Truncated Graph Laplacian on Manifolds with Boundary

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Introduction

Diffusion Maps [1] leverages an asymptotic expansion of the integral operator

$$K_\epsilon f(x) := \int_M \exp\left(\|x-y\|^2/4\epsilon\right) f(y) dV(y)$$

to estimate the Laplace-Beltrami operator on a manifold without boundary:

$$\Delta f(x) = L_\epsilon f(x) + O(\epsilon)$$

where $L_\epsilon f = \epsilon^{-1}(f - \frac{1}{K_\epsilon 1} K_\epsilon f)$.

Given a dataset of points sampled from an unknown manifold, discretizing integrals to sums results in a matrix $\mathbf{L}_{\epsilon,\mathbf{n}}$ estimating the Laplace-Beltrami operator.

Motivation

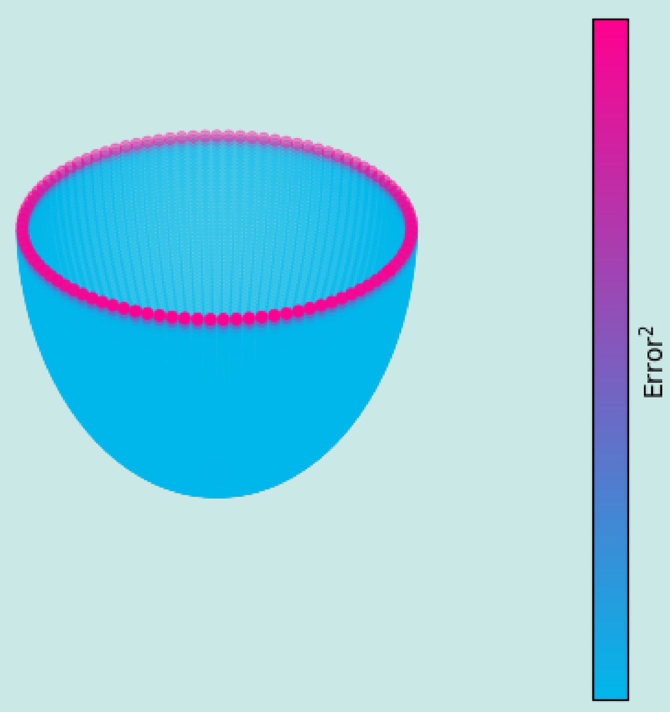
The key asymptotic expansion blows up near the boundary:

$$K_\epsilon f(x) = m_0^\epsilon(x) f(x_0) + \sqrt{\epsilon} m_1^\epsilon(x) \frac{\partial f}{\partial \nu}(x_0) + O(\epsilon)$$

Observation *Diffusion Maps applied to manifolds with boundary estimates the Neumann Laplacian.*

Question *Can Diffusion maps be modified to estimate the Dirichlet Laplacian?*

$$\Delta f = \lambda f, \qquad f|_{\partial M} = 0$$



Theoretical starting point:

Theorem *[3] The diffusion maps estimator is weakly consistent on manifolds with boundary:*

$$\langle L_\epsilon f, g \rangle = \langle \Delta f, g \rangle + O(\sqrt{\epsilon})$$

Symmetric Formulation

We can define a symmetrized version of the estimator L_ϵ:

$$L_\epsilon^{\text{sym}} = \frac{1}{2}(L_\epsilon + L_\epsilon^*)$$

Corollary *L_ϵ^{sym} is consistent on manifolds with boundary:*

$$\langle L_\epsilon^{\text{sym}} f, g \rangle = \langle \Delta f, g \rangle + O(\sqrt{\epsilon})$$

References

[1] R. Coifman, S. Laffon. Diffusion Maps In *Applied and Computational Harmonic Analysis 2008*

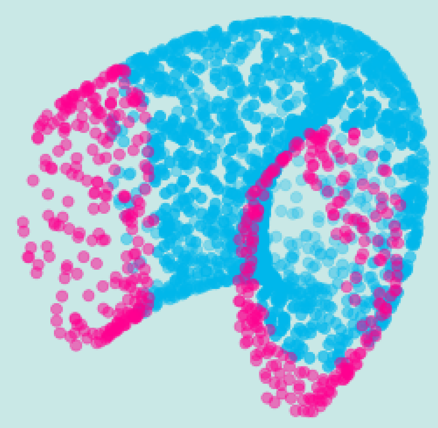
[2] J. Peoples, J. Harlim. Spectral Convergence of Symmetrized Graph Laplacian on Manifolds with Boundary. *arxiv preprint 2023*

[3] R. Vaughn. Diffusion Maps for Manifolds with Boundary. *PhD Thesis, George Mason University 2020*

Truncated Graph Laplacian

The Truncated Graph Laplacian (TGL) is the restriction of $\mathbf{L}_\epsilon^{\text{sym}}$ to points sufficiently far away from the boundary:

$$\mathbf{L}_\epsilon^{\text{sym}} = \begin{array}{c} \\ M_{\epsilon\gamma} \\ M\setminus M_{\epsilon\gamma} \end{array} \begin{array}{cc} M_{\epsilon\gamma} & M\setminus M_{\epsilon\gamma} \\ \left[\mathbf{L}_\epsilon^{\text{tgl}} \right. & * \\ * & \left. * \right] \end{array}$$



The weak truncation error is small on Dirichlet functions:

$$\langle (K_\epsilon - K_\epsilon^{\text{tgl}}) f, f \rangle = O(\epsilon^{3\gamma})$$

Spectral Convergence

Theorem *Let λ_i and $\lambda_i^{\epsilon,n}$ denote the i-th Dirichlet-eigenvalues of Δ and $\mathbf{L}_\epsilon^{\text{tgl}}$, respectively. Then with probability approaching 1 as $n \to \infty$,*

$$\lambda_i^{\epsilon,n} \to \lambda_i.$$

Convergence Rate *The rate of convergence is given by*

$$|\lambda_i - \lambda_i^{\epsilon,n}| = O\left(\sqrt{\epsilon}, \epsilon^{3\gamma-1}, \frac{\sqrt{\log(n)}}{\epsilon^{d/2+1}\sqrt{n}}\right)$$

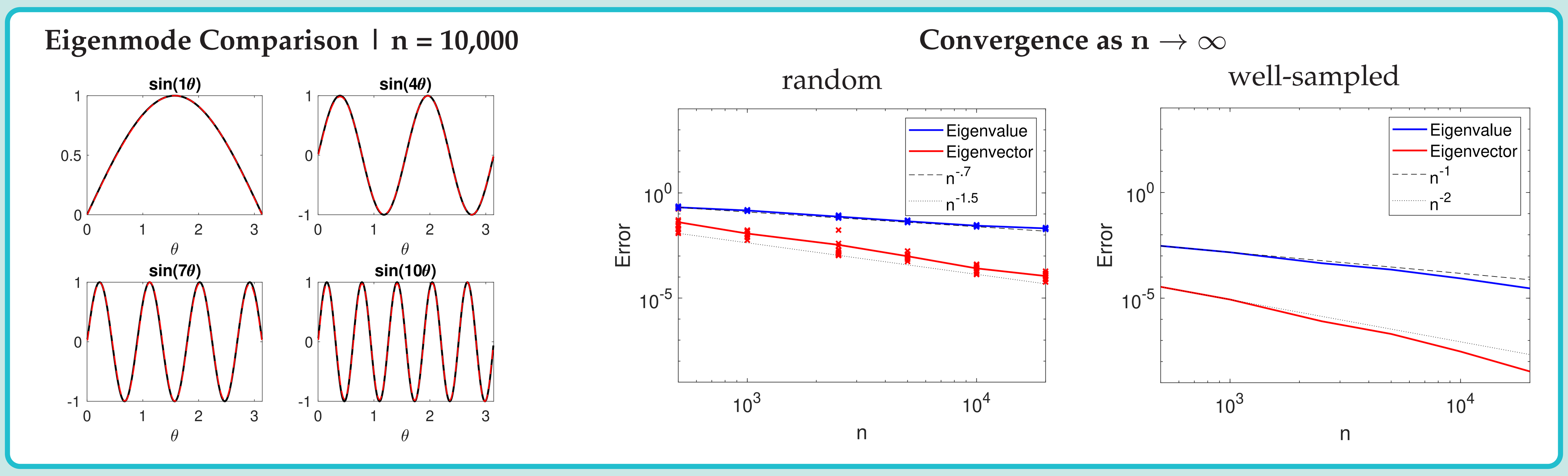
$$= \text{bias} + \text{truncation error}$$

$$+ \text{discretization error}$$

Theorem *For any eigenvector $\mathbf{u}$ of $\mathbf{L}_\epsilon^{\text{tgl}}$ with eigenvalue $\lambda_i^{\epsilon,n}$, there is a Dirichlet eigenfunction f of Δ with eigenvalue λ_i such that $\|\mathbf{f} - \mathbf{u}\|_{L^2(\mu_n)}$ is dominated by the same rate above.*

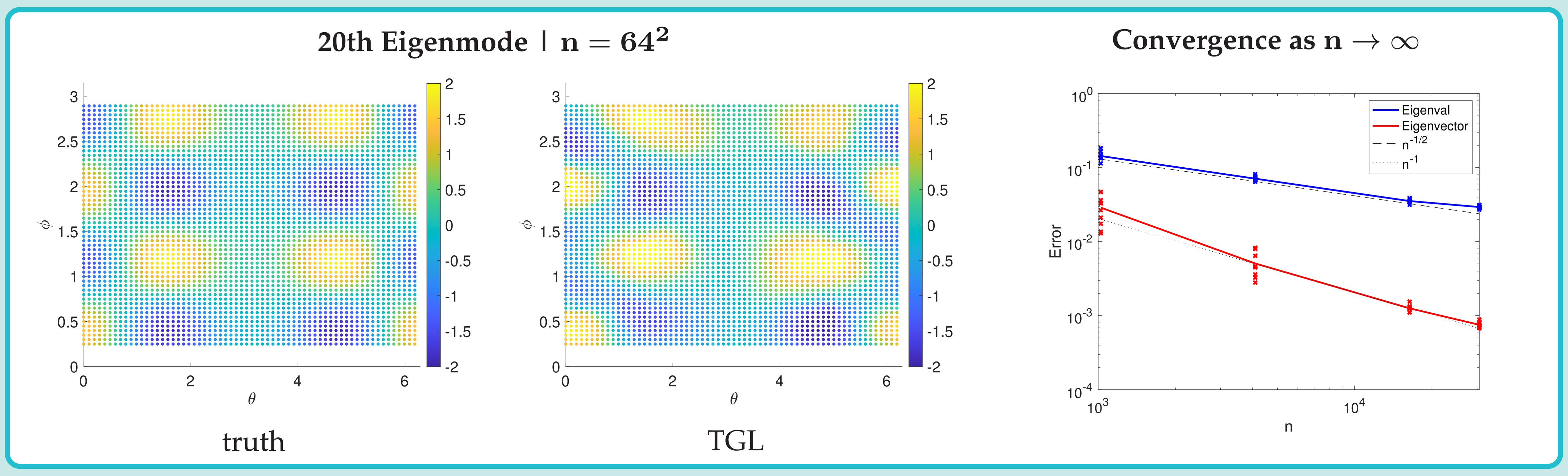
Numerical Results

Semicircle. Shown below are estimated eigenvectors for the semicircle using 10,000 data points sampled from a uniform distribution in the instrinsic coordinates (left). Also shown is convergence as $n \to \infty$ of the mean of relative eigenvalue error (blue) and mean of eigenvector MSE (red) for uniform random data (middle) and well-sampled data (right). Means are taken over the first 10 eigenmodes. For random data, 10 trials were performed.



Overall, Dirichlet eigenfunctions are well approximated by the TGL method, and observed convergence is slightly faster than the predicted rate.

Semitorus. Shown below is the 20th eigenvector of the Dirichlet Laplacian obtained via semi-analytic methods (left) and using TGL method with 64^2 data points sampled from a uniform distribution in the instrinsic coordinates (middle). Also shown is the convergence rate as $n \to \infty$ using the same metrics as for the semicircle (right).



Visually, we see that even high eigenmodes can be estimated using the TGL method. We also see the empirical convergence rate is slightly faster than predicted, even for random data.

Conclusions

Presented are the first results achieving spectral convergence to the Dirichlet Laplacian on an unknown manifold with boundary. To obtain such results, we introduced a novel estimator which has numerous theoretical advantages. Empirical findings further support the validity of this estimator.

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