the curvature tensor of $M \times(-\varepsilon, \varepsilon)$ is the direct sum of the curvature of $M$ and the curvature of $(-\varepsilon, \varepsilon)$ which is zero. Moreover, we have due to the block-diagonal structure of the curvature tensor $\frac{\partial^{c}}{\partial t} R_{a c b}^{M}{ }^{d}=0$. Therefore we get in total

$$
\begin{aligned}
\frac{\partial^{c}}{\partial t} \nabla_{c}^{\prime} \nabla_{a}^{\prime} d \phi_{b}^{r} & =\nabla_{a}^{\prime} \nabla_{b}^{\prime} \frac{\partial \phi^{r}}{\partial t}+\frac{\partial^{c}}{\partial t} R_{s u v}^{N}{ }^{r} d \phi_{a}^{s} d \phi_{c}^{u} d \phi_{b}^{v} \\
& =\nabla_{a}^{\prime} \nabla_{b}^{\prime} \frac{\partial \phi^{r}}{\partial t}+R_{s u v}^{N}{ }^{r} d \phi_{a}^{s} \frac{\partial \phi^{u}}{\partial t} d \phi_{b}^{v}
\end{aligned}
$$

The previous theorem basically tells us that the time derivative commutes with the pull-back connection. But the "Hessian" does not commute with the time derivative and one gets an additional curvature term.
Theorem 1 Let $M$ and $N$ be Riemannian manifolds with metric $g$ and $h$. Let $\phi(t, x):(-\varepsilon, \varepsilon) \times M \rightarrow N$ be a variation of the mapping $\phi=\phi(0, x)$ and $W^{b}=\left.\frac{\partial}{\partial t} \phi_{t}^{b}\right|_{t=0}$ the variational vector field at $t=0$. The variation of the Eells energy is given as,

$$
\begin{aligned}
\left.\frac{d}{d t} S_{\text {Eells }}\left(\phi_{t}\right)\right|_{t=0}= & 2 \int_{M} g^{a b} g^{c d} h_{r s} W^{r}\left[\nabla_{c}^{\prime} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{d}^{s}+R_{u v w}^{N}{ }^{s} d \phi_{a}^{w} d \phi_{c}^{u} \nabla_{b}^{\prime} d \phi_{d}^{v}\right] d V \\
& +2 \int_{\partial M} h_{r s} g^{a b} N^{d}\left[\nabla_{a}^{\prime} W^{r} \nabla_{d}^{\prime} d \phi_{b}^{s}-W^{r} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{d}^{s}\right] d \tilde{V}
\end{aligned}
$$

where $d \tilde{V}$ is the volume element of the boundary $\partial M, R_{u v w s}$ is the curvature tensor of $N$ and $N^{a}$ is the normal vector field at $\partial M$.
Proof: We use the commutator of Theorem 4 and obtain,

$$
\begin{aligned}
\frac{d}{d t} S_{\mathrm{Eells}}\left(\phi_{t}\right)= & 2 \int_{M} g^{a b} g^{c d} h_{r s}\left(\frac{\partial^{e}}{\partial t} \nabla_{e}^{\prime} \nabla_{a}^{\prime}\left(d \phi_{t}\right)_{c}^{r}\right) \nabla_{b}^{\prime}\left(d \phi_{t}\right)_{d}^{s} d V \\
= & 2 \int_{M} g^{a b} g^{c d} h_{r s} \nabla_{a}^{\prime} \nabla_{c}^{\prime} \frac{\partial \phi^{r}}{\partial t} \nabla_{b}^{\prime}\left(d \phi_{t}\right)_{d}^{s} d V \\
& +2 \int_{M} g^{a b} g^{c d} h_{r s} R_{u v w}^{N}{ }^{r}\left(d \phi_{t}\right)_{a}^{u} \frac{\partial \phi_{t}^{v}}{\partial t}\left(d \phi_{t}\right)_{c}^{w} \nabla_{b}^{\prime}\left(d \phi_{t}\right)_{d}^{s} d V
\end{aligned}
$$

One has $\left.\nabla_{b}^{\prime}\left(d \phi_{t}\right)_{d}^{s}\right|_{t=0}=\nabla_{b}^{\prime} d \phi_{d}^{s}$. Together with the extended Green's theorem we obtain

$$
\begin{aligned}
\left.\frac{d}{d t} S_{\mathrm{Eells}}\left(\phi_{t}\right)\right|_{t=0}= & 2 \int_{M} g^{a b} g^{c d} h_{r s} \nabla_{a}^{\prime} \nabla_{c}^{\prime} W^{r} \nabla_{b}^{\prime} d \phi_{d}^{s} d V \\
& +2 \int_{M} g^{a b} g^{c d} h_{r s} R_{u v w}^{N}{ }^{r} d \phi_{a}^{u} W^{v} d \phi_{c}^{w} \nabla_{b}^{\prime} d \phi_{d}^{s} d V \\
= & 2 \int_{\partial M} N^{b} g^{c d} h_{r s} \nabla_{c}^{\prime} W^{r} \nabla_{b}^{\prime}\left(d \phi_{t}\right)_{d}^{s} d \tilde{V} \\
& -2 \int_{M} g^{a b} g^{c d} h_{r s} \nabla_{c}^{\prime} W^{r} \nabla_{a}^{\prime} \nabla_{b}^{\prime}\left(d \phi_{t}\right)_{d}^{s} d V \\
& +2 \int_{M} g^{a b} g^{c d} h_{r s} R_{u v w}^{N}{ }^{r} d \phi_{a}^{u} W^{v} d \phi_{c}^{w} \nabla_{b}^{\prime} d \phi_{d}^{s} d V \\
= & 2 \int_{\partial M} N^{b} g^{c d} h_{r s} \nabla_{c}^{\prime} W^{r} \nabla_{b}^{\prime} d \phi_{d}^{s} d \tilde{V} \\
& -2 \int_{\partial M} g^{a b} N^{d} h_{r s} W^{r} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{d}^{s} d \tilde{V} \\
& +2 \int_{M} g^{a b} g^{c d} h_{r s} W^{r} \nabla_{c}^{\prime} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{d}^{s} d V \\
& +2 \int_{M} g^{a b} g^{c d} h_{r s} R_{u v w}^{N}{ }^{r} d \phi_{a}^{u} W^{v} d \phi_{c}^{w} \nabla_{b}^{\prime} d \phi_{d}^{s} d V \\
= & 2 \int_{M} g^{a b} g^{c d} h_{r s} W^{r}\left[\nabla_{c}^{\prime} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{d}^{s}+R_{v w u}^{N}{ }^{s} d \phi_{a}^{u} d \phi_{c}^{v} \nabla_{b}^{\prime} d \phi_{d}^{w}\right] d V \\
& +2 \int_{\partial M} h_{r s} g^{a b} N^{d}\left[\nabla_{a}^{\prime} W^{r} \nabla_{d}^{\prime} d \phi_{b}^{s}-W^{r} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{d}^{s}\right] d \tilde{V}
\end{aligned}
$$

where we have used in the last step $R_{u v w s}=R_{w s u v}$.

A necessary condition for a minimizer of the Eells energy is that

$$
\left.\frac{d}{d t} S_{\mathrm{Eells}}\left(\phi_{t}\right)\right|_{t=0}=0
$$

for all vector fields $W$. For points in the interior of $M$ this implies that

$$
\begin{equation*}
g^{a b} g^{c d}\left[\nabla_{c}^{\prime} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{d}^{s}+R_{v w u}^{N}{ }^{s} d \phi_{a}^{u} d \phi_{c}^{v} \nabla_{b}^{\prime} d \phi_{d}^{w}\right]=0 \tag{14}
\end{equation*}
$$

The boundary term clearly vanishes if on $\partial M$ we set

$$
\begin{equation*}
N^{a} \nabla_{a}^{\prime} d \phi_{b}^{r}=0, \quad N^{c} g^{a b} \nabla_{a}^{\prime} \nabla_{b}^{\prime} d \phi_{c}^{r}=0 . \tag{15}
\end{equation*}
$$

While these boundary conditions that we use in our implementation are not minimal, they allow for a very simple extrinsic formulation. With these boundary conditions we can avoid the use of the curvature tensor/second fundamental form of $N$ for expressing them in coordinates, see Theorem 2. Choosing non-minimal boundary conditions restricts the space of functions to optimize over more than necessary. However, our experiments show that the remaining set of function is still capable of representing all the effects that we were looking for.

## 5 Properties of the harmonic and the Eells energy

When performing approximation, we minimize the weighted sum of an energy functional $S(\phi)$ and a loss term such as the quadratic loss over all maps $\phi: M \rightarrow N$. In the limit where the weight of the loss term $\lambda$ tends to infinity we are effectively minimizing the following objective function

$$
\underset{\phi: M \rightarrow N}{\arg \min }\left\{\left.\frac{1}{n} \sum_{i=1}^{n} d^{2}\left(\phi\left(X_{i}\right), Y_{i}\right) \quad \right\rvert\, \quad S(\phi)=0 \quad \text { and BC hold }\right\}
$$

where $S(\phi)$ is either the harmonic or Eells energy and BC the corresponding boundary conditions. Thus, the solution is in the null space of $S(\phi)$. The null space is important even for finite $\lambda$ since this is the set of maps which are not penalized at all. In this section, we study the null space for the harmonic and the Eells energy.

It is well known, see [1], that the null space of the harmonic energy, $S_{\text {harmonic }}(\phi)=0$, consists of the constant maps $\phi=$ constant. Thus the null space of the harmonic energy is very restrictive. The boundary condition $N^{a} d \phi_{a}^{r}=0$ holds automatically since $S_{\text {harmonic }}(\phi)=0$ is equivalent to $d \phi_{a}^{r}=0$. The minimization of the objective function yields therefore the so-called Karcher mean [3] (given that it exists), which is the generalization of the mean of a set of points in Euclidean space to Riemannian manifolds. In the case of $M=\mathbb{R}^{d}$ and $N=\mathbb{R}^{p}$ this corresponds to the prediction of the mean $\frac{1}{n} \sum_{i=1}^{n} Y_{i}$.

For the usual thin plate spline energy for a mapping $\phi: \mathbb{R}^{m} \rightarrow \mathbb{R}^{n}$,

$$
S_{\text {ThinPlate }}(\phi)=\sum_{\mu=1}^{n} \int_{\mathbb{R}^{m}} \sum_{\alpha, \gamma=1}^{m}\left(\frac{\partial^{2} \Phi^{\mu}}{\partial x^{\alpha} \partial x^{\gamma}}\right)^{2} d x
$$

the null space consists of the linear mappings. This means we are free to fit the data with linear mappings but have to pay for any deviation from linearity. The concept of linearity breaks down for manifold-valued mappings since the output space has no linear structure. However, as shown in the following proposition taken from [1], there is an alternative property for manifold-valued mappings that can be interpreted as a an appropriate generalisation of linearity for manifold-valued mappings.
Proposition 1 [1] A map $\phi: M \rightarrow N$ is totally geodesic if $\phi$ maps geodesics of $M$ linearly to geodesics of $N$, i.e. the image of any geodesic in $M$ is also a geodesic in $N$ though potentially with a different constant speed. The following three properties are equivalent:

1. $\phi$ is totally geodesic,
2. $\phi$ preserves the connection, i.e.

$$
{ }^{N} \nabla_{d \phi(X)} d \phi(Y)=d \phi\left({ }^{M} \nabla_{X} Y\right)
$$

where $d \phi$ is the push-forward or differential of $\phi$,
3. $\nabla_{a}^{\prime} d \phi_{b}^{r}=0$.

Proof: We have for $X^{a}, Y^{b} \in T M, X^{a} \nabla_{a}^{\prime}\left(Y^{b} d \phi_{b}^{r}\right)=X^{a} Y^{b} \nabla_{a}^{\prime} d \phi_{b}^{r}+X^{a} d \phi_{b}^{r} \nabla_{a} Y^{b}$. This yields

$$
X^{a} Y^{b} \nabla_{a}^{\prime} d \phi_{b}^{r}=X^{a} \nabla_{a}^{\prime}\left(Y^{b} d \phi_{b}^{r}\right)-X^{a} d \phi_{b}^{r} \nabla_{a} Y^{b}
$$

The last equation can be rewritten in a more transparent way using the definition of the pull-back connection as

$$
X^{a} Y^{b} \nabla_{a}^{\prime} d \phi_{b}^{r}={ }^{N} \nabla_{d \phi(X)} d \phi(Y)-d \phi\left({ }^{M} \nabla_{X} Y\right)
$$

The above equation shows that $\phi$ is connection preserving if and only if $\nabla_{a}^{\prime} d \phi_{b}^{r}=0$. Moreover, $\nabla_{a}^{\prime} d \phi_{b}^{r}=0$ implies that geodesics are mapped onto geodesics. Suppose $\gamma:(-\varepsilon, \varepsilon) \rightarrow M$ is a geodesic on $M$. Then given $\nabla_{a}^{\prime} d \phi_{b}^{r}=0$ we obtain,

$$
0={ }^{N} \nabla_{d \phi(\dot{\gamma})} d \phi(\dot{\gamma})-d \phi\left({ }^{M} \nabla_{\dot{\gamma}} \dot{\gamma}\right)={ }^{N} \nabla_{d \phi(\dot{\gamma})} d \phi(\dot{\gamma})=0
$$

where we have used that ${ }^{M} \nabla_{\dot{\gamma}} \dot{\gamma}=0$ since $\gamma$ is a geodesic. Therefore the mapped curve $\gamma^{\prime}:(-\varepsilon, \varepsilon) \rightarrow N$ defined as $\gamma^{\prime}=\phi \circ \gamma$ is also a geodesic. Conversely, ${ }^{N} \nabla_{d \phi(\dot{\gamma})} d \phi(\dot{\gamma})-d \phi\left({ }^{M} \nabla_{\dot{\gamma}} \dot{\gamma}\right)=0$ for all geodesics implies $\nabla_{a}^{\prime} d \phi_{b}^{r}=0$.

Due to Proposition 1 we know that the null space of the Eells energy consists of the totally geodesic maps, that is the maps for which $\nabla_{b}^{\prime} d \phi_{a}^{r}=0$. As for the harmonic energy this implies automatically that also the boundary conditions $N^{b} \nabla_{b}^{\prime} d \phi_{a}^{r}=0$ and $N^{a} \nabla_{c}^{\prime} \nabla_{b}^{\prime} d \phi_{a}^{f}=0$ are fulfilled. Thus in the limit $\lambda \rightarrow \infty$ the minimization of the approximation objective function yields a map which maps geodesics of the input space to geodesics of the output space. In the case of $M=\mathbb{R}^{d}$ and $N=\mathbb{R}$ this corresponds to prediction of a linear function $\phi(x)=\langle w, x\rangle+b$. The set of maps which map geodesics to geodesics is therefore the natural generalization of linear maps in the Euclidean case. Since geodesics are curves on manifolds which are "straight" in the sense of having no acceleration, this set of maps is "straight" in the best possible way.

## 6 From intrinsic to extrinsic representation

The Eells energy written out in coordinates is quite complicated, see the expression of $\nabla_{a}^{\prime} d \phi_{b}^{r}$ in coordinates in eq. 5. If one minimizes the energy over maps $\phi: M \rightarrow N$ a direct implementation in coordinates also poses the problem of coordinate changes in $N$, if $\phi(x)$ is assigned to different charts during the course of the optimisation. Usually a manifold cannot be represented with one global coordinate chart. For example every global parametrization of the sphere has at least one coordinate singularity at the pole.

In this section, we show that an efficient optimization is nevertheless possible if $N$ is given as an isometrically embedded submanifold in Euclidean space $\mathbb{R}^{p}$. Such an isometric embedding is always possible for large enough $p$ [7]. For a huge class of manifolds an isometric embedding in Euclidean space is known. Often the manifold is even defined as a constrained set in $\mathbb{R}^{p}$ so that the metric is pull-back from $\mathbb{R}^{p}$ and the isometric embedding is trivial. Below, quantities which are defined on $N$ are called intrinsic, whereas quantities related to $\mathbb{R}^{p}$ are called extrinsic. The goal will be to represent the intrinsic expressions with simpler computable extrinsic ones. We have to stress that in doing this we neither lose the invariance with respect to parametrization nor do we change the regularizer.

Let $i: N \rightarrow \mathbb{R}^{p}$ be the isometric embedding and denote by $\Psi: M \rightarrow \mathbb{R}^{p}$ the composition $\Psi=i \circ \phi$. Let $z^{\mu}$ be standard Cartesian coordinates in $\mathbb{R}^{p}$. Then the differential of $\Psi$ is given as $d \Psi_{a}^{r}=\frac{\partial \Psi^{\mu}}{\partial x^{\alpha}} d x_{a}^{\alpha} \otimes \frac{\partial^{r}}{\partial z^{\mu}}$. As in the last section we can also define an pull-back connection $\tilde{\nabla}: T M \otimes \Psi^{-1} T \mathbb{R}^{p} \rightarrow \Psi^{-1} T \mathbb{R}^{p}$ for the mapping $\Psi$,

$$
\tilde{\nabla} \frac{\partial}{\partial x^{\alpha}} \frac{\partial^{r}}{\partial z^{\mu}}:=\mathbb{R}^{p} \nabla_{\Psi_{*} \frac{\partial}{\partial x^{\alpha}}} \frac{\partial^{r}}{\partial z^{\mu}}=0
$$

which is trivial due to the flatness of the connection of $\mathbb{R}^{p}$. Because of this property the expressions for the corresponding covariant derivatives expression will simplify significantly. However, note that the coordinate vector $\frac{\partial^{r}}{\partial y^{\mu}}$ of $N$ has the derivative $\tilde{\nabla}_{\frac{\partial}{\partial x^{\alpha}}}\left(i_{*} \frac{\partial^{r}}{\partial y^{\mu}}\right)=\frac{\partial^{2} i^{\rho}}{\partial y^{\nu} \partial y^{\mu}} \nabla_{a} \phi^{\nu} \frac{\partial^{r}}{\partial z^{\rho}}$. The following theorem shows how intrinsic expressions in $\phi$ can be expressed in terms of the extrinsic ones in $\Psi$. However, we first compute some geometric objects.
Lemma 5 Let $i: N \rightarrow \mathbb{R}^{p}$ be an isometric embedding and denote by $h$ the metric of $N$ and by $y^{\mu}$ coordinates in $N$. Then the following quantities can be computed using the embedding $i$,

$$
h_{\mu \nu}=\sum_{\alpha=1}^{p} \frac{\partial i^{\alpha}}{\partial y^{\mu}} \frac{\partial i^{\alpha}}{\partial y^{\nu}}, \quad h_{\mu \nu}^{N} \Gamma_{\omega \rho}^{\nu}=\sum_{\alpha=1}^{p} \frac{\partial^{2} i^{\alpha}}{\partial y^{\omega} \partial y^{\rho}} \frac{\partial i^{\alpha}}{\partial y^{\mu}}
$$

The projection $P: T_{z} \mathbb{R}^{p} \rightarrow T_{z} N, V \mapsto P V$ can be computed as

$$
(P V)^{r}=h^{r s} \delta_{s u} V^{u}=h^{\mu \nu} \sum_{\alpha=1}^{p} \frac{\partial i^{\alpha}}{\partial y^{\nu}} V^{\alpha} \frac{\partial^{r}}{\partial y^{\mu}}
$$

Proof: We have $h=i^{*} \delta$, where $\delta$ is the metric in $\mathbb{R}^{p}$. Thus, we obtain

$$
h_{r s}=\delta_{\alpha \beta}\left(i^{*} d z^{\alpha}\right)_{r} \otimes\left(i^{*} d z^{\beta}\right)_{s}=\delta_{\alpha \beta} \frac{\partial i^{\alpha}}{\partial y^{\mu}} \frac{\partial i^{\beta}}{\partial y^{\nu}} d y_{e}^{\mu} \otimes d y_{f}^{\nu}
$$

It holds $h_{\mu \nu}{ }^{N} \Gamma_{\omega \rho}^{\nu}=\frac{1}{2}\left(\partial_{\omega} h_{\rho \mu}+\partial_{\rho} h_{\omega \mu}-\partial_{\mu} h_{\omega \rho}\right)$. With

$$
\partial_{\omega} h_{\rho \mu}=\sum_{\alpha=1}^{p}\left[\frac{\partial^{2} i^{\alpha}}{\partial y^{\omega} \partial y^{\rho}} \frac{\partial i^{\alpha}}{\partial y^{\mu}}+\frac{\partial i^{\alpha}}{\partial y^{\rho}} \frac{\partial^{2} i^{\alpha}}{\partial y^{\omega} \partial y^{\mu}}\right],
$$

we arrive after a short calculation at the desired result. The projection $P: T_{z} \mathbb{R}^{p} \rightarrow T_{z} N$ can be written as $P=\sum_{i=1}^{n} e_{i}\left\langle e_{i}, \cdot\right\rangle$, where $\left\{e_{i}^{r}\right\}_{i=1}^{n}$ is an orthonormal basis in $T_{z} N$. Then $h^{r s}=\sum_{i=1}^{n} e_{i}^{r} e_{i}^{s}$ and thus $P_{b}^{r}=h^{r s} \delta_{s b}$. We have $\delta_{s b}=\sum_{\alpha=1}^{p} d z_{s}^{\alpha} d z_{b}^{\alpha}$, where $z^{\alpha}$ are Cartesian coordinates in $\mathbb{R}^{p}$. The tangential projection of $d z^{\alpha}$ is given as $\left(i^{*} d z^{\alpha}\right)_{b}=\frac{\partial i^{\alpha}}{\partial y^{\nu}} d y_{b}^{\nu}$. Thus $P_{b}^{r}=h^{\mu \nu} \sum_{\alpha=1}^{p} \frac{\partial i^{\alpha}}{\partial y^{\nu}} d z_{b}^{\alpha} \otimes \frac{\partial^{r}}{\partial y^{\mu}}$.

Definition 11 Let $\nabla^{\prime}$ be the connection pull-back by $\phi$ and $\tilde{\nabla}$ the connection pull-back by $\Psi=i \circ \phi$. The pull-back second fundamental from $\Pi: T M \otimes \phi^{-1} T N \rightarrow\left(\phi^{-1} T N\right)^{\perp}$ is defined as

$$
\Pi_{a s}^{r} X^{a} S^{s}=X^{a} \tilde{\nabla}_{a} S^{r}-X^{a} \nabla_{a}^{\prime} S^{r}
$$

Lemma 6 Let $i: N \rightarrow \mathbb{R}^{p}$ be an isometric embedding of $N$. The second fundamental form of $N$, ${ }^{N} \Pi_{g f}^{e}$ : $T N \otimes T N \rightarrow(T N)^{\perp}$ can be expressed in terms of the embedding $i$ as,

$$
{ }^{N} \Pi_{r s}^{u}=\left[\frac{\partial^{2} i^{\alpha}}{\partial y^{\mu} \partial y^{\nu}} \frac{\partial^{u}}{\partial z^{\alpha}}-P_{\beta}^{\rho} \frac{\partial^{2} i^{\beta}}{\partial y^{\mu} \partial y^{\nu}} \frac{\partial^{u}}{\partial y^{\rho}}\right] d y_{r}^{\mu} d y_{s}^{\nu}=\left(\frac{\partial^{2} i^{\alpha}}{\partial y^{\mu} \partial y^{\nu}} \frac{\partial^{u}}{\partial z^{\alpha}}\right)^{\perp} \otimes d y_{r}^{\mu} \otimes d y_{s}^{\nu}
$$

Then the pull-back second fundamental form $\Pi_{a b}^{\prime e}: T M \otimes \phi^{-1} T N \rightarrow \phi^{-1}(T N)^{\perp}$ can be computed as

$$
\Pi_{a s}^{\prime r}=d \phi_{a}^{u}{ }^{N} \Pi_{u s}^{r}=\left(\frac{\partial^{2} i^{\alpha}}{\partial y^{\mu} \partial y^{\nu}} \frac{\partial^{r}}{\partial z^{\alpha}}\right)^{\perp} \otimes d \phi_{a}^{\mu} \otimes d y_{s}^{\nu}
$$

Proof: The second fundamental form of $N$ can be computed for $\frac{\partial^{r}}{\partial y^{\mu}} \in T N$ as

$$
{ }^{N} \Pi_{s r}^{u} \frac{\partial^{r}}{\partial y^{\mu}}=\mathbb{R}^{p} \nabla_{s} \frac{\partial^{u}}{\partial y^{\mu}}-{ }^{N} \nabla_{s} \frac{\partial^{u}}{\partial y^{\mu}} .
$$

With $\frac{\partial^{r}}{\partial y^{\mu}}=\frac{\partial i^{\alpha}}{\partial y^{\mu}} \frac{\partial^{r}}{\partial z^{\alpha}}$ we have $\mathbb{R}^{p} \nabla_{s}\left(i_{*} \frac{\partial^{r}}{\partial y^{\mu}}\right)={ }^{\mathbb{R}^{p}} \nabla_{s}\left(\frac{\partial i^{\alpha}}{\partial y^{\mu}} \frac{\partial^{r}}{\partial z^{\alpha}}\right)=\frac{\partial^{2} i^{\alpha}}{\partial y^{\nu} \partial y^{\mu}} d y_{s}^{\nu} \otimes \frac{\partial^{r}}{\partial z^{\alpha}}$. Together with

$$
{ }^{N} \nabla_{s} \frac{\partial^{r}}{\partial y^{\mu}}={ }^{N} \Gamma_{s \mu}^{r}=h^{r \nu} \sum_{\alpha=1}^{p} \frac{\partial^{2} i^{\alpha}}{\partial y^{\omega} \partial y^{\mu}} \frac{\partial i^{\alpha}}{\partial y^{\nu}} d y_{s}^{\omega}=P_{\beta}^{r} \frac{\partial^{2} i^{\beta}}{\partial y^{\omega} \partial y^{\mu}} d y_{s}^{\omega}
$$

we obtain the result. The expression for $\Pi^{\prime}$ can be derived as follows. For $S^{r} \in \phi^{-1} T N$ one obtains

$$
\begin{aligned}
\tilde{\nabla}_{a} S^{r} & =d \Psi_{a}^{s} \mathbb{R}^{p} \nabla_{s} S^{r}=d \phi_{a}^{s} \mathbb{R}^{p} \nabla_{s} S^{r}=d \phi_{a}^{s}\left[{ }^{N} \nabla_{s} S^{r}+{ }^{N} \Pi_{s u}^{r} S^{u}\right] \\
& =\nabla_{a}^{\prime} S^{r}+d \phi_{a}^{s}{ }^{N} \Pi_{s u}^{r} S^{u}
\end{aligned}
$$

where we have used the result of Theorem 2 that $d \Psi_{a}^{f}=d \phi_{a}^{f}$. One can check that the result generalizes to covariant derivatives of $\otimes^{m} T^{*} M \otimes \phi^{-1} T N$.

Theorem 2 The following equivalences between intrinsic and extrinsic objects hold,

$$
\begin{aligned}
d \phi_{a}^{r} & =d \Psi_{a}^{r}, \quad \nabla_{c}^{\prime} d \phi_{a}^{r}=\left(\tilde{\nabla}_{c} d \Psi_{a}^{r}\right)^{\top} \\
\nabla_{d}^{\prime} \nabla_{c}^{\prime} d \phi_{a}^{r} & =\tilde{\nabla}_{d}\left(\tilde{\nabla}_{c} d \Psi_{a}^{r}\right)^{\top}-d \Psi_{d}^{s}{ }^{N} \Pi_{s u}^{r}\left(\tilde{\nabla}_{c} d \Psi_{a}^{u}\right)^{\top}
\end{aligned}
$$

where ${ }^{\top}$ denotes the projection onto the tangent space $T_{\Psi(x)} N$ and ${ }^{N} \Pi_{s u}^{r}$ is the second fundamental form of $N$. If $M$ is a domain in $\mathbb{R}^{d}$ we get,

$$
\begin{equation*}
S_{\text {harmonic }}=\int_{M} \sum_{\alpha=1}^{p} \sum_{\mu=1}^{d}\left(\frac{\partial^{2} \Psi^{\alpha}}{\partial x^{\mu}}\right)^{2} d x, \quad S_{\text {Eells }}=\int_{M} \sum_{\alpha=1}^{p} \sum_{\mu, \nu=1}^{d}\left[\left(\frac{\partial^{2} \Psi^{\alpha}}{\partial x^{\mu} \partial x^{\nu}}\right)^{\top}\right]^{2} d x \tag{16}
\end{equation*}
$$

The boundary conditions for the Eells energy are given in coordinates as

$$
\begin{equation*}
\sum_{\mu=1}^{d} N^{\mu}\left(\frac{\partial^{2} \Psi^{\alpha}}{\partial x^{\mu} \partial x^{\nu}}\right)^{\top}=0, \quad \sum_{\mu, \nu=1}^{d} N^{\mu} \frac{\partial}{\partial x^{\nu}}\left(\frac{\partial^{2} \Psi^{\alpha}}{\partial x^{\nu} \partial x^{\mu}}\right)^{\top}=0 \tag{17}
\end{equation*}
$$

Proof: We have $\Psi=i \circ \phi$, that is with $\frac{\partial^{r}}{\partial y^{\mu}}=\frac{\partial i^{\alpha}}{\partial y^{\mu}} \frac{\partial^{r}}{\partial z^{\alpha}}$ we obtain

$$
d \Psi_{a}^{r}=\frac{\partial \Psi^{\alpha}}{\partial x^{\beta}} d x_{a}^{\beta} \otimes \frac{\partial^{r}}{\partial z^{\alpha}}=\frac{\partial i^{\alpha}}{\partial y^{\mu}} \frac{\partial \phi^{\mu}}{\partial x^{\beta}} d x_{a}^{\beta} \otimes \frac{\partial^{r}}{\partial z^{\alpha}}=\frac{\partial \phi^{\mu}}{\partial x^{\beta}} d x_{a}^{\beta} \otimes \frac{\partial^{r}}{\partial y^{\mu}}=d \phi_{a}^{r}
$$

We have $\mathbb{R}^{p} \nabla_{s} V^{r}={ }^{N} \nabla_{s} V^{r}+\Pi_{s u}^{r} V^{u}$. Therefore we can decompose the pull-back connection $\tilde{\nabla}$ related to $\Psi$ and $\nabla^{\prime}$ related to $\phi$ as follows for $T_{a_{1} \ldots, a_{m}}^{s} \in \otimes^{m} T M \otimes \phi^{-1} T N$

$$
\tilde{\nabla}_{b} T_{a_{1} \ldots, a_{m}}^{s}=\nabla_{b}^{\prime} T_{a_{1} \ldots, a_{m}}^{s}+\Pi_{b r}^{s} T_{a_{1} \ldots a_{m}}^{r}
$$

where we have used the pull-back second fundamental form $\Pi_{b r}^{\prime s} \in \phi^{-1}(T N)^{\perp} \otimes T M \otimes \phi^{-1} T N, \Pi_{b r}^{\prime s}=$ $d \phi_{b}^{u}{ }^{N} \Pi_{u r}^{s}$. For the second part we assume that $M$ is a domain in $\mathbb{R}^{d}$. Then $g^{a b}=\delta^{a b}$ and we obtain

$$
\begin{aligned}
\delta^{a b} h_{r s} d \phi_{a}^{r} d \phi_{b}^{s} & =\delta^{a b} \delta_{r s} d \Psi_{a}^{r} d \Psi_{b}^{s}=\sum_{\alpha=1}^{p} \sum_{\mu=1}^{d}\left(\frac{\partial \Psi^{\alpha}}{\partial x^{\mu}}\right)^{2}, \\
\delta^{a c} \delta^{b d} h_{r s} \nabla_{b}^{\prime} d \phi_{a}^{r} \nabla_{d}^{\prime} d \phi_{c}^{s} & =\delta^{a c} \delta^{b d} \delta_{r s}\left(\tilde{\nabla}_{b} d \Psi_{a}^{r}\right)^{\top}\left(\tilde{\nabla}_{d} d \Psi_{c}^{s}\right)^{\top} \\
& =\sum_{\alpha=1}^{p} \sum_{\mu, \nu=1}^{d}\left[\left(\frac{\partial^{2} \Psi^{\alpha}}{\partial x^{\mu} \partial x^{\nu}}\right)^{\top}\right]^{2} .
\end{aligned}
$$

Moreover we have

$$
\begin{aligned}
N^{a} \nabla_{b}^{\prime} d \phi_{a}^{r} & =N^{a}\left(\tilde{\nabla}_{b} d \Psi_{a}^{r}\right)^{\top}=N^{\mu}\left(\frac{\partial^{2} \Psi^{\alpha}}{\partial x^{\mu} \partial x^{\nu}}\right)^{\top} \\
\delta^{c b} N^{a} \nabla_{c}^{\prime} \nabla_{b}^{\prime} d \phi_{a}^{r} & =\delta^{c b}\left[N^{a} \tilde{\nabla}_{c}\left(\tilde{\nabla}_{b} d \Psi_{a}^{r}\right)^{\top}-N^{a} d \Psi_{c}^{u} \Pi_{u s}^{r}\left(\tilde{\nabla}_{b} d \Psi_{a}^{s}\right)^{\top}\right] \\
& =\delta^{c b} N^{a} \tilde{\nabla}_{c}\left(\tilde{\nabla}_{b} d \Psi_{a}^{r}\right)^{\top}=\sum_{\mu, \nu=1}^{d} N^{\mu} \frac{\partial}{\partial x^{\nu}}\left(\frac{\partial^{2} \Psi^{\alpha}}{\partial x^{\nu} \partial x^{\mu}}\right)^{\top},
\end{aligned}
$$

where we used in the second condition that from the first condition we have $N^{a}\left(\tilde{\nabla}_{b} d \Psi_{a}^{r}\right)^{\top}=0$.

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