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A kernel class allowing for fast computations in shape spaces induced by diffeomorphisms

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ABSTRACT

Reproducing kernel Hilbert spaces play an important role in diffeomorphic matching of shapes and in which they intervene in the construction of Riemannian metrics on diffeomorphisms and shape spaces. In such contexts, they are directly involved in the expressions of geodesic equations, and in their numerical solutions via particle evolutions. Solving such equations, however, involves computing kernel sums over irregular grids which can be a big computational overhead if the number of particles is large. In this paper we introduce and establish properties of a finitely generated kernel class in which the kernel is defined using a double interpolation from a discrete kernel supported by a regular grid covering the domain of the system of particles under consideration. It not only speeds up the calculations by utilizing standard algorithms for faster computations over regular grids, but also maintains the exactness and consistency of the system. We provide experimental results in support of this, comparing in particular the computation time and accuracy to similar competing methods.

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1. Introduction

Because they make possible the analysis of complex nonlinear models within a convenient Hilbertian context, reproducing kernels, and their associated Hilbert spaces, provide a powerful framework that has found multiple applications in many domains, including approximation theory, probability, statistics, machine learning, or computer graphics. They also play an essential role in diffeomorphic shape analysis, which is our field of interest here, for which they provide elegant constructions of Riemannian metrics on diffeomorphisms and shape spaces, and constitute primary building components for the numerical solution of geodesic equations, parallel transport, optimal registration and other specific issues in this context. These operations are very naturally implemented as particle evolutions, and for large-scale problems (in which particles correspond, for example, to vertices of densely discretized triangulated surfaces), they require repeated evaluations of massive kernel sums, which induce a substantial computational burden. We address this issue in the present paper by selecting reproducing kernels for which the induced sums have controllable computational cost, while making sure that the most important theoretical requirements of the analysis remain satisfied. We will for this purpose use a class of discretely generated kernels, which induce a computational cost that remains linear in the number of particles.

Our test-bed algorithm will be the *Large Deformation Diffeomorphic Metric Matching* (LDDMM), in the context of surface registration. Several versions of LDDMM have been introduced for matching curves, surfaces and images in 2D and 3D. The surface case has been introduced in [1,2] and has become an important component of the computational anatomy toolkit. One of the main operations in computational anatomy, as introduced in [3], is the registration of anatomical structures via geodesic deformations on groups of diffeomorphisms. This consists in finding a time-dependent deformation of minimal

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energy (in the sense of a Riemannian metric defined on the diffeomorphism group) that transports (or almost transports) a template anatomy onto an observed one. The evolution in this context is driven by a geodesic equation (called EPDiff), which, in the case of objects represented as point sets (like triangulated surfaces) reduces to a high dimensional system of ordinary differential equations (ODEs). We will measure the impact of using our kernel class on the solution of the variational problem that consists in optimizing the initial conditions of the EPDiff equations to ensure that their solution at time 1 approaches the object of interest.

The EPDiff equation is a Hamiltonian form of the geodesic equation on diffeomorphisms. In d dimensions, its definition involves a positive kernel $(x, y) \mapsto K_V(x, y)$, which, in full generality, takes values in the set of d by d matrices, satisfying $K_V(y, x) = K_V(x, y)^T$ and, for all pairwise distinct $z_1, \dots, z_n \in \mathbb{R}^d$ and all $\beta_1, \dots, \beta_n \in \mathbb{R}^d$,

$$\sum_{i,j=1}^{n} \beta_i^T K_V(z_i, z_j)\beta_j \geq 0,$$

the above sum vanishing if and only if all β_j's are zero. EPDiff describes the time evolution of a point set, $x(t) = (x_i(t), i = 1, \dots, N)$, with $x_i(t) \in \mathbb{R}^d$, together with corresponding *momenta*, $\alpha(t) = (\alpha_1(t), \dots, \alpha_N(t))$, with $\alpha_i(t) \in \mathbb{R}^d$, and takes the following form:

$$\begin{cases} \partial_t x_k(t) = \displaystyle\sum_{l=1}^{N} K_V(x_k(t), x_l(t))\alpha_l(t) \\ \partial_t \alpha_k(t) = -\displaystyle\sum_{l=1}^{N} \sum_{i,j=1}^{d} \alpha_{k,i}(t)\alpha_{l,j}(t)\nabla_1 K_V^{i,j}(x_k(t), x_l(t)) \end{cases} \tag{1}$$

where $\alpha_{k,j}$ is the jth coordinate of α_k, $K_V^{i,j}$ is the (i, j) entry of K_V and ∇_1 denotes the gradient with respect to the first component.

Here, the kernel K_V generates a Hilbert space of vector fields on $\mathbb{R}^d$, according to the standard construction that completes the space of finite sums

$$V^0 = \left\{ v(.) = \sum_{k=1}^{n} K_V(\cdot, z_k)\beta_k, z_1, \dots, z_n, \beta_1, \dots, \beta_n \in \mathbb{R}^d, n \geq 0 \right\}$$

into a Hilbert space V for the norm:

$$\left\| \sum_{k=1}^{n} K_V(\cdot, z_k)\beta_k \right\|_V^2 = \sum_{k,l=1}^{n} \beta_k^T K_V(z_k, z_l)\beta_l.$$

In particular, the evolving sequence of points and momenta $(x_k,\ \alpha_k,\ k = 1, \dots, N)$ generated by (1) induces a time-dependent vector field $v(t, \cdot)$ defined by

$$v(t, x) = \sum_{k=1}^{N} K_V(x, x_k(t))\alpha_k(t). \tag{2}$$

This also defines a flow of diffeomorphisms, $\varphi(t, \cdot)$, via

$$\partial_t \varphi(t, x) = v(t, \varphi(t, x)) \tag{3}$$

(i.e., φ is the flow associated to the ODE $\partial_t y = v(t, y)$). One can also notice that the first equation in (1) is equivalent to $x_k(t) = \varphi(t, x_k(0))$, which says that the particles follow the flow of diffeomorphisms that they induce. Moreover, the path $t \mapsto \varphi(t, \cdot)$ in the group of diffeomorphisms is a geodesic for the right-invariant Riemannian metric on this group defined by

$$\|w\|_\varphi = \|w \circ \varphi^{-1}\|_V, \tag{4}$$

which implies that $\varphi(t, \cdot)$ minimizes

$$E_0(v) = \int_0^1 \|v(t, \cdot)\|_V^2 dt$$

subject to the constraint (3), with fixed boundary conditions at $t = 0$ and $t = 1$ (with $\varphi(0, \cdot) = \mathrm{id}_{\mathbb{R}^d}$). In particular, $E_0(v)$ for v given by (2) is the square of the Riemannian distance between $\mathrm{id}_{\mathbb{R}^d}$ and $\varphi(1, \cdot)$ for this metric.

Although the most general construction for reproducing kernels on spaces of vector fields involves matrix-valued kernels (as considered above), we will make in the following the simplifying assumption that K_V is derived from a scalar kernel, so that

$$K_V(x, y) = \tilde{K}_V(x, y)\mathrm{Id}_{\mathbb{R}^d}$$