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Out-of-sample extension of band-limited functions on homogeneous manifolds using diffusion maps

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ABSTRACT

In this paper, we address the problem of function extension when the available data lies on a homogeneous manifold (i.e. the domain of the function is a homogeneous manifold embedded in the Euclidean space) and the function is band-limited. We solve this problem in the general case in which the manifold is unknown. We assume that we have sufficient labeled data to reconstruct the function from labeled data. We also assume that we have enough data (at least exponential in the intrinsic dimension of the manifold) to approximate the Laplace–Beltrami operator on the manifold. The proposed method has a closed form solution and consists of matrix multiplication and inversion. As the size of data approaches infinity, the proposed method converges to the optimal solution as long as the function values are known on an appropriate sampling set. Simulation results demonstrate the advantage of the proposed method over commonly used function extension methods.

1. Introduction

Supervised learning is a machine learning task of inferring a function from labeled training data [1]. The type of data and properties of the function are application dependent. One of the most basic supervised learning problem in the field of signal processing is sampling and reconstruction of a band-limited function. When the data points are real numbers and the function is band-limited, the classical Nyquist theorem [2] states that the function can be perfectly reconstructed from its values on equally spaced points of reals, if the sampling rate is sufficiently high. The values of the function on points other than sampling points can be exactly calculated using SINC interpolator. Schoenberg [3] used cardinal splines for the reconstruction formula. There, it is shown that a band-limited function can be reconstructed from its values sampled at high enough rate (Nyquist rate) as accurately as needed using cardinal splines of sufficiently high degree. This result was further generalized to the case of nonuniform sampling by Lyubarskii and Madych [4]. More specifically, they showed that a band-limited function $f(x)$, whose Fourier transform is compactly supported between $[-\pi,\pi]$ can be completely reconstructed using spline functions, from its samples $f(x_n)$ taken at sampling points x_n, in the case when the functions $\exp(jx_n\omega)$, form a Riesz basis for $L_2([-\pi,\pi])$.

Pesenson [5] generalized the concept of band-limited functions to the case that the domain of the function is a homogeneous manifold and introduced the spectral entire functions of exponential type and Lagrangian splines on homogeneous manifolds. He also showed that on manifolds, the reconstruction of irregularly sampled spectral entire functions of exponential type (from now on band-limited functions) by splines is possible, as long as the distance between points of a sampling sequence is small enough.

Recently, using a different point of view, Coifman and Lafon [6] proposed a simple scheme, based on the Nyström

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method for supervised learning and extending empirical functions defined on a set X to a larger set $\overline{X}$. The extension process involves the construction of a specific family of functions termed geometric harmonics. These functions constitute a generalization of the prolate spheroidal wave functions of Slepian in the sense that they are optimally concentrated on X. Although being a powerful tool for function extension, this scheme does not make use of unlabeled data to improve the approximation of the Laplace–Beltrami operator on the manifold.

Supervised learning can be also regarded as the problem of function extension. The central dogma for studying the problem of function extension on manifolds is that the distribution of natural data is non-uniform and concentrates around low-dimensional structures. The shape (geometry) of the distribution can be exploited for efficient learning. As a justification for manifold assumption of natural data, see Jansen and Niyogi [7] for speech signals and Donoho and Grimes [8] for images. Geometrically derived methods have been used in applications such as image clustering [9,10], image completion [11], speech enhancement in presence of transient noise [12], voice activity detection in presence of transient noise [13], linear and nonlinear independent component analysis [14,15], parametrization of linear systems [16], and single channel source localization [17].

Zhu et al. [18] introduced an approach for supervised learning which is based on a Gaussian random field model. Labeled and unlabeled data were represented as vertices in a weighted graph, with edge weights encoding the similarity between instances. The learning problem was then formulated in terms of a Gaussian random field on this graph, where the mean of the field was characterized in terms of harmonic functions, and was efficiently obtained using matrix methods or belief propagation. In [19], it is shown that this method becomes ill posed as the number of unlabeled points tends to infinity. This observation was the motivation for Zhou and Belkin [20] to address the semi-supervised learning problem and propose a solution by using regularization based on an iterated Laplacian, which is equivalent to a higher order Sobolev semi-norm. Their proposed solution can alternatively be viewed as a generalization of the thin plate spline to an unknown submanifold in high dimensions.

In most practical applications, besides the function, the data manifold is also unknown and just some labeled data (the points that the value of function is known on them, i.e. sampling points) and unlabeled data (the points that the value of function on them must be determined, i.e. interpolation points) are available. This means that the sampling theorem on manifolds [5] cannot be utilized directly to learn and extend the function to unlabeled data because in [5], the manifold is assumed to be known.

In order to be able to use a sampling theorem on manifolds, one needs to completely know the manifold. This means that the Laplace–Beltrami operator on the manifold must be known and can be computed for every function. Many manifold learning algorithms have been introduced during the last decade, among them one can name isomap [21], Locally-linear embedding (LLE) [22], Laplacian eigenmaps [23] and diffusion maps [24]. Diffusion maps leverage the relationship between heat diffusion and a random walk on a graph. The heat diffusion on manifold, is the diffusion process whose infinitesimal generator is the Laplace–Beltrami operator. In [24], an analogy is drawn between the diffusion operator on a manifold and a Markov transition matrix operating on functions defined on the graph whose nodes were sampled from the manifold. It is also shown that one can approximate the Laplace–Beltrami operator using appropriately normalized Markov transition matrix.

In this paper, we propose a novel technique for supervised learning when the data is assumed to be located on a manifold. More specifically, we use diffusion maps as a tool for manifold learning and approximating the Laplace–Beltrami operator on a manifold. Next, we use sampling theorem of band-limited functions on manifolds [5] to extend the function onto the interpolation points. The solution coincides with the method proposed in [20], hence gives another justification for the method presented in [20]. This paper is organized as follows. In Section 2, we formulate the problem and introduce our function extension algorithm. In Section 3, we evaluate the performance of our method and compare it to several available function extension methods. We also discuss some applications of the proposed method. We conclude the paper in Section 4.

2. Problem formulation

Let $\mathcal{M}$ be a C^∞-homogeneous manifold and Δ be the Laplace–Beltrami operator in the corresponding Hilbert space $L^2(\mathcal{M})$. We say that a function $f(\cdot)$ from $L^2(\mathcal{M})$ is ω_0-band-limited if the function satisfies the Bernstein inequality [5]:

$$\|\Delta^{k/2} f\| \le \omega_0^k \|f\| \tag{1}$$

for every natural even k, where $\|f\|$ denotes $L^2(\mathcal{M})$ norm. Using Parseval's theorem, it can be easily verified that in the special case where $\mathcal{M} = \mathbb{R}$, this definition is equivalent to the definition of band-limited functions (i.e. the Fourier transform is compactly supported in $[-\omega_0, \omega_0]$).

A set of points $Z_\lambda = \{\boldsymbol{x}_\gamma\}$, is called a sampling sequence if

(a) $\inf_{\gamma \ne \mu} \operatorname{dist}(\boldsymbol{x}_\gamma, \boldsymbol{x}_\mu) > 0$,
(b) Balls $B(\boldsymbol{x}_\gamma, \lambda)$ form a cover of $\mathcal{M}$, and
(c) $\lambda < (c_0 \omega_0)^{-1}$,

where c_0 is a manifold-dependent constant. In the case $\mathcal{M} = \mathbb{R}$, the last condition becomes the Nyquist sampling condition if the sampling is uniform. It can be shown [5] that any ω_0-band-limited function can be exactly reconstructed from its samples as long as the value of the function is known on a sampling sequence.

In [5], it is shown that given an ω_0-band-limited function $f(\cdot)$ on a d-dimensional manifold $\mathcal{M}$, $\epsilon > 0$ and a sampling sequence Z_λ, there exists a function $\hat{f}^k$ such that

$$\|f - \hat{f}^k\| < \epsilon; \quad k = 2^l d, \quad l \in \mathbb{N} \tag{2}$$

for a sufficiently large l. The function $\hat{f}^k$ is the solution of the following optimization problem:

$$\hat{f}^k = \arg\min_u \|\Delta^{k/2} u\|$$