Geodesic Finite Elements of Higher Order

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Abstract

We generalize geodesic finite elements to obtain spaces of higher approximation order. Our approach uses a Riemannian center of mass with a signed measure. We prove well-definedness of this new center of mass under suitable conditions. As a side product we can define geodesic finite elements for non-simplex reference elements such as cubes and prisms. We prove smoothness of the interpolation functions, and various invariance properties. Numerical tests show that the optimal convergence orders of the discretization error known from the linear theory are obtained also in the nonlinear setting.

1 Introduction

In [19] we have introduced geodesic finite elements as a conforming finite element discretization for partial differential equations for functions with values in a Riemannian manifold M. Instances of such problems are the simulation of liquid crystals ([7], $M = S^2, \mathbb{RP}^2, \mathrm{SO}(3)$), Cosserat materials ([17], $M = \mathbb{R}^3 \times \mathrm{SO}(3)$), and image processing ([24], $M = S^2$). The core idea was to replace linear interpolation between values $v_i \in M$ at the corners of a simplex by the weighted average

$$\Upsilon(v_1, \dots, d_{d+1}; w) := \operatorname*{arg\,min}_{q \in M} \sum_{i=1}^{d+1} w_i \operatorname{dist}(v_i, q)^2, \tag{1}$$

where w are barycentric coordinates on the simplex. Based on this formula a finite element theory could be constructed that was completely covariant, i.e., it did not rely on any embedding or coordinates on M. Numerical tests showed optimal convergence orders for the discretization error.

In this paper we generalize the approach to obtain higher-order geodesic finite element spaces. As p-th order interpolation on a reference element we use

$$\Upsilon^p(v_1, \dots, v_m; \xi) := \operatorname*{arg\,min}_{q \in M} \sum_{i=1}^{m} \varphi_i^p(\xi) \operatorname{dist}(v_i, q)^2, \tag{2}$$

where the m functions φ_i^p are p-th order scalar Lagrangian shape functions, and ξ are coordinates on the reference element. It is easy to see that this produces p-th order Lagrangian interpolation if M is a linear space, and that (1) is a

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special case of (2). We restrict our attention to Lagrangian finite elements in this article, even though other more general interpolation functions can also be used in (2).

The new interpolation rule shares many important properties with the first-order rule (1). In particular, it is infinitely differentiable with respect to its arguments. Also, it is invariant under various symmetries of the domain and M. In particular, it is equivariant under isometries of M. This is an important fact, because it implies, e.g., that an objective continuous model in mechanics will remain objective after discretization. Partly, the proofs for these results carry over verbatim from the first-order case [19].

We use the new interpolation method to construct p-th order geodesic finite element spaces. These are a direct generalization of the standard Lagrangian finite element spaces used for scalar partial differential equations. The geodesic finite element spaces are conforming; no variational crimes are committed. This is particularly advantageous from a theoretical point of view, because many properties of discrete models can be inferred directly from the continuous model. In numerical experiments we observe optimal discretization error rates (Chapter 7). The theoretical analysis of our method is the subject of a separate paper [10].

As in the first-order case the well-posedness of the defining minimization problem (2) is an important but nontrivial question. For the first-order case this question was answered by recognizing the interpolation rule (1) as a special case of the Riemannian center of mass with a positive measure of unit weight, and using the now classic result of Karcher [14]. This approach does not work in the higher-order case, as the interpolation weights $\varphi_i^p(\xi)$ can become negative. To our knowledge, a Riemannian center of mass with a signed measure has never been investigated in the literature. Based on ideas by Groisser [11], we prove well-posedness of the Riemannian center of mass for a signed measure, provided the measure is contained in a small enough ball, and certain curvature bounds are obeyed. From this follows the well-posedness of (2) under similar conditions.

The use of barycentric coordinates in (1) has restricted first-order geodesic finite elements to grids with simplex elements only. With the barycentric coordinates replaced in (2) by the more general Lagrangian shape functions, we can now define geodesic finite elements on any type of reference element that admits a Lagrange basis. We therefore obtain a geodesic finite element theory also for cube and mixed grids.

The availability of higher-order interpolation methods opens the door to a whole new range of geodesic finite element methods. Besides the obvious p-th order Lagrangian methods it becomes now possible to generalize DG and mixed element methods to problems with manifold-valued functions. Also, the theory of hierarchical error estimators [2] relies on higher-order interpolation. With a good error estimation technique, hp-adaptive methods become conceivable. These techniques may become subject of future papers.

Very little can be found in the literature on higher-order discretization for PDEs with values in a nonlinear space. The main obstacle has been the definition of suitable interpolation rules on a nonlinear manifold M. For the first-order case Bartels and Prohl [3] have used an embedding into a Euclidean space for problems in the unit sphere. While this is cheap and simple, it is not known whether generalizations to higher orders show good error behavior. Also, with this method the discrete solution depends on the embedding. This is problematic in cases like $M = \mathrm{SO}(3)$, for example, where it is equally plausible to embed M into the 3×3-matrices or the quaternions.

An alternative approach notes that the interpolation function is needed only at the quadrature points. The values there can be treated as additional variables. In the framework of an iterative solver they are initialized with known values, and only corrections—which live in linear spaces—are ever interpolated. This method was used by Simo and Vu-Quoc [21] to simulate Cosserat rods and by Simo et al. [22] for Cosserat shells. However, as was shown later [6], at least for the rod model the method introduces spurious dependencies of the solution on the initial iterate and the parameters of the path-following mechanism.

A third method singles out a tangent space T_pM of M, and retracts the values v_i onto T_pM using the exponential map. The retracted values are then interpolated on T_pM, and projected back onto M. This approach has been used by Münch [16] and Müller [15] to discretize Cosserat continua with interpolation functions of second order. However, it works only as long as the values v_i stay away from the cut locus of p, and both Münch and Müller have observed problems when dealing with large rotations for this reason. Also, the dependence on a fixed tangent space T_pM breaks objectivity.

While writing this article the author learned of the work of Philipp Grohs [9], who independently came up with the same approach (2) to higher-order interpolation in nonlinear spaces, using splines as interpolation functions. While concentrating on approximating functions of a single variable, he clearly recognized that the resulting interpolation could form the basis of a finite element theory. Even more importantly, his work contains the first rigorous interpolation error estimates.

The idea to use shape functions as the weight functions in a Riemannian center of mass to obtain higher order interpolation also appeared in the work of Buss and Fillmore [5], who used it to construct spline curves on the sphere.

The content of this article is as follows. Chapter 2 formally introduces p-th order geodesic interpolation for functions with values in a Riemannian manifold. We prove well-posedness of this construction in Chapter 3. A variety of useful properties of the interpolation is demonstrated in Chapter 4. The new concept is then used in Chapter 5 to construct geodesic finite element spaces. Chapter 6 discusses various algorithmic aspects of the numerical solution of the algebraic minimization problems. In particular we show how geodesic finite element functions and some of their derivatives can be evaluated. Finally, Chapter 7 gives a numerical example, computing harmonic maps from a domain in $\mathbb{R}^3$ to the unit sphere S^2. We numerically measure the discretization errors for Lagrangian geodesic finite element spaces of up to third order, and observe that they behave optimally.

2 Geodesic Interpolation

The basis of our higher-order finite element method is a generalization of Lagrangian interpolation of arbitrary order to functions that map into a nonlinear manifold M. To motivate our definition we briefly revisit the following generalization of linear interpolation, which was introduced in [19].

Definition 2.1. *Let $\Delta = \{w \in \mathbb{R}^{d+1} \mid w_i \geq 0, \ \sum_{i=1}^{d+1} w_i = 1\}$ be the d-dimensional standard simplex, with barycentric coordinates w. Let M be a connected smooth manifold and* $\operatorname{dist}(\cdot,\cdot) : M \times M \to \mathbb{R}$ *a distance metric on M. For a set of values $v = (v_1, \dots, v_{d+1}) \in M^{d+1}$ at the simplex corners we call*

$$\Upsilon \ : \ M^{d+1} \times \Delta \to M$$
$$\Upsilon(v,w) := \operatorname*{arg\,min}_{q \in M} \sum_{i=1}^{d+1} w_i \operatorname{dist}(v_i, q)^2 \tag{3}$$

simplicial geodesic interpolation on M.

This definition is motivated by the corresponding formula for linear spaces. If $M = \mathbb{R}$, then (3) reduces to

$$\Upsilon(v,w) = \operatorname*{arg\,min}_{q \in \mathbb{R}} \sum_{i=1}^{d+1} w_i |v_i - q|^2,$$

and it is well known that this expression is equivalent to linear interpolation.

We now generalize Definition 2.1 to Lagrangian interpolation of higher order. At the same time, we allow non-simplex reference elements. Let T_{ref} be an open connected domain in $\mathbb{R}^d$, with coordinates ξ. We call T_{ref} a reference element. On its closure $\overline{T_{\text{ref}}}$ we have a set of distinct Lagrange nodes $\nu_i, 1 \leq i \leq m$, and corresponding Lagrangian interpolation functions φ_i^p, i.e., p-th order polynomial functions with $\varphi_i^p(\nu_j) = \delta_{ij}$. We assume that the φ_i^p and ν_i are such that the corresponding interpolation problem is well posed, i.e., for given $v_i \in \mathbb{R}$, $i = 1, \dots, m$ there is a single function $\pi : T_{\text{ref}} \to \mathbb{R}$ in the span of the φ_i^p such that $\pi(\nu_i) = v_i$ for all $1 \leq i \leq m$.

For values v_i in $\mathbb{R}$, p-th order Lagrangian interpolation is given by

$$\Upsilon^p(v,\xi) = \sum_{i=1}^{m} \varphi_i^p(\xi) v_i.$$

To generalize this to values in a manifold M, we write it as a minimization problem in the spirit of (3). This is surprisingly easy; we find that

$$\sum_{i=1}^{m} \varphi_i^p(\xi) v_i = \operatorname*{arg\,min}_{q \in \mathbb{R}} \sum_{i=1}^{m} \varphi_i^p(\xi) |v_i - q|^2.$$

This motivates the following definition, which is visualized in Figure 1.

Definition 2.2. *Let $T_{ref} \subset \mathbb{R}^d$ be open and connected, and M a connected smooth manifold with a distance metric* $\operatorname{dist}(\cdot,\cdot) : M \times M \to \mathbb{R}$. *Let $\{\varphi_1^p, \dots, \varphi_m^p\}$ be a set of p-th order scalar Lagrangian shape functions, and let $v = \{v_1, \dots, v_m\} \subset M$ be values at the corresponding Lagrange nodes. We call*

$$\Upsilon^p \ : \ M^m \times T_{ref} \to M$$
$$\Upsilon^p(v,\xi) := \operatorname*{arg\,min}_{q \in M} \sum_{i=1}^{m} \varphi_i^p(\xi) \operatorname{dist}(v_i, q)^2 \tag{4}$$

p-th order geodesic interpolation on M.

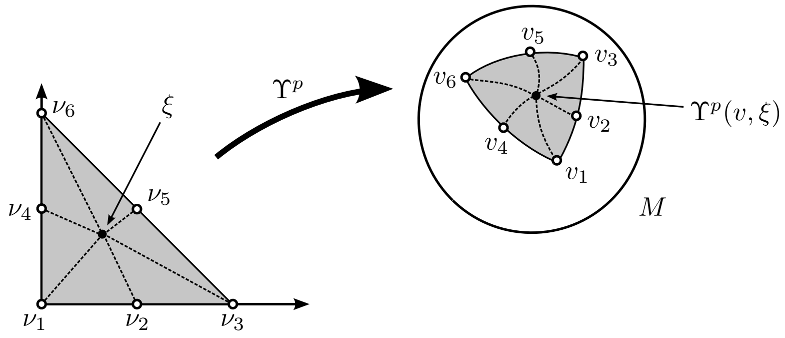

Figure 1: Second-order geodesic interpolation from the reference triangle into a sphere

Remark 2.1. We use Lagrange shape functions mainly for simplicity, and because they are the most common in finite element analysis. In a similar fashion, Grohs [9] and Buss and Fillmore [5] have used splines to achieve higher-order approximation. It is equally possible to build a geodesic finite element theory on spline interpolation functions. This would allow to generalize recent developments like isogeometric analysis.

Obviously, the construction (4) produces an interpolation function of the values v_i. Indeed at the k-th Lagrange node ν_k we get

$$\Upsilon^p(v,\nu_k) = \arg\min_{q\in M} \sum_{i=1}^m \varphi_i^p(\nu_k)\operatorname{dist}(v_i,q)^2 = \arg\min_{q\in M} \operatorname{dist}(v_k,q)^2 = v_k. \tag{5}$$

Also, this definition comprises the previous Definition 2.1 for the first-order case, because we have $w_i(\xi) = \varphi_i^1(\xi)$, $i = 1,\dots,d+1$ for all ξ in the d-dimensional reference simplex. For that reason, we drop the index p from Υ^p for the rest of the article, and use Υ to mean the interpolation function from Definition 2.2 for all orders. Similarly, we write φ_i instead of φ_i^p for a scalar p-th order Lagrangian shape function.

The definition of Υ can be further generalized. As the construction uses only metric information of M, it is possible to define Υ in the more general context of metric spaces. Finite element theories would be difficult, however, without some minimal level of smoothness.

On the other hand, for a Riemannian manifold M it is known that at minimizers $q \in M$ of (3) we have $\sum_{i=1}^{d+1} w_i \exp_q^{-1}(v_i) = 0$. The corresponding formula for the higher order case is

$$\sum_{i=1}^m \varphi_i(\xi)\exp_q^{-1}(v_i) = 0. \tag{6}$$

Using this as the definition of geodesic interpolation allows to define geodesic finite elements for manifolds with metrics that are only pseudo-Riemannian.

Finally, we would like to point out that in [18] it was shown that if M has zero sectional curvature then for each set of coefficients $v_1,\dots,v_{d+1} \in M$ suitably close together there exists a coordinate function $\psi : M \supset U \to \mathbb{R}^{\dim M}$

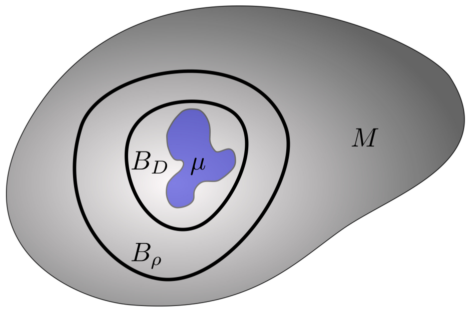

Figure 2: Schematic setting of the well-posedness result. If the support of the measure μ is contained in a ball of radius D, then there is a unique center of mass in a possibly larger concentric ball of radius ρ.

such that

$$\Upsilon^1(v,\xi) = \psi^{-1}\Big(\sum_{i=1}^{d+1} w_i(\xi)\psi(v_i)\Big). \tag{7}$$

An analogous formula holds for the higher-order case.

3 Well-Posedness of the Riemannian Center of Mass with a Signed Measure

Using the Riemannian center of mass for the definition of a function $\Upsilon(v,\cdot) : T_{\text{ref}} \to M$ is only meaningful if the minimizer in (4) is well-defined. However it is not immediately clear from Definition 2.1 whether this is the case. Even for the first-order case examples can be constructed where the minimization problem has either several solutions or no solution at all (see [19, Sec. 2.2]). Some problems can be avoided by requiring that M be connected and complete, which we do for the rest of this article.

Existence and uniqueness of a minimizer can be obtained, however, if the nodal values are "close together" in a certain sense. For the first-order case this follows from a corresponding result by Karcher [14] for the general Riemannian center of mass

$$\mathcal{C}(\mu) = \operatorname*{arg\,min}_{q\in M} \int_M \operatorname{dist}(p,q)^2 \, d\mu(p), \tag{8}$$

with μ a positive measure of unit weight on M. Evidently, the interpolation formula (1) is a special case of this for a discrete measure.

Karcher's existence and uniqueness proof uses the positivity of the interpolation weights. However, while the interpolation weights of (4) still sum up to 1, they may become negative if the polynomial order p is larger than one. The appropriate more general framework for this is the Riemannian center of mass *with a signed measure*, which looks formally like (8), but where μ is now a signed measure, still of weight 1. To our knowledge, except for a brief comment in [14] such a center of mass has never been discussed in the literature.

Karcher's result states that if the support of μ is contained in a certain geodesic ball, then there is a unique center of mass in this ball. This fails to hold for $p \geq 2$ even if M is a linear space. A well-posedness result for signed measures needs to involve two balls, see Figure 2. We will prove the following result, the conditions of which are made precise in Theorem 3.4.

Theorem 3.1. *Let μ be a signed measure on M of weight 1. Let $B_D \subset B_\rho$ be two concentric geodesic balls in M of radii D and ρ, respectively. There are numbers D and ρ such that if the support of μ is contained in B_D, then the Riemannian center of mass*

$$\mathcal{C}(\mu) = \arg\min_{q \in M} \int_M \operatorname{dist}(p, q)^2 \, d\mu(p),$$

has a unique minimizer in B_ρ.

Our proof takes its core ideas from a corresponding proof by Groisser [11] for unsigned measures. Indeed, relatively few generalizations are needed to adapt it to signed measures. We therefore only present a simplified version. Groisser's proof reaches sharper bounds, at the price of being more technical. We believe that his sharper results can also be extended to unsigned measures.

The main idea of the proof is that minimizers of the functional

$$f_\mu(q) := \frac{1}{2} \int \operatorname{dist}(p, q)^2 \, d\mu(p) \tag{9}$$

are zeros of the vector field

$$Y_\mu(q) := \int \exp_q^{-1}(p) \, d\mu(p) \in T_q M. \tag{10}$$

We use a fixed-point argument to show that Y_μ has a unique zero in a ball B_ρ if μ is contained in a possibly smaller concentric ball B_D. Then we use convexity to show that this zero must be a minimizer of f_μ.

Information about μ enters the theorem only in form of the total variation $\|\mu\|$. Recall that by the Jordan decomposition theorem [8], for any finite signed measure μ on M there are unsigned finite measures μ_+, μ_- such that $\mu = \mu_+ - \mu_-$. The total variation is then defined as $\|\mu\| := \mu_+(M) + \mu_-(M)$. Note that $\|\mu\| \geq 1$ if μ has unit weight, with equality holding when the measure is unsigned.

We briefly discuss the importance of the total variation in the context of geodesic interpolation. The connection to discrete measures is given in the following result.

Lemma 3.1. *If μ is a signed discrete measure with weights $\omega_i \in \mathbb{R}$, then $\|\mu\| = \sum_i |\omega_i|$.*

From Theorem 3.4 (the quantitative version of Theorem 3.1) we will see that the bounds on D and ρ get more restrictive if $\|\mu\|$ is increased. If the weights ω_i are given by Lagrange shape functions φ_i, then $\|\mu_\xi\| = \sum_{i=1}^m |\varphi_i(\xi)|$ for any point $\xi \in T_{\text{ref}}$. This value is 1 if ξ is a Lagrange node. Otherwise, for a Lagrange basis with $p \geq 2$, this value may be much higher. The maximum over all $\xi \in T_{\text{ref}}$ turns out to be the Lebesgue constant $\lambda_p = \max_{\xi \in T_{\text{ref}}} \sum_{i=1}^m |\varphi_i^p(\xi)|$ of the Lagrange polynomials. It is well-known that this constant increases with increasing p, and that the speed of the increase depends on the spacing of the

Lagrange nodes. We arrive at the surprising result that the Lebesgue constant not only governs the quality of polynomial interpolation, but also the well-posedness of interpolation in nonlinear spaces.

For practical applications, only the well-posedness of Υ at quadrature points matters. Hence an appropriately chosen quadrature rule may allow to encounter only much better-posed problems than what the Lebesgue constant λ_p would suggest. This topic is left for further research.

Of course, $\|\mu_\xi\| = 1$ if μ_ξ remains a positive measure for all $\xi \in T_{\mathrm{ref}}$. This suggests to investigate geodesic finite element methods with alternative interpolation functions, such as the B-spline functions in [9].

3.1 Fixed Points of Mappings

In this section we state a fixed-point result of Groisser [11] for certain maps generated by vector fields on M. This is the foundation of our well-posedness proof. We start with a few technical preliminaries.

Definition 3.1. *A subset $U \subset M$ is convex if for all $p, q \in U$ there is a unique minimal geodesic segment γ in M from p to q, and γ lies entirely in U.*

For any subset $U \subset M$, let $\Delta(U)$ and $\delta(U)$ denote, respectively, the supremum and the infimum of the sectional curvatures of U.

Definition 3.2 (Hildebrandt [12])**.** *Let $r_{inj}(p_0)$ be the injectivity radius of M at a point p_0. An open ball $B = B_r(p_0)$ with radius r is a regular geodesic ball if $r < r_{inj}(p_0)$ and $r \max(0, \Delta(B))^{1/2} < \pi/2$. For $p_0 \in M$ define the regularity radius*

$$r_{reg}(p_0) := \sup\{\, r \mid B_r(p_0) \text{ is a regular geodesic ball}\}.$$

The fixed-point theorem uses that contractivity of a map $\Psi : M \to M$ can be guaranteed by an upper bound on $\|\Psi_{*p}\|$, where $\Psi_{*p} : T_pM \to T_{\Psi(p)}M$ is the derivative of Ψ at a point $p \in M$. To bound this norm we need two helper functions (see [11, Chap. 2] for details)

$$\phi : [0,\infty) \to \mathbb{R}, \qquad \phi(x) = \cosh(x) - \frac{\sinh(x)}{x}$$

and

$$C : \mathbb{R} \times [0,\infty) \to \mathbb{R}, \qquad C(\lambda, r) = \begin{cases} 1, & \lambda \geq 0, \\ \frac{\sinh(|\lambda|^{1/2} r)}{|\lambda|^{1/2} r}, & \lambda < 0. \end{cases}$$

Note that both are continuous, and that $C(\lambda, r)$ is monotone increasing in each variable.

Lemma 3.2. *The function ϕ is monotonically increasing, convex, and $\phi(0) = 0$.*

The following main fixed-point result is a special case of [11, Thm. 2.8].

Theorem 3.2. *Let $B \subset M$ be a convex ball of radius ρ centered in $p_0 \in M$. Assume that Y is a vector field defined on B, and define $\Psi_Y := \exp \circ Y : B \to M$. Assume further that there are positive constants $\epsilon_0 < r_{inj}(B)$ and ϵ_1 such that at each point of B we have $\|Y\| \leq \epsilon_0$ and $\|\nabla Y + I\| \leq \epsilon_1$. With these constants define*

$$\kappa(\Psi_Y) := \phi\big(\max(|\delta(B)|, |\Delta(B)|)^{1/2}\epsilon_0\big) + C(\delta(B), \epsilon_0)\epsilon_1. \tag{11}$$

1. (Contractivity) *If ϵ_0, ϵ_1 are small enough so that $\kappa(\Psi_Y) < 1$, then $\Psi_Y : B \to M$ is a contraction with constant $\kappa(\Psi_Y)$, and therefore has at most one fixed point in B. Equivalently, the vector field Y has at most one zero in B.*

2. (Self-mapping) *If additionally*

$$\|Y(p_0)\| < (1 - \kappa(\Psi_Y))\rho, \tag{12}$$

then $\Psi_Y : B \to M$ has a unique fixed point. Equivalently, the vector field Y has a unique zero in B.

In the following we will apply this result to the specific map Ψ_μ generated by the vector field Y_μ given by (10).

3.2 Bounds on the Vector Field Y_μ

We first compute the bounds on Y_μ that appear in Theorem 3.2. Assume that the measure μ has its support contained in a ball B_D around a point $p_0 \in M$. We analyze the vector field Y_μ on a concentric ball B_ρ, still assumed to be convex, with $\rho \geq D$ (Figure 2).

Lemma 3.3. *For all $q \in B_\rho$ we have $\|Y_\mu(q)\| \leq \|\mu\|(\rho + D)$. In particular, we have $\|Y_\mu(p_0)\| \leq \|\mu\| D$.*

Proof. By the Jordan decomposition theorem, for any integrable function f we get

$$\Big\| \int f \, d\mu \Big\| \leq \Big(\int d\mu_+ + \int d\mu_- \Big) \sup_{\operatorname{supp} \mu} \|f\| = \|\mu\| \sup_{\operatorname{supp} \mu} \|f\|. \tag{13}$$

Using this and the definition of Y_μ yields

$$\|Y_\mu(q)\| = \Big\| \int \exp_q^{-1}(p) \, d\mu(p) \Big\| \leq \|\mu\| \sup_{p \in B_D} \big\| \exp_q^{-1}(p) \big\|$$

for all $q \in B_\rho$. Since $\|\exp_q^{-1}(p)\| = \operatorname{dist}(p, q)$ this proves the assertions. □

To get a quantitative bound on $\|\nabla Y_\mu + I\|$ we need some curvature information. Define the function

$$h(\lambda, r) := \begin{cases} |\lambda|^{1/2} r \cot(|\lambda|^{1/2} r) & \text{if } \lambda > 0, \\ 1 & \text{if } \lambda = 0, \\ |\lambda|^{1/2} r \coth(|\lambda|^{1/2} r) & \text{if } \lambda < 0, \end{cases}$$

which is monotone decreasing (hence ≤ 1) in $|\lambda|^{1/2} r$ if $\lambda > 0$, while it is monotone increasing in $|\lambda|^{1/2} r$ (hence ≥ 1) if $\lambda < 0$. It is an analytic function of λr^2, with $h(\lambda, r) = \frac{1}{3}\lambda r^2 + O((\lambda r^2)^2)$. Later, λ will be a curvature bound, and r will be a radius.

With the help of the function h define

$$\psi(\lambda, r) := \operatorname{sign}(\lambda)(1 - h(\lambda, r)).$$

For every λ the function $r \mapsto \psi(\lambda, r)$ is nonnegative, monotone increasing on $[0, \pi)$ if $\lambda > 0$ and on $[0, \infty)$ if $\lambda \leq 0$, and $\psi(\lambda, r) = \frac{1}{3}|\lambda| r^2 + O((\lambda r^2)^2)$. For $\delta \leq \Delta \in \mathbb{R}$, $r \geq 0$, and $r < \pi \Delta^{-1/2}$ if $\Delta > 0$, define

$$\psi_{\max}(\delta, \Delta, r) := \max(\psi(\Delta, r), \psi(\delta, r)),$$

and note that

$$\psi_{\max}(\delta, \Delta, r) = \frac{1}{3} K r^2 + O(K^2 r^4),$$

where $K = \max(|\delta|, |\Delta|)$. The following properties of $\psi_{\max}$ are straightforward to see.

Lemma 3.4. *The function ψ_{max} is monotone increasing in Δ and r, and monotone decreasing in δ. It is a convex function in each argument with the other two held fixed.*

The new function $\psi_{\max}$ can be used to bound the difference between $-\nabla Y_\mu$ and the identity.

Lemma 3.5. *Let $p \in B_D, q \in B_\rho$, $D \leq \rho$, and let δ and Δ be lower and upper bounds, respectively, for the sectional curvatures of B_ρ. If $\Delta > 0$ also assume* $\operatorname{dist}(p, q) < \pi \Delta^{-1/2}$. *Then*

$$\|\nabla Y_\mu(q) + I\| \leq \|\mu\| \cdot \psi_{max}(\delta, \Delta, \rho + D)$$

for all $q \in B_\rho$.

Proof. For any function $f : M \to \mathbb{R}$ let $\operatorname{Hess} f$ be the covariant Hessian, and $\operatorname{Hess}' f := g^{-1} \operatorname{Hess}$, with g the metric tensor. From [14, Thm. 1.5] (see also Groisser [11, (4.1)]) and (13) we get

$$\begin{aligned} \|\nabla Y_\mu(q) + I\| &= \left\| \int \left(\operatorname{Hess}' \left(\frac{1}{2} \operatorname{dist}(p, \cdot)^2 \right) \Big|_q - I \right) d\mu(p) \right\| \\ &\leq \|\mu\| \sup_{p \in \operatorname{supp} \mu} \left\| \operatorname{Hess}' \left(\frac{1}{2} \operatorname{dist}(p, \cdot)^2 \right) \Big|_q - I \right\|. \end{aligned}$$

By Groisser [11, (4.7)] we know that $\left\| \operatorname{Hess}' \left(\frac{1}{2} \operatorname{dist}(p, \cdot)^2 \right) \Big|_q - I \right\| < \psi_{\max}(\delta, \Delta, d(p, q))$ under the given assumptions. Since finally $d(p, q) < \rho + D$ under the same assumptions and $\psi_{\max}$ is monotone in its third argument we obtain

$$\|\nabla Y_\mu(q) + I\| \leq \|\mu\| \cdot \psi_{\max}(\delta, \Delta, \rho + D).$$

□

We have now found bounds for $\|Y_\mu\|$ and $\|\nabla Y_\mu + I\|$ which can be used for ϵ_0 and ϵ_1 in Theorem 3.2. Since they primarily depend on the two radii ρ and D we express the quantity κ of (11) in terms of ρ and D.

Definition 3.3. *For $0 \leq D \leq \rho \leq r_{reg}(p_0)$, let $\Delta : [0, \infty)$ be a monotone increasing function such that $\Delta(\rho)$ is an upper bound for the sectional curvatures of $B_\rho(p_0)$. Analogously, let $\delta : [0, \infty)$ be a monotone decreasing function such that $\delta(\rho)$ is a lower bound for the sectional curvatures of $B_\rho(p_0)$. Set $K(\rho) :=$* $\max(|\delta(\rho)|, |\Delta(\rho)|)$, *and define*

$$\begin{aligned} \kappa_\mu(\rho, D) := {} & \phi\big(\|\mu\|(\rho + D) K(\rho)^{1/2}\big) \\ & + C\big(\delta(\rho), \|\mu\|(\rho + D)\big) \|\mu\| \psi_{max}\big(\delta(\rho), \Delta(\rho), \rho + D\big). \end{aligned} \tag{14}$$

Suitable choices for δ and Δ are constant functions, but also sharp curvature-bounding functions if available.

We will need the following properties of κ_μ.

Lemma 3.6. *For each D, the function $\kappa_\mu(\cdot, D)$ is continuous, monotone increasing, and convex.*

Proof. Continuity of κ_μ is evident by continuity of the functions ϕ, C, and $\psi_{\max}$. The function κ_μ is monotone increasing and convex in ρ, because the three terms $\phi\big(\|\mu\|(\rho+D)K(\rho)^{1/2}\big)$, $C\big(\delta(\rho), \|\mu\|(\rho+D)\big)$, and $\psi_{\max}\big(\delta(\rho), \Delta(\rho), \rho+D\big)$ are monotone increasing and convex in ρ. For the first this follows from the monotonicity of K and Lemma 3.2, for the second, directly from the definition of C, and for the third from Lemma 3.4 and the monotonicity properties of $\delta(\rho)$ and $\Delta(\rho)$. □

3.3 Zeros of Y_μ

To show existence of a unique zero of Y_μ in B_ρ we need two things. First we need to show that Ψ_μ is a contraction. By Theorem 3.2 this is the case if $\kappa_\mu(\rho, D) < 1$. Additionally, Ψ_μ has to be a self-map on B_ρ, for which $\|Y_\mu(p_0)\| < (1-\kappa_\mu(\rho, D))\rho$ is a sufficient condition. We show in this section that radii ρ and D can be found such that both properties hold.

For a simpler notation we first define

$$s(\rho, D) := (1-\kappa_\mu(\rho, D))\rho,$$

and investigate some properties of the functions κ_μ and s. The arguments here are all taken from Groisser [11], who gives them for the simpler case $\|\mu\| = 1$.

Define the constants

$$\begin{aligned} D_{\max} &:= \sup\{D \in [0, r_{\mathrm{reg}}(p_0)) \mid \kappa_\mu(D, D) < 1\} \qquad (15)\\ D_{\mathrm{crit}} &:= \sup\{D \in [0, r_{\mathrm{reg}}(p_0)) \mid \exists \rho \in [D, r_{\mathrm{reg}}(p_0)) \text{ for which } s(\rho, D) > \|\mu\|D\}. \end{aligned}$$

Note that $\kappa_\mu(0,0) = 0$, and hence the supremum in (15) is taken over a nonempty set. Since κ_μ is continuous we get $D_{\max} > 0$.

Lemma 3.7. $D_{crit} > 0$.

Proof. From Lemma 3.6 follows that $s(\cdot, D)$ is continuous, and concave. As the product of a concave function with ρ it is also nonconstant on any interval of positive length. Since $\kappa_\mu(\rho, 0) = O(\rho^2)$, $s(\rho, 0) > 0$ for $\rho > 0$ sufficiently small. Hence for each $r_1 < r_{\mathrm{reg}}(p_0)$, the set $J_0 := \{\rho \in [0, r_1] \mid 0 < s(\rho, 0)\}$ is nonempty, and by continuity so is $J_D := \{\rho \in [0, r_1] \mid \|\mu\|D < s(\rho, D)\}$ for sufficiently small positive D. Hence $D_{\mathrm{crit}} > 0$. □

For $0 \le D < D_{\mathrm{crit}}$ we define

$$\begin{aligned} \rho_1(D) &:= \inf\{\rho \in [D, r_{\mathrm{reg}}(p_0)] \mid s(\rho, D) > \|\mu\|D\} \qquad (16)\\ \rho_3(D) &:= \sup\{\rho \in [D, r_{\mathrm{reg}}(p_0)] \mid s(\rho, D) > \|\mu\|D\}, \end{aligned}$$

which will be shown to bound the range of ρ where Ψ_μ is a self-map. Finally, for $0 \le D < D_{\max}$ we define

$$\rho_4(D) := \sup\{\rho \in [D, r_{\mathrm{reg}}(p_0)] \mid \kappa(\rho, D) < 1\}. \qquad (17)$$

This ρ_4 is the upper bound on ρ to ensure contractivity of Ψ_μ. We have to show that bounds ρ_1, ρ_3, ρ_4 exist and are compatible.

Lemma 3.8. *Let $r_1 \in (0, r_{reg}(p_0))$. For each $D \in [0, r_1]$, the set $J_D := \{\rho \in [0, r_1] \mid \|\mu\| D < s(\rho, D)\}$ is an interval with endpoints $\rho_1(D), \rho_3(D)$ if $D < D_{crit}$, and empty otherwise.*

Proof. Let D be fixed. Since $s(\cdot, D)$ is concave and locally nonconstant, it achieves its maximum value $\rho_c(D)$ on $[0, r_1]$ at a unique point. Furthermore, for any $\alpha < \rho_c(D)$ the set $\{\rho \in [0, r_1] \mid s(\rho) > \alpha\}$ is an interval. This holds in particular for each set J_D. If $D > D_{\text{crit}}$ the set J_D is empty by the definition of D_{crit}. □

Lemma 3.9. *For each $D < D_{crit}$ we have $\rho_3(D) < \rho_4(D)$.*

Proof. By the definition of s, the condition $\kappa_\mu(\rho, D) < 1$ is equivalent to $s(\rho, D) > 0$. Since s is concave and has a maximum at $\rho_c \leq \rho_3$ we get $\rho_3(D) < \rho_4(D)$. □

We can now plug everything together and obtain existence of a unique zero of Y_μ in B_ρ if D and ρ are properly chosen.

Theorem 3.3. *Let $0 < r_1 < r_{reg}(p_0)$ and such that $B_{r_1}(p_0)$ is convex. For $0 < \rho \leq r_1$, let $\Delta(\rho)$, $\delta(\rho)$ be upper and lower bounds on the curvature on $B_\rho(p_0)$ as in Definition 3.3, respectively. Let μ be a signed measure of unit weight, with support contained in $B_{r_1}(p_0)$, and define Y_μ by (10). Then the following is true.*

1. *For all $D \in (0, r_1]$, if $\operatorname{supp}\mu \subset B_D$ and $\rho < \rho_4(D)$, then the map $\Psi_\mu : B_\rho(p_0) \to M$ is a contraction with constant $\kappa_\mu(\rho, D) < 1$.*
2. *For all $D \in (0, r_1]$, if $\operatorname{supp}\mu \subset B_D$, $D < D_{crit}$, and $\rho_1(D) < \rho < \rho_3(D)$, then Ψ_μ preserves each ball $B_\rho(p_0)$.*
3. *Under the assumptions of 2, there exists a unique fixed point of Ψ_μ in B_ρ. Consequently, Y_μ has a unique zero in B_ρ.*

Proof. 1. By construction of ρ_4, from the assumption $\rho < \rho_4(D)$ follows that $\kappa_\mu(\rho, D) < 1$. Hence we can use the first part of Theorem 3.2 to conclude that Ψ_μ is a contraction with constant $\kappa_\mu(\rho, D) < 1$. Note that the curvature assumption of Lemma 3.5 holds since B_ρ is a regular ball.

2. Let $D < D_{\text{crit}}$ and ρ such that $\rho_1 < \rho < \rho_3$. Then by construction of ρ_1, ρ_3 and Lemma 3.8 we have $s(\rho, D) > \|\mu\| D$. From this follows

$$(1 - \kappa(\rho, D))\rho = s(\rho, D) > \|\mu\| D \geq \|Y_\mu(p_0)\|,$$

where the last inequality is Lemma 3.3. This is (12), and we can invoke the second part of Theorem 3.2 to obtain the assertion.

3. By Lemma 3.9, if the assumptions of Part 2 are satisfied, we also have $\rho < \rho_4$ and hence contractivity of Ψ_μ. Hence from Theorem 3.2 we obtain existence of a unique fixed point of Ψ_μ in B_ρ, which is a zero of Y_μ by construction.

□

3.4 Minimizers of f_μ

It remains to show that the zero of Y_μ in B_ρ is indeed a minimizer of f_μ. For this we need convexity of f_μ.

The proof of the following result can be found in [11, Lem. 4.1].

Lemma 3.10. *Let $p, q \in M$ with $\operatorname{dist}(p,q) \cdot \max(0,\Delta)^{1/2} < \pi/2$. Then the Hessian $\operatorname{Hess}'\big(\frac{1}{2}\operatorname{dist}(p,\cdot)^2\big)\big|_q$ is positive definite.*

From this, convexity of f_μ on suitably small balls follows immediately if μ is unsigned. For signed μ we need an additional argument.

Lemma 3.11. *Assume that $(\rho + D)\cdot \max(0,\Delta(\rho))^{1/2} < \pi/2$, and that ρ and D are small enough such that $\|\mu\| \cdot \psi_{max}(\delta, \Delta, \rho + D) < 1$. Then $\operatorname{Hess}'(f_\mu)(q)$ is positive definite for all $q \in B_\rho(p_0)$.*

Proof. Let $H := \operatorname{Hess}'(f_\mu)(q)$. From Lemma 3.5 (using $H = -\nabla Y_\mu$) we know that

$$\|H - I\| \le \|\mu\| \cdot \psi_{\max}(\delta, \Delta, \rho + D).$$

Using this, for any $v \in T_qM$ we can estimate

$$\begin{aligned} v^T H v &= v^T I v + v^T (H - I) v \\ &\ge \|v\|^2 - |v^T(H-I)v| \\ &\ge \|v\|^2 - \|v\|^2 \|(H-I)\| \\ &\ge \|v\|^2\big(1 - \|\mu\| \cdot \psi_{\max}(\delta, \Delta, \rho + D)\big). \end{aligned}$$

Hence H is positive definite if $\|\mu\| \cdot \psi_{\max}(\delta, \Delta, \rho + D)$ is less than 1. $\square$

The last step is to show that the curvature bound in Lemma 3.11 can be complied with by a radius ρ that also fulfills the conditions of Theorem 3.3. The proof follows closely the one by Groisser for the case $\|\mu\| = 1$ [11]; we restate it here for completeness.

Lemma 3.12. *For each $D < D_{crit}$ we have*

$$(\rho_4(D) + D) \cdot \max(0, \Delta(\rho_4(D)))^{1/2} < \pi/2.$$

Proof. We prove the assertion in two steps. We claim first that for all $D < D_{\text{crit}}$ we have

$$(\rho_1(D) + D) \cdot \max(0, \Delta(\rho_1(D)))^{1/2} < \pi/2. \tag{18}$$

This is true for $D = 0$, so if it is false for some $D < D_{\text{crit}}$ then there must exist a $D \in (0, D_{\text{crit}})$ for which $\Delta(\rho_1(D)) > 0$ and $(\rho_1(D) + D)\Delta(\rho_1(D))^{1/2} = \pi/2$. Since $\cot\frac{\pi}{2} = 0$, the latter can be transformed to

$$\Delta(\rho_1(D))^{1/2} \cdot (\rho_1(D) + D) \cdot \cot\big[\Delta(\rho_1(D))^{1/2} \cdot (\rho_1(D) + D)\big] = 0,$$

which is just

$$h(\Delta(\rho_1(D)), \rho_1(D) + D) = 0.$$

Since $\Delta(\rho_1(D)) > 1$ we can write this as

$$\operatorname{sign}(\Delta(\rho_1(D))) \cdot \big(1 - h(\Delta(\rho_1(D)), \rho_1(D) + D)\big) = 1,$$

which is

$$\psi(\Delta(\rho_1(D)), \rho_1(D) + D) = 1.$$

Note that from its definition (14) we have

$$\kappa_\mu(\rho, D) \geq \psi_{\max}(\delta(\rho), \Delta(\rho), \rho + D) \geq \psi(\Delta(\rho), \rho + D), \tag{19}$$

and hence $\kappa_\mu(\rho_1(D), D) \geq 1$. Since $D > 0, \Delta > 0$, this inequality is even strict. This leads to a contradiction, since then $s(\rho_1(D), D) < 0$; but from the definition of ρ_1 we have $s(\rho_1(D), D) \geq D$. Hence (18) holds for all $D < D_{\text{crit}}$.

We now extend the result from ρ_1 to ρ_4. Assume that the assertion is false. Then there exists $\rho \in (\rho_1(D), \rho_4(D))$ for which $(\rho+D)\Delta(\rho)^{1/2} = \pi/2$. From (19) we again conclude that $\kappa(\rho, D) > 1$, and since $\rho \geq \rho_1(D) > 0$ this implies the strict inequality $s(\rho, D) < 0$, a contradiction since $\rho \in (0, \rho_4(D))$. This proves the assertion. □

We finally arrive at our main result. It gives existence and uniqueness of the Riemannian center of mass with a signed measure.

Theorem 3.4. *Let $p_0 \in M$, and $r_1 < r_{reg}(p_0)$ a radius such that $B_{r_1}(p_0)$ is convex. For $0 < \rho \leq r_1$ write B_ρ for $B_\rho(p_0)$. Let μ be a signed measure on M of weight 1, and define f_μ by* (9)*. Define the functions ρ_1 and ρ_4 as in* (16) *and* (17)*, respectively. If $D < D_{crit}$ and $\operatorname{supp}\mu \subset B_D$, then f_μ has a unique critical point in B_{ρ_4}, and this critical point lies in $\overline{B_{\rho_1}}$. At the same point, f_μ achieves its minimum value in B_{ρ_4}. Hence μ has exactly one center of mass in B_{ρ_4} if $\operatorname{supp}\mu \subset B_{D_{crit}}$.*

Proof. By Theorem 3.3, the vector field Y_μ has a unique zero in B_ρ for $\rho_1 < \rho < \rho_3$. Since Ψ_μ is a contraction even for $\rho_3 \leq \rho < \rho_4$, this zero is even unique in B_{ρ_4}. By the definition of Y_μ this zero is a critical point of f_μ.

Lemma 3.12 ensures that $(\rho+D)\cdot\max(0, \Delta(\rho))^{1/2} < \pi/2$ is met for all $\rho \leq \rho_4$. Then we can use Lemma 3.11 to show that $\operatorname{Hess}(f_\mu)(p)$ is positive definite for all $p \in B_{\rho_4}(p_0)$. From this follows that f_μ is strictly convex in $B_{\rho_4}(p_0)$. Hence the critical point of f_μ is a minimizer. □

If μ is an unsigned measure, a much stronger result holds for M with nonpositive curvature [19, Cor. 2.1]. We expect this to hold also for the more general signed Riemannian center of mass, but we have no proof.

Conjecture 3.1. *Let M be a complete, simply connected Riemannian manifold with sectional curvatures bounded from above by zero. Then for any signed measure μ on M of unit weight, the functional f_μ defined by* (9) *has a unique minimizer in M.*

4 Properties of the Interpolation

We now discuss various properties of the geodesic interpolation (4). Arguably the most important one for finite element applications is smoothness in ξ and the coefficients v_i.

Theorem 4.1. *Let M be a complete and connected Riemannian manifold, and let $v = \{v_1, \dots, v_m\}$ be coefficients on M with respect to a Lagrange basis $\{\varphi_i\}$ on a domain T_{ref}. Assume that the situation is such that the assumptions of Theorem 3.4 hold. Then the function*

$$\Upsilon(v, \xi) \;:\; M^m \times T_{ref} \to M$$

is infinitely differentiable with respect to the v_i and ξ.

Proof. The proof follows the same argument as the proof for the first-order case in [19]. Namely, using that the squared distance on M is differentiable away from the cut loci ([19, Lem. 2.4]), and that the Hessian of $f_{v,\xi}(\cdot) = \sum_{i=1}^{m} \varphi_i(\xi) \operatorname{dist}(v_i, \cdot)^2$ is positive definite in a sphere of large enough radius (Lemma 3.11), the assertion follows from the implicit function theorem. □

The next property concerns restrictions of geodesic interpolation functions to faces of the reference elements. If the standard Lagrange basis is used, the restricted functions are geodesic interpolation functions in their own right. In Chapter 5 this will be important for the construction of globally continuous finite element functions. We show the result for the reference simplex Δ^d only. The corresponding results for other reference elements can be shown analogously.

Lemma 4.1. *Let $\Delta^d \subset \mathbb{R}^d$ be the d-dimensional reference simplex. On Δ^d consider the p-th order Lagrange shape functions $\{\varphi_i\}$ with respect to the equidistant Lagrange nodes $\{\nu_i\}$. Let δ be a face of the reference simplex Δ^d of any dimension, and let $\Upsilon_v : \Delta^d \to M$ be the geodesic interpolation of the fixed values $v = \{v_1, \dots, v_m\} \subset M$ with the shape functions $\varphi_1, \dots, \varphi_m$. Then its restriction $\Upsilon_v|_\delta$ is also a p-th order geodesic interpolation, namely of the values corresponding to Lagrange nodes on δ.*

Proof. It is well known that only the Lagrange shape functions pertaining to Lagrange nodes on δ are nonzero there. Moreover, they form a p-th order Lagrange basis (in particular a partition of unity) on δ. Hence

$$\Upsilon_v|_\delta(\xi) = \operatorname*{arg\,min}_{q \in M} \sum_{\substack{i=1 \\ \nu_i \in \delta}}^{m} \varphi_i(\xi)|_\delta \operatorname{dist}(v_i, q)^2$$

is a p-th order geodesic interpolation between the values $\{v_i \in v \mid v_i \in \delta\}$. □

Polynomial functions are nested in the sense that p-th order polynomial interpolation of a q-th order polynomial yields the original polynomial if $p \geq q$. One may ask whether the same holds for the interpolating functions Υ. If M has zero curvature then the affirmative result follows directly from the representation formula (7). In the general case we can only prove nestedness for $d = 1$ and $q = 1$. This means that a p-th order interpolating function in one variable is a geodesic if its nodal values v_i are placed on a geodesic (cf. [5]). Numerical experiments suggest that this result is optimal, i.e., geodesic interpolation functions are not nested if $d > 1$ and/or $q > 1$.

Lemma 4.2 (Nestedness). *Let $\Upsilon^1(v^1, \cdot) : [0, 1] \to M$ be a first-order geodesic interpolation function between two values $v_1^1, v_2^1 \in M$. Correspondingly, let*

$\Upsilon^p(v^p, \cdot) : [0,1] \to M$ be a p-th order geodesic interpolation function of values $v_1^p, \dots, v_{p+1}^p$. We assume that Υ^p interpolates Υ^1 in the sense that

$$v_i^p = \Upsilon^p(v^p, \nu_i^p) = \Upsilon^1(v^1, \nu_i^p) \tag{20}$$

for all Lagrange nodes $\nu_i^p \in [0,1]$ of Υ^p. Then

$$\Upsilon^p(v^p, \xi) = \Upsilon^1(v^1, \xi) \qquad \text{for all } \xi \in [0,1].$$

Proof. Pick any $\xi \in [0,1]$, and set $x := \Upsilon^1(v^1, \xi) \in M$. By (6) we have

$$\sum_{i=1}^{2} \varphi_i^1(\xi) \exp_x^{-1}(v_i^1) = 0. \tag{21}$$

Consider normal coordinates $\phi : U \to \mathbb{R}^{\dim M}$ on a neighborhood U around x that includes v_1^1 and v_2^1. In these coordinates, (21) reads

$$\sum_{i=1}^{2} \varphi_i^1(\xi)\phi(v_i^1) = 0. \tag{22}$$

We call the left hand side $c(\cdot) := \sum_{i=1}^{2} \varphi_i^1(\cdot)\phi(v_i^1)$ and view it as a function $[0,1] \to \mathbb{R}^{\dim M}$. It is linear and connects the two points $\phi(v_1^1)$ and $\phi(v_1^2)$. On the other hand, by [19, Lem. 2.2] the function $\Upsilon^1(v^1, \cdot)$ is a geodesic, and therefore c is the coordinate representation of Υ^1

$$c(\zeta) = \phi(\Upsilon^1(\zeta)) \qquad \forall\, \zeta \in [0,1]. \tag{23}$$

By the nestedness of polynomials there is a representation of c in the p-th order Lagrangian basis $\{\varphi_i^p\}$

$$c(\zeta) = c^p(\zeta) := \sum_{i=1}^{p+1} \varphi_i^p(\zeta)(c(\nu_i^p)) \qquad \forall\, \zeta \in [0,1].$$

But by (23) and (20) we have $c(\nu_i^p) = \phi(v_i^p)$, and hence from (22) we get

$$c^p(\xi) = \sum_{i=1}^{p+1} \varphi_i^p(\xi)\phi(v_i^p) = 0.$$

This is equivalent to $\sum_{i=1}^{p+1} \varphi_i^p(\xi) \exp_x^{-1}(v_i^p) = 0$, and since that zero is unique we have $x = \Upsilon^p(v^p, \xi)$. □

Geodesic interpolation enjoys various symmetry properties expected from a finite element interpolation procedure. We distinguish symmetry under transformations of the domain T_{ref}, and symmetry under transformation of the codomain M. For finite element applications the first symmetry implies that for a given element T of a grid it is irrelevant which affine transformation from T onto the reference element is used for the assembly of the stiffness matrix on T. The crucial second one means that invariances of a continuous model (such as frame invariance in mechanics) are not lost by discretization.

We first show symmetry under transformations of the domain. We do this separately for simplices and cubes. For other more exotic reference elements the proofs are similar. For simplicity we also only consider the standard Lagrangian shape functions on equidistant grids.

Lemma 4.3. *Let Δ be a d-dimensional simplex, and $\{\nu_i\}$ the set of uniformly spaced Lagrange nodes on Δ, for the corresponding p-th order Lagrange interpolation functions $\{\varphi_i\}$. Let S be the group of symmetries of Δ (the* symmetric group*). S acts on sets of coefficients $v = \{v_1, \dots, v_m\} \subset M$ by permutations, and on Δ by coordinate transformations. For any set of coefficients $v = \{v_1, \dots, v_m\}$, $s \in S$, and $\xi \in \Delta$ we have*

$$\Upsilon(s(v), s(\xi)) = \Upsilon(v, \xi).$$

Proof. We use barycentric coordinates $w \in \mathbb{R}^{d+1}$ on Δ. Then the regularly spaced Lagrange nodes can be indexed by a multi-index $\alpha = (\alpha_1, \dots, \alpha_{d+1})$. More concretely, for a Lagrange node ν_l we write ν_α if $w(\nu_l) = (\alpha_1/p, \dots, \alpha_{d+1}/p)$, where $w(\nu_l)$ are the barycentric coordinates of ν_l. Analogously, we label shape functions φ_α and nodal values v_α. Note that $|\alpha| := \sum_{i=1}^{d+1} \alpha_i = p$ for all multi-indices corresponding to a Lagrange node.

The symmetry group S is generated by reflections at planes perpendicularly bisecting the simplex edges [13], and in barycentric coordinates these reflections correspond to transpositions of axes. We label the generators s_{ij}, and show invariance of Υ under these generators. A generator s_{ij} acts on a multi-index α by exchanging α_i and α_j. It acts on the coefficient sets by $s_{ij}(v_\alpha) = v_{s_{ij}(\alpha)}$, on barycentric coordinates w by exchanging w_i and w_j, and on points $\xi \in \Delta$ by $s_{ij}(\xi) = \xi(s_{ij}(w(\xi)))$, where $w(\xi)$ are the barycentric coordinates of ξ, and $\xi(\cdot)$ the local coordinates on Δ of the argument. To see how s_{ij} acts on the simplex shape functions we write them as [23]

$$\varphi_l(\xi) = \prod_{k=1}^{d+1} \prod_{j=1}^{I_{k,l}} \big[p w_k(\xi) - j + 1\big]/j,$$

where

$$I_{k,l} := p w_k(\nu_l) \in \mathbb{N}.$$

It follows that $\varphi_\alpha(s_{ij}(\xi)) = \varphi_{s_{ij}(\alpha)}(\xi)$. Hence for any $\xi \in \Delta$

$$\begin{aligned}
\Upsilon(s_{ij}(v), s_{ij}(\xi)) &= \arg\min_{q \in M} \sum_{|\alpha|=p} \varphi_\alpha(s_{ij}(\xi)) \operatorname{dist}(s_{ij}(v_\alpha), q)^2 \\
&= \arg\min_{q \in M} \sum_{|\alpha|=p} \varphi_{s_{ij}(\alpha)}(\xi) \operatorname{dist}(v_{s_{ij}(\alpha)}, q)^2 \\
&= \Upsilon(v, \xi).
\end{aligned}$$

□

We show the same result for cube reference elements.

Lemma 4.4. *Let $\square = [-1, 1]^d$ be a d-dimensional cube, and $\{\nu_i\}$ the set of uniformly spaced Lagrange nodes on $\square$, for the corresponding p-th order Lagrange interpolation functions $\{\varphi_i\}$. Let B be the group of symmetries of $\square$ (the* hyperoctahedral group*). B acts on sets of coefficients $v = \{v_1, \dots, v_m\} \subset M$ by permutations, and on $\square$ by coordinate transformations. For any set of coefficients $v = \{v_1, \dots, v_m\}$, $b \in B$, and $\xi \in \square$ we have*

$$\Upsilon(b(v), b(\xi)) = \Upsilon(v, \xi).$$

Proof. The hyperoctahedral group B is the semidirect product of the group of reflections at the coordinate planes, and the group of permutations of the axes [13]. It is therefore sufficient to show invariance under transposition of axes and reflections at coordinate planes. Let again $\alpha = (\alpha_1, \dots, \alpha_d)$, $1 \leq \alpha_i \leq p+1$, be a multi-index and use it to label shape functions and values in the natural way.

A transposition of axes b_{ij} acts on φ_α and v_α by swapping the corresponding indices in α, and on $\xi \in \square$ by swapping the coordinate entries. Since Lagrange shape functions on cubes are constructed as tensor products

$$\varphi_\alpha(\xi) = \theta_{\alpha_1}(\xi_1) \cdot \ldots \cdot \theta_{\alpha_d}(\xi_d)$$

of one-dimensional p-th order Lagrange shape functions θ_i, we see that $\varphi_\alpha(b_{ij}(\xi)) = \varphi_{b_{ij}(\alpha)}(\xi)$. Hence

$$\begin{aligned} \Upsilon(b_{ij}(v), b_{ij}(\xi)) &= \operatorname*{arg\,min}_{q \in M} \sum_\alpha \varphi_\alpha(b_{ij}(\xi)) \operatorname{dist}(b_{ij}(v_\alpha), q)^2 \\ &= \operatorname*{arg\,min}_{q \in M} \sum_\alpha \varphi_{b_{ij}(\alpha)}(\xi) \operatorname{dist}(v_{b_{ij}(\alpha)}, q)^2 \\ &= \Upsilon(v, \xi). \end{aligned} \tag{24}$$

A reflection r_i at a plane normal to axis i acts on ξ by replacing the i-th coordinate ξ_i with $-\xi_i$, and on α by replacing α_i with $(p+2) - \alpha_i$. Since for one-dimensional Lagrange shape functions functions θ on $[-1, 1]$ on a uniform partition we have $\theta_i(\xi_i) = \theta_{p+2-i}(-\xi_i)$ the invariance of Υ under reflections at axes follows. Together with (24) we get the assertion for any $b \in B$. □

The second important symmetry of geodesic interpolation is equivariance of the interpolation under isometries of M. In mechanics, where usually $M = \mathbb{R}^3$ and the corresponding isometries are the special Euclidean group $\mathbb{R}^3 \rtimes \mathrm{SO}(3)$, this property is known as frame-invariance or objectivity.

Lemma 4.5. *Let M be a Riemannian manifold and G a group that acts on M by isometries. Let $v_1, \dots, v_m \in M$ be such that the assumptions of Theorem 3.4 hold. Then*

$$Q\Upsilon^p(v_1, \dots, v_m; \xi) = \Upsilon^p(Qv_1, \dots, Qv_m; \xi)$$

for all $\xi \in T_{ref}$, $Q \in G$, and interpolation orders p.

As geodesic interpolation is defined using metric quantities only, this result is straightforward. We therefore omit the proof and refer the reader to the corresponding proof for the first-order case given in [19, Lem. 2.6], which can be adapted easily. We point out, however, that Lemma 4.5 is very general, and in particular not restricted to Lagrangian interpolation on equidistant nodes.

5 Geodesic Finite Elements

In this section we use the interpolation method presented above to construct global finite element spaces. These spaces are conforming in the sense that they are subsets of $H^1(\Omega, M)$, and we discuss the relationship between geodesic finite element functions and coefficient vectors. The important equivariance result of the previous section (Lemma 4.5) extends naturally to global geodesic finite element functions.

Let Ω be an open bounded subset of $\mathbb{R}^d$, $d \geq 1$. For simplicity we assume that Ω has a polygonal boundary. Let $\mathcal{G}$ be a conforming grid for Ω with elements of arbitrary type. We denote by $x_i \in \Omega$, $i = 1, \dots, n$ the union of the sets of Lagrange nodes of the individual elements.

Definition 5.1*a* (Geodesic Finite Elements)**.** *Let $\mathcal{G}$ be a conforming grid on Ω, and let M be a Riemannian manifold. We call $v_h : \Omega \to M$ a p-th order geodesic finite element function if it is continuous, and if for each element $T \in \mathcal{G}$ the restriction $v_h|_T$ is a p-th order geodesic interpolation in the sense that*

$$v_h|_T(x) = \Upsilon\big(v_{T,1}, \dots, v_{T,m}; \mathcal{F}_T(x)\big),$$

where $\mathcal{F}_T : T \to T_{ref}$ is affine or multilinear, T_{ref} is the reference element corresponding to T, and the $v_{T,i}$ are values in M. The space of all such functions v_h will be denoted by $V^M_{p,h}$.

For completeness we also define geodesic finite elements for $p = 0$. These are not directly a special case of Definition 5.1a, because they are not continuous. Note, however, that $\Upsilon = \Upsilon^p$ does produce constant functions when $p = 0$.

Definition 5.1*b*. *Let $\mathcal{G}$ be a grid on Ω, and let M be a Riemannian manifold. We call $v_h : \Omega \to M$ a 0-th order geodesic finite element function if it is constant on each element of $\mathcal{G}$.*

Remark 5.1. For simplicity we assume an identical polynomial order p for all grid elements. An extension of the construction to locally varying order (as needed, e.g., for *hp*-refinement) is straightforward.

Definitions 5.1a and 5.1b obviously form a generalization of the first-order geodesic finite elements proposed in [19]. Setting $M = \mathbb{R}$ we also recover the definition of standard p-th order Lagrangian finite elements. On the other hand, the well-posedness of Definition 5.1a is again unclear, as we inherit the corresponding well-posedness problems from the definition of geodesic interpolation (4). We will see below, when we discuss the relationship between geodesic finite element functions and coefficient vectors, that the spaces $V^M_{p,h}$ do contain sufficiently many functions for finite element analysis.

We begin our investigations by showing that geodesic finite element functions are conforming. We first introduce Sobolev spaces for manifold-valued functions (see, e.g., [20]).

Definition 5.2. *Let M be a Riemannian manifold isometrically embedded in $\mathbb{R}^k$ for some $k \in \mathbb{N}$. Then*

$$H^l(\Omega, M) := \{v \in H^l(\Omega, \mathbb{R}^k) \mid v(x) \in M \text{ a.e.}\}$$

is called the l-th order Sobolev space for functions with values in M.

It is now easy to show that geodesic finite element functions are indeed Sobolev functions in the sense of this definition.

Theorem 5.1. *$V^M_{p,h}(\Omega) \subset H^1(\Omega, M)$ for all $p \geq 1$.*

As in the first-order case this is proved by embedding M into a suitable Euclidean space, and using that a function is in H^1 if it is continuous and piecewise C^1. See [19] for details.

The classical linear finite element method distinguishes the discrete problem, which deals with finite element functions, from the algebraic problem, which deals with vectors of coefficients. The latter is used to implement numerical algorithms. Both formulations are equivalent, because a classical finite element function uniquely corresponds to a coefficient vector once a basis of the finite element space has been chosen. In the simplest case the basis is the nodal basis and the coefficients are the function values at the Lagrange nodes.

The distinction between discrete and algebraic formulations persists in the theory of geodesic finite elements. However, the relationship between geodesic finite element functions $v_h \in V_{p,h}^M$ and sets of coefficients $\bar{v} \in M^n$ is more subtle. Since any $v_h \in V_{p,h}^M$, $p \geq 1$, is continuous we can associate to it the coefficient set consisting of the values of v_h at the Lagrange nodes. However, given a set of coefficients $\bar{v} \in M^n$ it is not clear whether there is a corresponding geodesic finite element function, and whether this function is unique, if there is one. The difficulty stems mainly from the corresponding problem for geodesic interpolation, but it is also not obvious whether individual geodesic interpolation functions can be stitched together continuously.

To formally investigate the relationship between geodesic finite element functions and sets of coefficients we define the nodal evaluation operator

$$\begin{aligned} \mathcal{E}_p \;:\; V_{p,h}^M &\to M^n \\ (\mathcal{E}_p(v_h))_i &= v_h(x_i), \qquad x_i \text{ the } i\text{-th Lagrange node of } \mathcal{G}. \end{aligned}$$

To each geodesic finite element function $v_h \in V_{p,h}^M$ it associates the set of function values at the Lagrange nodes. Since functions in $V_{p,h}^M$ are continuous for all $p \geq 1$ the operator $\mathcal{E}_p$ is well-defined and single-valued for all $v_h \in V_{p,h}^M$.

We are now interested in the inverse operator $\mathcal{E}_p^{-1}$, which associates geodesic finite element functions to a given set of coefficients. For arbitrary $\bar{v} \in M^n$ it may be multi-valued. Using Theorem 3.4 the sets of coefficients for which $\mathcal{E}_p^{-1}$ is single-valued can be characterized in principle. However, unlike in the first-order case, the bounds ρ, D in Theorem 3.4 depend on the interpolation weights. Therefore it does not directly follow from this theorem that for fixed values $v_1, \dots, v_m$ the interpolation function $\Upsilon(v, \cdot) : T_{\text{ref}} \to M$ is well-defined on all of T_{ref}. The gap is filled by the following lemma.

Lemma 5.1. *Let $v_1, \dots, v_m$ be a set of values in M, and let $B_D(p_0)$ be a regular convex geodesic ball in M of radius D and center p_0 such that $v_i \in B_D(p_0)$ for all $i = 1, \dots, m$. For a point $\xi \in T_{ref}$ let μ_ξ be the signed measure on M with $\mu_\xi(\{v_i\}) = \varphi_i(\xi)$ and $\mu_\xi(M \setminus \{v_1, \dots, v_m\}) = 0$. Let $D_{crit,\xi} \in \mathbb{R}$ be the value D_{crit} of Theorem 3.4 for the measure μ_ξ. If $D < D_{crit,T} := \inf_{\xi \in T_{ref}} D_{crit,\xi}$ then $\Upsilon(v, \cdot) : T_{ref} \to M$ is a well-defined function.*

The proof of this is evident, but it is important to note that $D_{\text{crit},T}$ is positive by Lemma 3.7, compactness of T_{ref} and continuity of $D_{\text{crit},\xi}$ with respect to ξ. However, note again that for practical applications only well-posedness of Υ at quadrature points is relevant.

Lemma 5.2. *Let $\mathcal{G}$ be a grid, and let $\bar{v} \in M^n$ be a set of coefficients with respect to the standard scalar p-th order Lagrange basis on $\mathcal{G}$. If for each element T of $\mathcal{G}$ with associated coefficients $\bar{v}_{T,1}, \dots, \bar{v}_{T,m}$ there exists an open geodesic ball B_D of radius $D < D_{crit,T}$ (with $D_{crit,T}$ defined in Lemma 5.1) such that $\bar{v}_{T,i} \in B_D$ for each $i = 1, \dots, m$, then there is a unique function $v_h \in V_{p,h}^M$ with $v_h = \mathcal{E}^{-1}(\bar{v})$.*

Proof. For each $x \in \Omega$ let T be an element of $\mathcal{G}$ with $x \in T$ and nodal values $\bar{v}_{T,i}$, $i = 1, \dots, m$. Set $\mathcal{F}_T$ an affine mapping from T onto the corresponding reference element and define the function $v_h : \Omega \to M$ by

$$v_h(x) = \Upsilon(\bar{v}_{T,1}, \dots, \bar{v}_{T,m}; \mathcal{F}_T(x)).$$

By the assumptions on the grid and the coefficients we can invoke Lemma 5.1 to get that v_h is single-valued on each T. By Lemmas 4.3 and 4.4 it is independent of the choice of $\mathcal{F}_T$. By (5), v_h is an interpolation of the nodal values $\bar{v}$, i.e., we have that $\mathcal{E}(v_h) = \bar{v}$. Finally, by Lemma 4.1, v_h varies continuously between adjacent elements. Hence $v_h \in V_{p,h}^M$. □

In Chapter 3 we have conjectured that Υ is well-defined without restrictions if M is a space of nonpositive curvature (Conjecture 3.1). A direct consequence would be the following result.

Conjecture 5.1. *Let M be complete, simply connected, and have nonpositive sectional curvatures. Then $\mathcal{E}_p : V_{p,h}^M \to M^n$ is a bijection.*

For general M, the unique correspondence between geodesic finite element functions and sets of coefficients can still be obtained, but only in the following asymptotic sense.

Theorem 5.2. *Let M be a Riemannian manifold, and let $v : \Omega \to M$ be Lipschitz continuous in the sense that there exists a constant L such that*

$$\operatorname{dist}(v(x), v(y)) \leq L\|x - y\|$$

for all $x, y \in \Omega$. Let $\mathcal{G}$ be a grid of Ω and h the length of the longest edge of $\mathcal{G}$. Set $\bar{v} = \mathcal{E}_p(v)$, tacitly extending the definition of $\mathcal{E}_p$ to all continuous functions $\Omega \to M$. For h small enough, the inverse of $\mathcal{E}_p$ has only a single value in $V_{p,h}^M$ for each $\tilde{v} \in M^n$ in a neighborhood of $\bar{v}$.

Proof. Let T be an element of $\mathcal{G}$ with Lagrange nodes $x_{T,1}, \dots, x_{T,m} \in \overline{\Omega}$, and let $v_{T,1}, \dots, v_{T,m} \in M$ be the values of v at these nodes. For any pair $v_{T,i}$, $v_{T,j}$ we have

$$\operatorname{dist}(v_{T,i}, v_{T,j}) \leq L\|x_{T,i} - x_{T,j}\| \leq Lh,$$

and hence the $v_{T,i}$ are contained in a single open geodesic ball B of radius $D < Lh$. If h is small enough such that the radius is less than $D_{\text{crit},T}$ then we can use Lemma 5.2 to conclude that there is a unique function $v_h \in V_{p,h}^M$ with $\mathcal{E}(v_h) = \bar{v}$. Since B is open we can even perturb the $v_{T,i}$ without leaving B. Hence for h small enough, the inverse of $\mathcal{E}_p$ has only a single value in $V_{p,h}^M$ for each $\tilde{v} \in M^n$ in a neighborhood of $\bar{v}$. □

This result implies that for a given problem with a Lipschitz-continuous solution we can always find a grid fine enough such that we can disregard the distinction between $V_{p,h}^M$ and M^n in the vicinity of the solution. Hence locally a geodesic finite element problem can be represented by a corresponding algebraic problem on the product manifold M^n. In numerical experiments, this requirement of locality does not appear to pose a serious obstacle.

Remark 5.2. Locally around functions where Theorem 5.2 applies, the function space $V_{p,h}^M$ inherits the differentiable manifold structure of M^n, because functions defined by geodesic interpolation depend differentiably on their corner values (Theorem 4.1). The global geometric structure of the spaces $V_{p,h}^M$ is unclear.

We close the chapter showing equivariance of geodesic finite elements under isometries of M. This is a central result of geodesic finite element theory, because it implies that the invariance of a continuous model under isometries will not be lost by discretization. In mechanics, e.g., it allows for discrete problem formulations that are exactly frame-indifferent. The proof is trivial with the help of Lemma 4.5, which is in turn straightforward since the definition of $V_{p,h}^M$ relies on metric properties of M exclusively.

Theorem 5.3. *Let M be a Riemannian manifold and G a group that acts on M by isometries. Let $V_{p,h}^M$ be a geodesic finite element space for n nodal values on a domain Ω. Extend the action of G to M^n by setting*

$$(Q\bar{v})_i = Q\bar{v}_i \qquad \forall \bar{v} \in M^n, \quad i = 1, \dots, n,$$

and to $V_{p,h}^M$ by setting

$$(Qv_h)(x) = Q(v_h(x)) \qquad \forall v_h \in V_{p,h}^M, \quad x \in \Omega.$$

Then

$$\mathcal{E}_p(Qv_h) = Q\mathcal{E}_p(v_h)$$

for all $Q \in G$ and $v_h \in V_{p,h}^M$, whenever these expressions are well defined.

6 Minimization Problems in Geodesic Finite Element Spaces

We will now use geodesic finite elements to solve partial differential equations for functions in $H^1(\Omega, M)$. We restrict our attention to time-independent PDEs that have a minimization formulation. That is, we assume that there is an energy functional

$$\mathcal{J} : H^1(\Omega, M) \to \mathbb{R}$$

such that the (stable) problem solutions are minimizers of $\mathcal{J}$ subject to suitable boundary conditions. For simplicity we consider Dirichlet boundary conditions only. More formally, our continuous problem is then to find a function $u \in H^1(\Omega, M)$ such that

$$\mathcal{J}(u) \le \mathcal{J}(v) \tag{25}$$

for all v in a neighborhood of u in $H^1(\Omega, M) \cap \{v \mid v|_{\partial\Omega} = u_D\}$, and

$$u = u_D \qquad \text{on } \partial\Omega, \tag{26}$$

with $u_D : \partial\Omega \to M$ sufficiently smooth. We assume that this problem is well-posed in the sense that at least local minimizers exist.

6.1 Discrete and Algebraic Minimization Problems

Remember that Ω is polygonally bounded and let $\mathcal{G}$ be a conforming grid of Ω. Stating the discrete problem corresponding to (25)–(26) is straightforward, since we have shown in Theorem 5.1 that the geodesic finite element space $V_{p,h}^M$ is a subspace of $H^1(\Omega, M)$. Consequently, the energy functional $\mathcal{J}$ is well-defined on $V_{p,h}^M$. We can formulate a discrete version of Problem (25)–(26) by restricting the ansatz space to $V_{p,h}^M$. The discrete problem then reads: Find a function $u_h \in V_{p,h}^M(\Omega)$ such that

$$\mathcal{J}(u_h) \le \mathcal{J}(v_h) \tag{27}$$

for all v_h in a neighborhood $U \subset V_{p,h}^M \cap \{v_h \mid v_h|_{\partial\Omega} = u_{h,D}\}$ of u_h, and with

$$u_h = u_{h,D} \qquad \text{on } \partial\Omega,$$

where $u_{h,D}$ is a suitable approximation of the Dirichlet data u_D.

For a numerical treatment of (27) we need the corresponding algebraic formulation. Let u be a solution of the continuous problem (25) and assume that it is Lipschitz continuous. By Theorem 5.2 there is a number $h_0 > 0$ and a neighborhood V of $\mathcal{E}_p(u)$ in M^n such that for all coefficient sets $\bar{v} \in V$ there is a unique discrete function $\mathcal{E}_p^{-1}(\bar{v}) \in V_{p,h}^M$ if the maximum grid edge length is less than h_0. We assume that $\mathcal{E}_p(u_h) \in V$, which allows us to formulate the algebraic minimization problem corresponding to (27): Find $\bar{u} \in M^n$ such that

$$\mathcal{J}(\mathcal{E}_p^{-1}(\bar{u})) \le \mathcal{J}(\mathcal{E}_p^{-1}(\bar{v})) \tag{28}$$

for all $\bar{v} \in M^n$ such that $\bar{v} \in \mathcal{E}_p(U) \cap V$, and subject to the boundary conditions

$$\bar{u}_i = (\mathcal{E}_p(u_{h,D}))_i \qquad \text{for all Lagrange nodes } x_i \text{ on } \partial\Omega.$$

For simplicity of notation we define the algebraic energy functional

$$J : M^n \to \mathbb{R}, \qquad J(\bar{v}) := \mathcal{J}(\mathcal{E}_p^{-1}\bar{v}).$$

With this functional we can rewrite the algebraic problem (28) as: Find $\bar{u} \in M^n$ such that

$$J(\bar{u}) \le J(\bar{v}) \tag{29}$$

for all $\bar{v}$ from the same space as for (28), and subject to the boundary conditions

$$\bar{u}_i = (\mathcal{E}_p(u_{h,D}))_i$$

for all Lagrange nodes x_i on $\partial\Omega$.

6.2 Numerical Evaluation of Geodesic Finite Elements

The algorithmic treatment of geodesic finite element problems needs particular attention, because the finite element functions can only be evaluated numerically (unless M has zero curvature, see (7)). Higher derivatives in particular can be challenging.

For the rest of this article we restrict our attention to energy functionals of the form

$$\mathcal{J}(v) = \int_\Omega W(\nabla v(x), v(x), x)\, dx, \qquad v \in H^1(\Omega, M),$$

where W is a scalar energy density assumed to be as smooth as necessary. These functionals are important in many applications. For a given grid $\mathcal{G}$ the corresponding algebraic energy is

$$J(\bar{v}) = \int_\Omega W\big(\nabla(\mathcal{E}_p^{-1}(\bar{v}))(x), (\mathcal{E}_p^{-1}(\bar{v}))(x), x\big)\, dx, \qquad \bar{v} \in M^n. \tag{30}$$

To compute this energy numerically for a given function $v_h = \mathcal{E}_p^{-1}(\bar{v}) \in V_{p,h}^M$ we have to evaluate geodesic finite element function values $v_h(x)$ and derivatives $\nabla v_h(x)$ at (quadrature) points x in Ω. For the minimization of J by Newton-type methods we further need to evaluate first and second derivatives of J with respect to the coefficients $\bar{v}$. By the chain rule, this in turn requires derivatives of $v_h(x)$ and $\nabla v_h(x)$ with respect to the finite element coefficients. In principle, these derivatives can all be evaluated algorithmically. Unfortunately, for higher derivatives the expressions get fairly unwieldy. We work out the expressions needed for the first derivatives of J in this section. In our numerical example the Hessian of J has been approximated by finite differences.

Remark 6.1. Just as for linear finite elements it is sufficient to compute the relevant quantities on a reference element. The real values and derivatives on an element T can then be obtained by concatenating with $\mathcal{F}_T : T \to T_{\text{ref}}$ or its derivative. For first-order geodesic finite elements this is worked out in more detail in [19].

The formulas we obtain are very similar to the formulas for the first-order case. Again, all information about the manifold M enters only in form of different derivatives of the squared distance function $\operatorname{dist}(\cdot,\cdot)^2 : M \times M \to \mathbb{R}$. We will need the following expressions, which are the same as for the first-order case:

$$\frac{\partial}{\partial q}\operatorname{dist}(p,q)^2, \qquad \frac{\partial^2}{\partial p \partial q}\operatorname{dist}(p,q)^2, \qquad \frac{\partial^2}{\partial q^2}\operatorname{dist}(p,q)^2,$$
$$\frac{\partial^3}{\partial p \partial q^2}\operatorname{dist}(p,q)^2, \qquad \frac{\partial^3}{\partial q^3}\operatorname{dist}(p,q)^2.$$

For $M = S^k$ (the unit sphere in $\mathbb{R}^{k+1}$) these have been worked out in the appendix of [19]. For the hyperbolic half-space H^k they appear in [10].

6.2.1 Evaluation of Function Values

Let T_{ref} be a reference element, and $v_T : T_{\text{ref}} \to M$ a geodesic interpolation function. We denote its values at the m Lagrange nodes by $\bar{v}_T = \{v_{T,1}, \dots, v_{T,m}\}$. For a given $\xi \in T_{\text{ref}}$ we want to compute $v_T(\xi) \in M$. By construction of v_T, the value $v_T(\xi)$ is given by

$$v_T(\xi) = \Upsilon_{\bar{v}_T}(\xi) = \operatorname*{arg\,min}_{q \in M} f_{\bar{v}_T,\xi}(q), \qquad f_{\bar{v}_T,\xi}(\cdot) := \sum_{i=1}^m \varphi_i(\xi)\operatorname{dist}(v_{T,i},\cdot)^2. \tag{31}$$

In general the minimization problem (31) can only be solved numerically. Under the assumptions of Lemma 5.1, $f_{\bar{v}_T,\xi}$ is C^∞ [19, Lem. 2.4], and strictly convex on an open geodesic ball containing the $v_{T,i}$ (Lemma 3.11). We use a Riemannian trust-region method as presented in [1] to minimize $f_{\bar{v}_T,\xi}$. With k

the trust-region iteration number let $q_k \in M$ be the current iterate. We use the exponential map $\exp_{q_k} : T_{q_k}M \to M$ to define lifted functionals

$$\hat{f}_k \;:\; T_{q_k}M \to \mathbb{R}$$
$$\hat{f}_k(s) := \sum_{i=1}^{m} \varphi_i(\xi) \operatorname{dist}(v_{T,i}, \exp_{q_k} s)^2,$$

and corresponding quadratic models

$$m_k(s) = \hat{f}_k(0) + g_{q_k}(\nabla \hat{f}_k(0), s) + \frac{1}{2} g_{q_k}(\operatorname{Hess} \hat{f}_k(0)s, s),$$

where g_{q_k} is the Riemannian metric of M at q_k. This model is then minimized under a norm constraint $\|s\| \le \rho_k$, using, e.g., a preconditioned truncated conjugate gradient method as described in [1].

Using $\nabla \exp 0 = I$ we see that the gradient of $\hat{f}_k$ at $0 \in T_{q_k}M$ is

$$\nabla \hat{f}_k(0) = \sum_{i=1}^{m} \varphi_i(\xi) \frac{\partial}{\partial q} \operatorname{dist}(v_{T,i}, q)^2,$$

and that the Hessian is

$$\operatorname{Hess} \hat{f}_k(0) = \sum_{i=1}^{m} \varphi_i(\xi) \frac{\partial^2}{\partial q^2} \operatorname{dist}(v_{T,i}, q)^2.$$

Hence the derivatives $\frac{\partial}{\partial q} \operatorname{dist}(v_{T,i}, q)^2$ and $\frac{\partial^2}{\partial q^2} \operatorname{dist}(v_{T,i}, q)^2$ need to be available for a given manifold M to be able to evaluate geodesic finite element functions.

Remark 6.2. Note that the number of variables in the minimization problem (31) depends on the dimension of M, but not on the polynomial order.

6.2.2 Evaluation of Gradients

Next we compute derivatives of a geodesic finite element function with respect to ξ. In an abuse of vocabulary we call them gradients, because they generalize the gradient of linear finite elements. Let again $v_T : T_{\text{ref}} \to M$ be a geodesic interpolation function with nodal values $\bar{v}_T = \{v_{T,1}, \dots, v_{T,m}\}$, and let $\xi \in T_{\text{ref}}$. The derivative of v_T at ξ is a linear map

$$\nabla v_T(\xi) \;:\; T_\xi T_{\text{ref}} \to T_{v_T(\xi)}M,$$

which exists by Theorem 4.1, and which can be computed using the implicit function theorem. Recall the definition of geodesic interpolation on T_{ref} as the minimization problem (31). By [19, Lem. 2.4] the functional $f_{\bar{v}_T,\xi}$ is smooth, and the minimizer can hence also be characterized by

$$F\big(\bar{v}_T, \xi, \Upsilon(\bar{v}_T, \xi)\big) = 0, \tag{32}$$

where

$$F \;:\; M^m \times T_{\text{ref}} \times M \to TM$$
$$F(\bar{v}_T, \xi, q) = \frac{\partial}{\partial q} f_{\bar{v}_t,\xi}(q) = \sum_{i=1}^{m} \varphi_i(\xi) \frac{\partial}{\partial q} \operatorname{dist}(v_{T,i}, q)^2, \tag{33}$$

which is just another way of writing (6). Taking the total derivative of (32) with respect to ξ we get

$$\frac{\mathrm{d}}{\mathrm{d}\xi} F(\bar{v}_T, \xi, \Upsilon(\bar{v}_T, \xi)) = \frac{\partial F(\bar{v}_T, \xi, q)}{\partial \xi} + \frac{\partial F(\bar{v}_T, \xi, q)}{\partial q} \cdot \frac{\partial \Upsilon(\bar{v}_T, \xi)}{\partial \xi} = 0.$$

By Lemma 3.11 the matrix

$$\frac{\partial F}{\partial q} = \operatorname{Hess} f_{\bar{v}_T, \xi} \tag{34}$$

is invertible, and hence $\partial v_T(\xi)/\partial \xi = \partial \Upsilon(\bar{v}_T, \xi)/\partial \xi$ can be computed as the solution of the linear system of equations

$$\frac{\partial F(\bar{v}_T, \xi, q)}{\partial q} \cdot \frac{\partial \Upsilon(\bar{v}_T, \xi)}{\partial \xi} = -\frac{\partial F(\bar{v}_T, \xi, q)}{\partial \xi}. \tag{35}$$

Using the definition (33) we see that in coordinates $\partial F/\partial \xi$ is a $(\dim M) \times d$-matrix with entries

$$\Big(\frac{\partial F}{\partial \xi}\Big)_{ij} = \sum_{k=1}^{m} \frac{\partial \varphi_k(\xi)}{\partial \xi_j} \frac{\partial}{\partial q_i} \operatorname{dist}(v_{T,k}, q)^2.$$

Hence evaluating the gradient of a geodesic interpolation function v_T amounts to an evaluation of its value $v_T(\xi)$ (to know where to evaluate the derivatives of F) and the solution of the symmetric linear system (35).

6.2.3 Derivatives of Values with Respect to Coefficients

Let $v_T : T_{\mathrm{ref}} \to M$ be a function given by geodesic interpolation, $\bar{v}_T = \{v_{T,1}, \dots, v_{T,m}\}$ its coefficients, and let $\xi \in T_{\mathrm{ref}}$ be arbitrary but fixed coordinates. We now want to compute the derivatives

$$\frac{\partial}{\partial v_{T,i}} v_T(\xi) = \frac{\partial}{\partial v_{T,i}} \Upsilon(v_{T,1}, \dots, v_{T,m}; \xi)$$

for all $i = 1, \dots, m$. For each i, the derivative is a linear map from $T_{v_{T,i}}M$ to $T_{v_T(\xi)}M$. By definition of Υ we have

$$F\big(\bar{v}_T,\ \xi,\ \Upsilon(\bar{v}_T, \xi)\big) = 0,$$

the function F again given by (33). Taking the total derivative of this with respect to a $v_{T,i}$, $i = 1, \dots, m$, gives

$$\frac{\mathrm{d}F}{\mathrm{d}v_{T,i}} = \frac{\partial F}{\partial v_{T,i}} + \frac{\partial F}{\partial q} \cdot \frac{\partial \Upsilon(\bar{v}_T, \xi)}{\partial v_{T,i}} = 0,$$

with

$$\frac{\partial F}{\partial v_{T,i}} = \varphi_i(\xi) \frac{\partial}{\partial v_{T,i}} \frac{\partial}{\partial q} \operatorname{dist}(v_{T,i}, q)^2$$

and $\partial F/\partial q$ as in (34). By Lemma 3.11 the matrix $\partial F/\partial q$ is invertible. Hence the derivative of $\Upsilon(\bar{v}_T, \xi)$ with respect to one of the coefficients $v_{T,i}$ can be computed as a minimization problem to obtain the value $\Upsilon(\bar{v}_T, \xi)$, and the solution of the linear system of equations

$$\frac{\partial F}{\partial q} \cdot \frac{\partial \Upsilon(\bar{v}_T, \xi)}{\partial v_{T,i}} = -\frac{\partial F}{\partial v_{T,i}}.$$

6.2.4 Derivatives of the Gradient with Respect to Coefficients

Let v_T be a geodesic interpolation function with nodal values $\bar{v}_T = \{v_{T,1}, \dots, v_{T,m}\}$ on a reference element T_{ref}. Its gradient at a $\xi \in T_{\text{ref}}$ as computed in Section 6.2.2 is $\nabla v_T(\xi) : T_\xi T_{\text{ref}} \to T_{v_T(\xi)} M$. This map depends implicitly on the coefficients $v_{T,i}$, and for each $i = 1, \dots, m$ we want to compute the derivative $\frac{\partial}{\partial v_{T,i}} \nabla v_T(\xi)$. Note that since $\nabla v_T(\xi)$ is a linear map, its derivative is a trilinear form, with three indices if written in coordinates. To compute it we use the same technique as previously, but applied on top of the result of Section 6.2.2.

Let v_T^* be one of the coefficients $v_{T,1}, \dots, v_{T,m}$. To compute the derivative of ∇v_T with respect to v_T^* we take the total derivative of expression (35) with respect to v_T^* and obtain

$$\frac{\partial F}{\partial q} \cdot \frac{\partial^2 \Upsilon}{\partial v_T^* \, \partial \xi} = -\frac{\partial^2 F}{\partial v_T^* \, \partial q} \cdot \frac{\partial \Upsilon}{\partial \xi} - \frac{\partial \Upsilon}{\partial v_T^*} \cdot \frac{\partial^2 F}{\partial q^2} \cdot \frac{\partial \Upsilon}{\partial \xi} - \frac{\partial^2 F}{\partial v_T^* \, \partial \xi} - \frac{\partial \Upsilon}{\partial v_T^*} \cdot \frac{\partial^2 F}{\partial q \, \partial \xi}. \tag{36}$$

In coordinates (and using the Einstein convention), this is

$$\frac{\partial F_j}{\partial q_l} \frac{\partial^2 \Upsilon_l}{\partial (v_T^*)_i \, \partial \xi_k} = -\frac{\partial^2 F_j}{\partial (v_T^*)_i \, \partial q_l} \frac{\partial \Upsilon_l}{\partial \xi_k} - \frac{\partial \Upsilon_l}{\partial (v_T^*)_i} \left[\frac{\partial^2 F_j}{\partial q^2}\right]_{lm} \frac{\partial \Upsilon_m}{\partial \xi_k} - \frac{\partial^2 F_j}{\partial (v_T^*)_i \, \partial \xi_k} - \frac{\partial \Upsilon_l}{\partial (v_T^*)_i} \frac{\partial^2 F_j}{\partial q_l \, \partial \xi_k}.$$

This time we need to compute the value of $v_T(\xi)$, solve a linear system for $\partial \Upsilon / \partial \xi$, and then solve the linear system (36) to obtain the desired value of $\partial^2 \Upsilon / \partial v_T^* \partial \xi$. Various new derivatives of F appear. These are

$$\begin{aligned}
\frac{\partial^2 F_j}{\partial (v_T^*)_i \, \partial \xi_k} &= \frac{\partial \varphi_*}{\partial \xi_k} \frac{\partial}{\partial (v_T^*)_i} \frac{\partial}{\partial q_j} \operatorname{dist}(v_T^*, q)^2, \\
\frac{\partial^2 F_j}{\partial (v_T^*)_i \, \partial q_k} &= \varphi_* \frac{\partial}{\partial (v_T^*)_i} \left[\frac{\partial^2}{\partial q^2} \operatorname{dist}(v_T^*, q)^2\right]_{jk}, \\
\left[\frac{\partial^2 F_j}{\partial q^2}\right]_{ik} &= \sum_{l=1}^m \varphi_l \left[\frac{\partial^3}{\partial q^3} \operatorname{dist}(v_{T,l}, q)^2\right]_{ijk}, \\
\frac{\partial^2 F_j}{\partial q_i \, \partial \xi_k} &= \sum_{l=1}^m \frac{\partial \varphi_l}{\partial \xi_k} \cdot \left[\frac{\partial^2}{\partial q^2} \operatorname{dist}(v_{T,l}, q)^2\right]_{ij}.
\end{aligned}$$

Note that these are all third-order objects. To implement the geodesic finite element method for a particular manifold M, these quantities need to be available.

7 Example: Harmonic Maps in Liquid Crystals

We close this article showing numerically that the higher-order interpolation functions introduced here really lead to higher convergence orders of the discretization error. In [19] it was already shown with a numerical example that

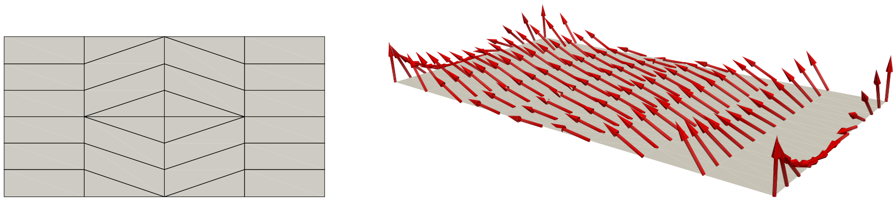

Figure 3: Example problem. Left: coarse grid. Right: solution field

the convergence order of the discretization error is optimal in the first-order case. Now we show the same for higher orders.

As in [19] we want to look for minimizers of the harmonic energy for maps into the sphere. Let Ω be a domain in $\mathbb{R}^d$ and $M = S^2$ the unit sphere in $\mathbb{R}^3$. We solve the Dirichlet problem

$$\text{minimize} \quad \mathcal{J}(v) = \int_\Omega |\nabla v|^2 \, dx \qquad \text{in } H^1(\Omega, S^2) \tag{37}$$

subject to

$$v = v_D \qquad \text{on } \partial\Omega,$$

with v_D a given set of boundary conditions. This is a standard model for equilibrium states of nematic liquid crystals, known as the one-constant approximation [7]. Solutions of this are harmonic maps.

As coordinates on the unit sphere S^2 we use the canonical embedding into $\mathbb{R}^3$ (see the appendix of [19] for details). With the metric on S^2 induced by the embedding we obtain the coordinate representation

$$|\nabla v|^2 = \sum_{i=1}^{d} \sum_{\alpha=1}^{3} \Big(\frac{\partial v^\alpha}{\partial x^i} \Big)^2,$$

that is, ∇v is a $3 \times d$-matrix and $|\cdot|$ the Frobenius norm.

Unlike [19] we solve a problem on a two-dimensional domain. This is strictly for simplicity, and our discretization can also be used in three dimensions. As the domain Ω we choose the rectangle $\Omega = [-2, 2] \times [-1, 1]$, which we discretize by a mixed grid $\mathcal{G}_0$ consisting of 35 vertices, 20 quadrilaterals, and 4 triangles (Figure 3, left). This is to emphasize that geodesic finite elements are not restricted to simplex grids.

We want to test geodesic finite elements of up to third order. Optimal convergence can only be expected if the continuous solution is sufficiently smooth. To construct a problem with sufficient regularity we first define $R_x(\alpha)$ and $R_y(\alpha)$ as the 3×3 rotation matrices of an angle α around the x- and y-axes, respectively. Then, with $\zeta \in [0, 1]^2$ the local coordinates on Ω we define

$$v_D = R_y(0.5\pi \sin(\pi\zeta_1)) \cdot R_x(0.5\pi \sin(\pi\zeta_2)) e_3,$$

where $e_3 = (0, 0, 1)$ is the third canonical basis vector. Figure 3, right, shows a numerical solution of (37) with these boundary conditions.

We use the Riemannian trust-region method introduced by Absil et al. [1] together with the inner monotone multigrid solver described in [19] to solve the

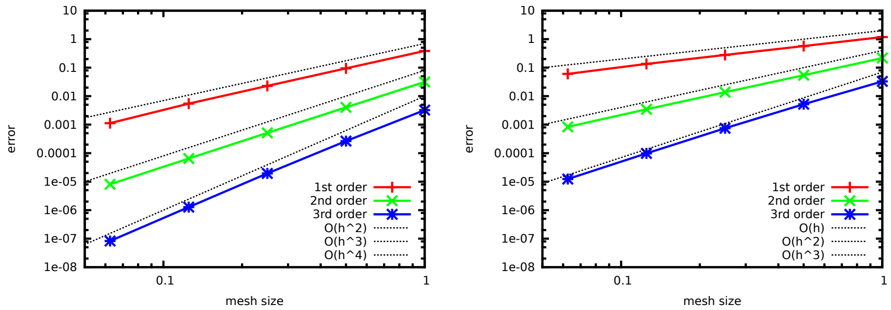

Figure 4: Discretization error as a function of normalized grid edge length. Left: error in the L^2-norm. Right: error in the H^1-seminorm

algebraic minimization problem (29) with the energy from (37). The gradient of the energy functional in (37) in the geodesic finite element space $V_{p,h}^{S^2}$ is computed analytically using the formulas of Chapter 6, whereas its Hessian is approximated by a finite difference method. The discretization and solution algorithms are implemented in C++ using the DUNE libraries [4].

We cover the cases $p = 1, 2, 3$. To estimate the discretization error we compute reference solutions $\hat{v}_p$ on a grid $\mathcal{G}_5$ obtained from $\mathcal{G}_0$ by five steps of uniform refinement. The solver is set to iterate until machine precision is reached. We then compute solutions v_p^k, $k = 0, \dots, 4$, $p = 1, 2, 3$ on grids $\mathcal{G}_k$ obtained from $\mathcal{G}_0$ by k steps of uniform refinement, and compute the errors

$$e_p^k = \|\mathcal{E}^{-1}(v_p^k) - \mathcal{E}^{-1}(\hat{v}_p)\|, \qquad k = 0, \dots, 4, \qquad p = 1, 2, 3$$

where $\|\cdot\|$ is either the norm in $L^2(\Omega, \mathbb{R}^3)$, or the seminorm in $H^1(\Omega, \mathbb{R}^3)$. Note that since geodesic finite element functions are not piecewise polynomials in $\mathbb{R}^3$, the norms can only be computed with an additional error due to numerical quadrature.

Figure 4 shows the errors e_p^k as functions of the normalized mesh size h. We see that for p-th order finite elements the L^2-error decreases like h^{p+1}, and the H^1-error decreases like h^p. Hence we can reproduce the optimal convergence behavior well-known from the linear theory even in this nonlinear case. A rigorous proof of this is subject of a forthcoming paper [10].

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