Extrinsic and Intrinsic Operator Estimations for Manifold Learning

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Overview

1. **Extrinsic Approximation**

2. **Intrinsic Approximation for manifolds with boundary**

Basic Setup

- (M, g) is a closed Riemannian manifold of dimension d.
- $M \subseteq \mathbb{R}^n$, where $n \gg d$.
- A data set $X = \{x_1, \ldots, x_N\}$ of points sampled i.i.d. from M.

Goal of Manifold Learning

Use the data to construct a matrix which approximates an operator which encodes information about the manifold.

Example

$\Delta_g : C^\infty(M) \to C^\infty(M)$, the Laplace-Beltrami operator. In smooth local coordinates,

$$\Delta_g f = \frac{-1}{\sqrt{\det g}} \frac{\partial}{\partial \theta^i} \left(g^{ij} \sqrt{\det g} \frac{\partial f}{\partial \theta^j} \right).$$

Existing works and our contribution

Pointwise approximation

- The existing literature reports mostly the formulation for operators on functions[a]. We extend it to tensor fields. This includes gradient and divergence of vector fields, divergence of $(2, 0)$ tensor fields, vector Laplacians (Bochner, Hodge, Licnerowicz), and covariant derivative.
- We develop an improved numerical method to approximate the local tangent bundles.

[a] Narcowich & Ward, J. Approx. Theory 1991

Weak estimation

Laplace-Beltrami and vector Laplacians (Bochner, Hodge, Licnerowicz).

- Many theoretical issues encountered with the pointwise approximation, which motivate the weak approximation.
- We prove convergence of eigenvalue and eigenvector/eigenvector-field for the Laplace-Beltrami and Bochner Laplacian approximations.

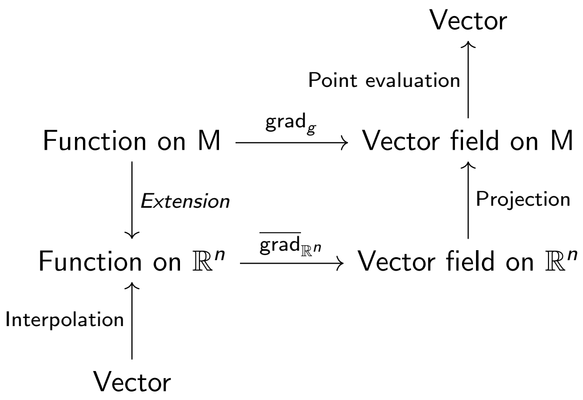
Interpolation, Differentiation, and Projection

$$\text{Function on M} \xrightarrow{\text{grad}_g} \text{Vector field on M}$$

Interpolation, Differentiation, and Projection

$$
\begin{array}{ccc}
\text{Function on M} & \xrightarrow{\mathrm{grad}_g} & \text{Vector field on M} \\
\Big\downarrow \textit{Extension} & & \Big\uparrow \text{Projection} \\
\text{Function on } \mathbb{R}^n & \xrightarrow{\overline{\mathrm{grad}}_{\mathbb{R}^n}} & \text{Vector field on } \mathbb{R}^n
\end{array}
$$

Interpolation, Differentiation, and Projection



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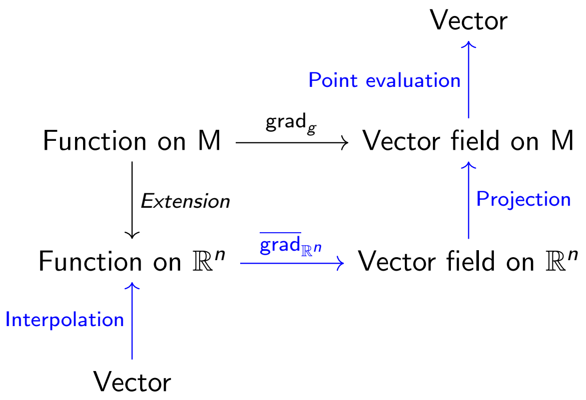

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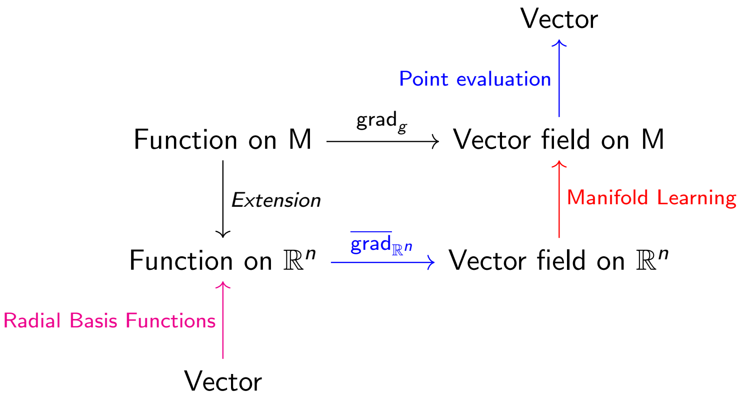

$$\mathrm{grad}_g f(x) = \mathbf{P}\overline{\mathrm{grad}}_{\mathbb{R}^n} F(x) \approx \hat{\mathbf{P}}\overline{\mathrm{grad}}_{\mathbb{R}^n}(I_{\phi_s}\mathbf{f})(x),$$

where $\mathbf{P} = P(x), \hat{\mathbf{P}}$, and $I_{\phi_s} : \mathbb{R}^N \to C^{\alpha}(\mathbb{R}^n)$ will be defined below.

Learning P

- At each $x \in M$, consider $T_x M \subseteq T_x \mathbb{R}^n$.
- There is an $n \times n$ matrix orthogonal projection matrix $\mathbf{P} := T_x\mathbb{R}^n \to T_x M \subseteq T_x\mathbb{R}^n$.
- The entries of $\mathbf{P}$ can be written in terms of the Riemanian matrix g and the embedding $(\theta^1, \ldots, \theta^d) \to (X^1, \ldots, X^n)$:

$$[\mathbf{P}]_{ij} = \frac{\partial X^i}{\partial \theta^r} g^{rs} \frac{\partial X^j}{\partial \theta^s}.$$

- Methods exist for approximating $\mathbf{P}$ [2].

[2] Zhang & Zha J. Approx. Theory 2004, Tyagi, Vural & Frossard, Information and Inference 2013

Learning $\mathbf{P}$

- Note that if $\mathbf{T} = (\tau_1, \ldots, \tau_d)$ denotes a matrix with orthonormal columns that span $T_x M$, then $\mathbf{P} := \mathbf{T}\mathbf{T}^\top$.

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- Methods for learning $\mathbf{P}$ relate the distance $y - x$, for points y close to x, to the directions τ_i. Denoting $(s_1, \ldots, s_d)$ to be the geodesic normal coordinates of y from the based point x.

$$y - x = \iota(\mathbf{s}) - \iota(\mathbf{0}) = \sum_{i=1}^{d} s_i \frac{\partial \iota(\mathbf{0})}{\partial s_i} + \frac{1}{2} \sum_{i,j=1}^{d} s_i s_j \frac{\partial^2 \iota(\mathbf{0})}{\partial s_i \partial s_j} + O(s^3). \tag{1}$$

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- We propose a novel, related method which achieves a faster convergence rate by correcting for curvature. We approximate $\{s_i\}$, the Hessian components $\frac{\partial^2 \iota(\mathbf{0})}{\partial s_i \partial s_j}$, then

$$y - x - \frac{1}{2} \sum_{i,j=1}^{d} s_i s_j \frac{\partial^2 \iota(\mathbf{0})}{\partial s_i \partial s_j} = \sum_{i=1}^{d} s_i \frac{\partial \iota(\mathbf{0})}{\partial s_i} + O(s^3). \tag{2}$$

Second order approximation

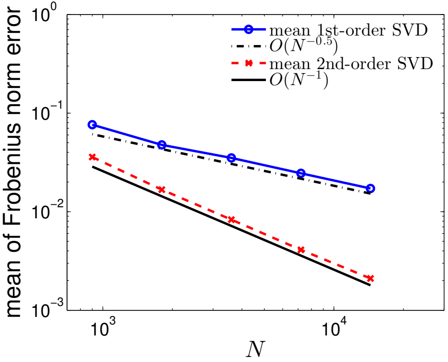
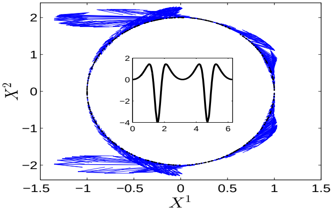


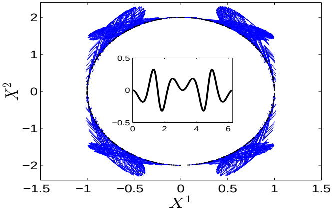
Figure: Mean of Frobenius error $\|\mathbf{P} - \hat{\mathbf{P}}\|_F$ as a function of N, on the $2D$ torus in $\mathbb{R}^3$. We show convergence rate of order $N^{-2/d}$ improving from the first-order estimate $N^{-1/d}$.

Pointwise operator estimation (on a 1D ellipse)

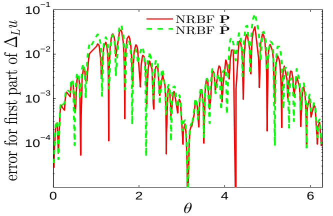
(a) Truth of Lich. Laplacian



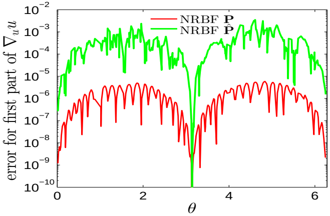
(b) Truth of $\nabla_u u$.



(c) Error of Lich. Laplacian



(d) Error of Covariant Deriv.



Interpolation using RBFs

- Given function values $\mathbf{f} := (f(x_1), \ldots, f(x_N))^\top$ at $X = \{x_j\}_{j=1}^{N}$, the radial basis function (RBF) interpolant of f at x takes the form

$$I_{\phi_s}\mathbf{f}(x) := \sum_{k=1}^{N} c_k \phi_s \left(\|x - x_k\|\right).$$

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- Theoretical advantage with Matérn class kernels is to have Reproducing Kernel Hilbert Space norm that is equivalent to Sobolev space norms [Fuselier and Wright, SINUM 2012].
- We extend their result to probabilistic setting, where if $\{x_1, \ldots, x_N\}$ are random i.i.d. samples of uniform distribution on M, then if ϕ_s is a Matérn kernel with Sobolev norm of regularity $\alpha > n/2$, then for any $f \in H^{\alpha - \frac{n-d}{2}}(M)$, w.p.h. than $1 - \frac{1}{N}$,

$$\|I_{\phi_s} f - f\|_{L^2(M)} = O\left(N^{\frac{-2\alpha+(n-d)}{2d}}\right).$$

Laplace-Beltrami Estimators

- Let $\mathbf{G} : \mathbb{R}^N \to \mathbb{R}^{nN}$ denote the estimate of grad_g,

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- The classical pointwise approximation to Δ_g with

$$\mathbf{L}_N := \mathbf{G}_1\mathbf{G}_1 + \cdots + \mathbf{G}_n\mathbf{G}_n : \mathbb{R}^N \to \mathbb{R}^N,$$

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- In weak form, it is natural to consider

$$\int_M f \Delta_M f d\mathrm{Vol} = \int_M \langle \mathrm{grad}_g f, \mathrm{grad}_g f \rangle d\mathrm{Vol} \approx \frac{1}{N}\mathbf{f}^\top \mathbf{G}^\top \mathbf{Gf}$$

  or $\mathbf{G}^\top\mathbf{G}$ as a symmetric estimator of Δ_M.

Convergence of Eigenvalues

Theorem

Let λ_i denote the i-th eigenvalue of Δ_M, enumerated $\lambda_1 \leq \lambda_2 \leq \ldots$. Suppose that $I_{\phi_s} : \mathbb{R}^N \to C^{\alpha - \frac{n-d}{2}}(M)$ is a stable interpolator. For any i, there exists a sequence $\hat{\lambda}_i^{(N)}$ of eigenvalues of $\mathbf{G}^\top \mathbf{G}$ such that

$$\left| \lambda_i - \hat{\lambda}_i^{(N)} \right| = O\left(\frac{1}{\sqrt{N}} \right) + O\left(N^{\frac{-2\alpha + (n-d)}{2d}} \right).$$

w.p.h. $1 - \frac{12}{N}$ as $N \to \infty$.

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w.p.h. $1 - \frac{12}{N}$ as $N \to \infty$. Also, if $\mathbf{u}$ denotes any normalized eigenvector of $\mathbf{G}^\top \mathbf{G}$, then there exists a normalized f eigenfunction of Δ_g corresponds to non-simple eigenvalue λ with geometric multiplicity m such that w.p.h. $1 - \left(\frac{2m^2+4m+24}{N}\right)$,

$$\|f|_X - \mathbf{u}\|_{L^2(\mu_N)} = O\left(\frac{1}{\sqrt{N}}\right) + O\left(N^{\frac{-2\alpha+(n-d)}{2d}}\right).$$

Some remarks

- Proof uses min-max principle and several interpolation error estimates.
- In this case, we have Monte-Carlo rate.
- We also have equivalent result for the estimation of Bochner Laplacian.
- We can also show consistency of the spectral estimates for the non-symmetric estimator, $\mathbf{L}_N$, using a Gershgorin circle argument under appropriate spectral gap assumption. However, this consistency may break down for $d > 4$.
- The non-symmetric approximation is numerically suffer from spectral pollution issue and theoretically needs to be reconsidered differently.

Numerical Results: Laplace-Beltrami

(a) DM Eigenvalues (b) SRBF Eigenvalues

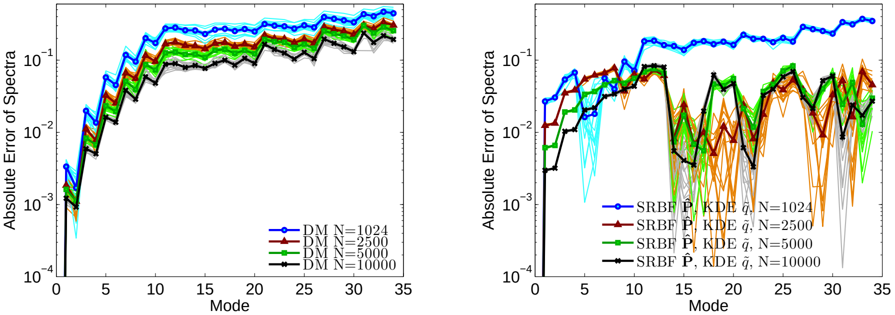

Figure: 2D general torus in $\mathbb{R}^{21}$. Comparison of errors of eigenvalues for (a) DM, (b) SRBF. For each N, 16 independent trials are run and depicted by light color. For each N, the average of all 16 trials are depicted by dark color.

Numerical Results: Laplace-Beltrami

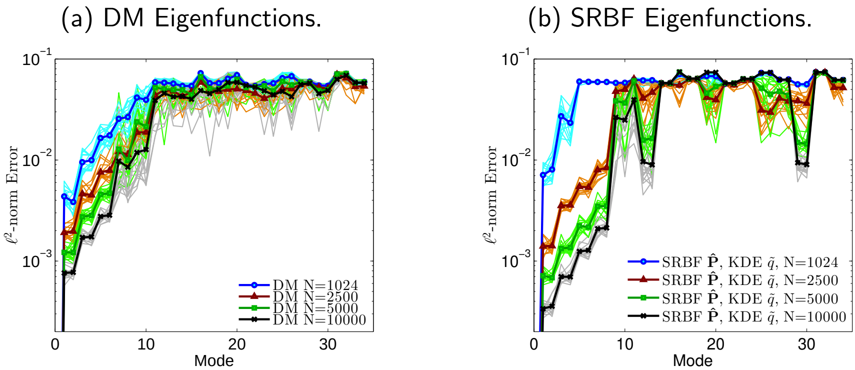

Figure: 2D general torus in $\mathbb{R}^{21}$. Comparison of errors of eigenfunctions for (a) DM, (b) SRBF. For each N, 16 independent trials are run and depicted by light color. For each N, the average of all 16 trials are depicted by dark color.

Numerical Results: Vector Laplacians

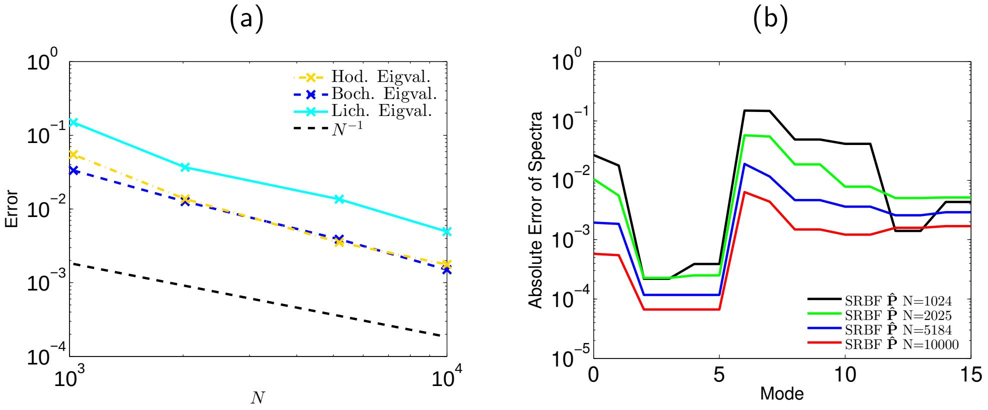

Figure: 2-Sphere in $\mathbb{R}^3$. (a) Mean absolute error of the leading 16 modes for Bochner and Hodge Laplacians and 20 modes for the Lichnerowicz Laplacian, plotted against N. (b) Absolute error between the eigenvalues of the Bochner Laplacian and its approximation, over the leading 15 modes.

Numerical Results

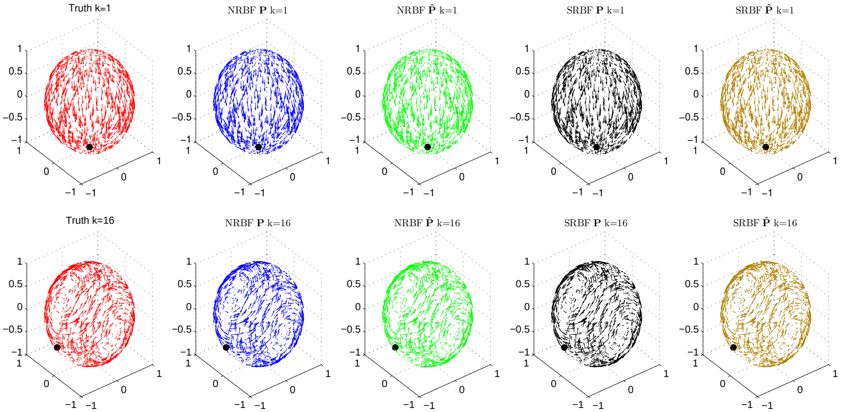

Figure: **2D Sphere in $\mathbb{R}^3$.** Comparison of eigen-vector fields of Bochner Laplacian for $k = 1, 16$. For NRBF, GA kernel with $s = 1.0$ is used, and for SRBF, IQ kernel with $s = 0.5$ is used. The $N = 1024$ data points are randomly distributed on the manifold.

Graph Laplacian (intrinsic) approach

Let $M \subseteq \mathbb{R}^n$ be a compact Riemannian manifold and define,

$$G_\epsilon f(x) := \epsilon^{-d/2} \int_M K_\epsilon(x,y) dV(y).$$

with exponentially decaying kernel $K_\epsilon : M \times M \to \mathbb{R}$.

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- For any $x \in M$ sufficiently far **away from the boundary** and $f \in C^3(M)$,

  $$L_\epsilon f(x) := \frac{G_\epsilon f(x) - f(x) G_\epsilon 1(x)}{\epsilon} := m_2 \Delta_g f(x) + \mathcal{O}(\epsilon), \quad \text{as } \epsilon \to 0,$$

  for some $m_2 > 0$.

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  for some $m_2 > 0$.

- For $x \in M$ whose $d_g(x, \partial M) \leq \epsilon^\gamma$, $0 < \gamma \leq 1/2$,

$$L_\epsilon f(x) = \frac{m_1^\epsilon(x) \frac{\partial f}{\partial \nu}(x_0)}{\sqrt{\epsilon}} + O(1), \qquad \text{as } \epsilon \to 0,$$

  where $x_0 = \arg\inf_{y \in \partial M} d_g(x,y)$.

Existing convergence results

- **Closed manifolds**
  - Pointwise convergence: Belkin & Niyogi 2005, Hein, Audibert, & Von Luxburg 2005, Singer 2006.
  - Spectral convergence: Belkin & Niyogi 2007, Burago-Kurylev 2014, Garcia-Trillos, Gerlach, Hein & Slepcev 2022, Calder & Garcia-Trillos 2022, Dunson, Wu, & Wu 2021.
- **Compact manifolds with boundary**
  - Weak convergence: Hein 2006, Vaughn, Berry, & Antil 2022.
  - Spectral convergence (Neumann Laplacian): Singer & Wu 2017, Lu 2020, Tao & Shi 2020.

Q: How about studying Dirichlet Laplacian?

Motivations for Dirichlet Laplacian

Solving PDEs on point clouds.

- **Mean passage problem, computing committor functions:**
  - Thiede, Giannakis, Dinner, & Weare 2019, Evans, Cameron, & Tiwary, 2022.
- **Elliptic and parabolic PDEs:**
  - S.W. Jiang and J. Harlim, *Ghost Point Diffusion Maps for solving elliptic PDE's on Manifolds with Classical Boundary Conditions*, Comm. Pure Appl. Math. `https://doi/10.1002/cpa.22035`
  - Q. Yan, S.W. Jiang, and J. Harlim, *Kernel-based methods for solving time-dependent advection-diffusion equations on manifolds*, arXiv:2105.13835.
- **Inverse problems**:
  - J. Harlim, S.W. Jiang, H. Kim, and D. Sanz-Alonso, *Graph-based prior and forward models for inverse problems on manifolds with boundaries*, Inverse Problems 38(3) 035006, 2022.

Symmetrized Gaussian Kernels[3]

- Given a Gaussian kernel, $k_\epsilon(x, y) = \exp\left(-\frac{\|x-y\|^2}{\epsilon}\right)$, define a symmetric kernel,

$$\hat{k}_\epsilon(x, y) := \epsilon^{-d/2} k_\epsilon(x, y) \left(\frac{1}{2\rho(x)} + \frac{1}{2\rho(y)}\right),$$

where, $\rho(x) := \epsilon^{-d/2} \int_M k_\epsilon(x, y) dV(y)$.

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  where, $\rho(x) := \epsilon^{-d/2}\int_M k_\epsilon(x,y)dV(y)$.

- Numerically, given data $X = \{x_1, \ldots, x_N\} \subset M$, we approximate the kernel $\hat{k}_\epsilon$ with,

$$\tilde{k}_{\epsilon,n}(x_i,x_j) = k_\epsilon(x_i,x_j)\left(\frac{1}{\frac{2}{n}\sum_{k=1}^n k_\epsilon(x_i,x_k)} + \frac{1}{\frac{2}{n}\sum_{k=1}^n k_\epsilon(x_j,x_k)}\right).$$

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Symmetrized Graph-Laplacian (SGL) matrices

Theorem (Neumann and no boundary Laplacian)

For $X = \{x_1, \ldots, x_N\} \subset M$, we define the SGL as,

$$\tilde{L}_{\epsilon,N} u(x) = \frac{2}{m_2 \epsilon} \left(u(x) - \frac{1}{N} \sum_{i=1}^{N} \tilde{k}_{\epsilon,N}(x, x_i) u(x_i) \right).$$

For closed manifold and manifold with homogeneous Neumann boundaries, given uniformly sampled X, in high probability,

$$|\lambda_i - \tilde{\lambda}_i^{\epsilon,N}| = O\Big(N^{-\frac{1}{2d+6}}\Big), \quad as \quad N \to \infty.$$

where λ_i and $\tilde{\lambda}_i$ are the ith eigenvalues of Δ_g and $\tilde{L}_{\epsilon,N}$, respectively.

Outline of the proof

We use min-max argument on:

$$\|\nabla f\|_{L^2(M)} - \tilde{\lambda}_i^{\epsilon,N} = \underbrace{\|\nabla f\|_{L^2(M)} - \langle L_\epsilon f, f\rangle_{L^2(M)}}_{\text{approximation error}} + \underbrace{\langle L_\epsilon f, f\rangle_{L^2(M)} - \tilde{\lambda}_i^{\epsilon,N}}_{\text{discretization error}}$$

over i-dim subspace $\mathcal{G}_i \subset C^\infty(M) \subset H^1(M)$, where

$$L_\epsilon f := \frac{2}{m_2\epsilon}(f - \hat{K}_\epsilon f) = \frac{2}{m_2\epsilon}\left(f - \int_M \hat{k}_\epsilon(\cdot, y)dV(y)\right).$$

1. Bound the approximation error using the weak consistency (Vaughn et al 2019).
2. The main point of choosing $\hat{K}_\epsilon$ to be compact, self-adjoint with positive definite kernel allows one to characterize,
$$\lambda_i^\epsilon = \min_{S\in\mathcal{G}_i} \max_{f\in S\setminus\{0\}} \frac{\langle L_\epsilon f, f\rangle_{L^2(M)}}{\|f\|^2_{L^2(M)}}.$$
3. Once the min-max is taken, the discretization error can be bounded by
$$|\lambda_i^\epsilon - \tilde{\lambda}_i^{\epsilon,N}| \leq \underbrace{|\lambda_i^\epsilon - \lambda_i^{\epsilon,N}|}_{\text{Rosasco et al. 2010}} + \underbrace{|\lambda_i^{\epsilon,N} - \tilde{\lambda}_i^{\epsilon,N}|}_{\text{spectral error of perturbed matrix}}$$

Additional results:

Remarks:

1. For closed manifold, the rate can be improved to $O(N^{-\frac{1}{d+4}})$, which is equivalent to results reported by Calder & García-Trillos, 2022. One can replace the approximation error with a stronger L^2-error bound such as in H, Sanz-Alonso, & Yang, 2020.
2. Following the method of proof from Calder & García-Trillos paper, we deduce the convergence of eigenvectors in $L^2(\mu_N)$ with rate $N^{-\frac{1}{8d+20}}$, which again can be improved for closed manifolds.
3. For non-uniformly sampled data, the error rate for eigenvalue estimation is of order-$N^{-\frac{1}{4d+6}}$. The extra factor $N^{-\frac{1}{2d}}$ is due to the estimation of non-uniform sampling density. For the eigenvectors estimation is of order-$N^{-\frac{1}{16d+20}}$.

Truncated SGL matrices

Definition

Define $M_r := \{x \in M : \inf_{y \in \partial M} d_g(x, y) > r\}$. Let $N_1 = |X \cap M_r|$.

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Let's re-order the data to $\{x_i\}_{i=1}^{N_1} \subset M^r$ and define a truncated SGL matrix of size $N_1 \times N_1$ as,

$$\left(L^r_{\epsilon,N}\right)_{ij} := \left(\tilde{L}_{\epsilon,N}\right)_{ij}, \qquad i,j = 1,\dots,N_1,$$

where we truncate components of SGL matrix $\tilde{L}_{\epsilon,N}$ corresponding to data points whose distance from the boundary is less than some parameter $r > 0$.

Convergence results for truncated SGL:

Theorem (eigenvalue)

Let λ_i be the ith eigenvalue of Dirichlet Laplacian,

$$\Delta_g \varphi_i = \lambda_i \varphi_i, \quad \varphi_i|_{\partial M} = 0,$$

and $\lambda_i^{r,\epsilon,n}$ be the ith eigenvalue of the truncated SGL matrix $L^r_{\epsilon,n}$. For $r \geq c\epsilon^{\frac{d+3}{2d}}$, in high probability,

$$|\lambda_i - \tilde{\lambda}_i^{r,\epsilon,n}| = O\left(N_1^{-\frac{1}{2d+6}}\right), \quad as \quad N_1 \to \infty.$$

Outline of the proof

- In this case, Dirichlet Laplacian eigenfunction φ_i corresponding to eigenvalue λ_i is attained on span$\{\varphi_1, \ldots, \varphi_i\} \subset C_0^\infty(M) \subset H_0^1(M)$.

Outline of the proof

- In this case, Dirichlet Laplacian eigenfunction φ_i corresponding to eigenvalue λ_i is attained on $\text{span}\{\varphi_1, \ldots, \varphi_i\} \subset C_0^\infty(M) \subset H_0^1(M)$.
- Consider

$$L_\epsilon^c f := \frac{2}{m_2 \epsilon}\left(f - \int_{M_r} \hat{k}_\epsilon^c(\cdot, y) dV(y)\right),$$

where $\hat{k}_c : M \times M \to \mathbb{R}$ is supported in $M_r \times M_r$ and its L^2-distance to $\hat{k}_\epsilon$ is small, ϵ^3.

Outline of the proof

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where $\hat{k}_c : M \times M \to \mathbb{R}$ is supported in $M_r \times M_r$ and its L^2-distance to $\hat{k}_\epsilon$ is small, ϵ^3.
- By design, its eigenfunctions vanish on $M \backslash M_r$ for all $r > 0$, so
$$\lambda_i^{c,\epsilon} = \min_{S_i \subset C_0^\infty(M)} \max_{f \in S_i, \|f\|=1} \langle L_\epsilon^c f, f \rangle_{L^2(M)}.$$

Outline of the proof

Then we consider min-max over $C_0^\infty(M)$ on,

$$\|\nabla f\|^2_{L^2(M)} - \tilde{\lambda}_i^{r,\epsilon,n} = \underbrace{\|\nabla f\|^2_{L^2(M)} - \langle L_\epsilon f, f\rangle_{L^2(M)}}_{(I)} + \underbrace{\langle L_\epsilon f, f\rangle_{L^2(M)} - \langle L_\epsilon^c f, f\rangle_{L^2(M)}}_{(II)} + \underbrace{\langle L_\epsilon^c f, f\rangle_{L^2(M)} - \tilde{\lambda}_i^{r,\epsilon,n}}_{(III)}.$$

- To bound term (I), we use the weak covergence result of Vaughn et al 2019.
- To bound term (III), we need to show $|\lambda_i^{c,\epsilon} - \lambda_i^{r,\epsilon}| = O(\epsilon^{1/2})$, then use Rosasco et al. 2010 to bound $|\lambda_i^{r,\epsilon} - \lambda_i^{r,\epsilon,n}|$ and the matrix perturbation theory to bound $|\lambda_i^{r,\epsilon,n} - \tilde{\lambda}_i^{r,\epsilon,n}|$.
- As for term (II), one can deduce that

  $$|\langle L_\epsilon - L_\epsilon^c f, f\rangle_{L^2(M)}| = O(\epsilon^{1/2}) + \int_M f(x)\frac{2}{m_2\epsilon}\int_{M\backslash M_r} \hat{k}(x,y)f(y)dV(y),$$

  which suggests that $\mathrm{Vol}(M\backslash M_r) = \epsilon^{\frac{d+3}{2}}$.
- This implies that $r > c\epsilon^{\frac{d+3}{2d}}$ and $N - N_1 := N_0 \sim \epsilon^{\frac{d+3}{2}} N$.

Homogeneous Dirichlet Laplacian example

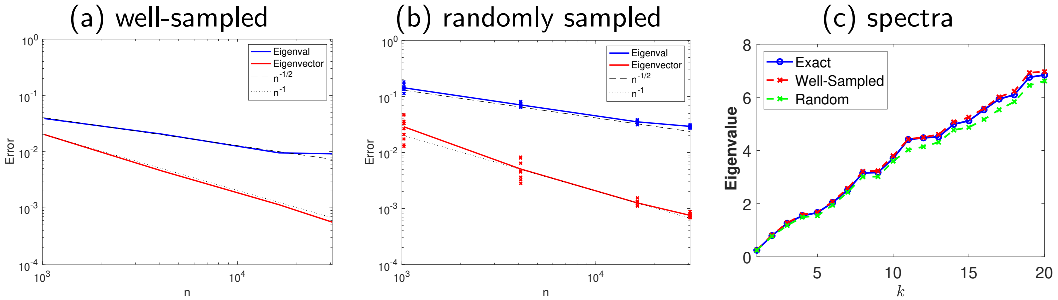
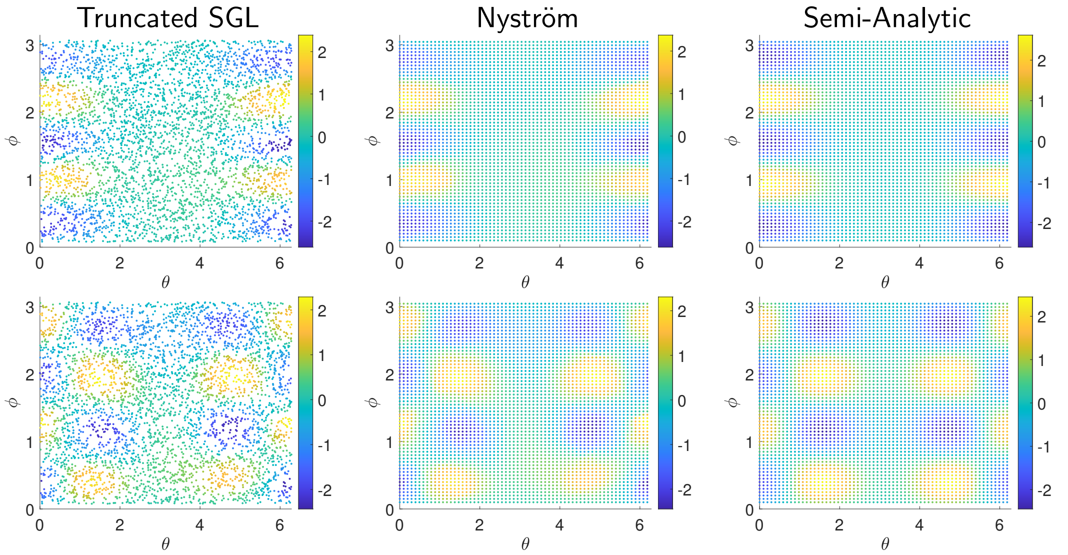


Figure: Semi-Torus Example, uniform sampling distribution.

Remarks

- The theoretical predicted eigenvalue is $O\left(N^{-\frac{1}{2d+6}}\right)$.
- In this numerical experiment, we set $r = \sqrt{\epsilon}$.

$N = 64^2$. Mode 10 (row 1) and mode 20 (row 2).



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