The SPDE Approach to Matérn Fields: Graph Representations

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Abstract

This paper investigates Gaussian Markov random field approximations to nonstationary Gaussian fields using graph representations of stochastic partial differential equations. We establish approximation error guarantees building on and generalizing the theory of spectral convergence of graph Laplacians. Graph representations allow inference and sampling with linear algebra methods for sparse matrices, thus reducing the computational cost. In addition, they bridge and unify several models in Bayesian inverse problems, spatial statistics and graph-based machine learning. We demonstrate through examples in these three disciplines that the unity revealed by graph representations facilitates the exchange of ideas across them.

1 Introduction

The stochastic partial differential equation (SPDE) approach to Gaussian fields (GFs) has been one of the key developments in spatial statistics over the last decade [59]. The main idea is to represent GFs as finite element solutions to SPDEs, reducing the computational cost of inference and sampling by invoking a Gaussian Markov random field (GMRF) approximation [72]. This paper investigates graph representations of stationary and nonstationary Matérn fields following the SPDE perspective, contributing to and unifying the extant theoretical, computational and methodological literature on GFs in Bayesian inverse problems, spatial statistics and graph-based machine learning. We demonstrate through transparent mathematical reasoning that graph representations give GMRF approximations with error guarantees, and we illustrate through numerical examples that they do so without the pre-processing burden of finite element representations, an essential advantage when interpolating manifold data living in a high dimensional ambient space.

Recall that a random function \( u(x), x \in \mathbb{R}^d \), is a GF if all finite collections \( \{u(x_i)\}_{i=1}^n \) have self-consistent multivariate Gaussian distributions [1, 2]. A GF can be specified using a mean function \( \mu(\cdot) \) and a covariance function \( c(\cdot, \cdot) \), so that the mean vector and covariance matrix of the finite dimensional distributions are \( \{\mu(x_i)\} \in \mathbb{R}^n \) and \( \Sigma = \{c(x_i, x_j)\} \in \mathbb{R}^{n \times n} \). GFs are natural models for spatial, temporal and spatio-temporal data. They have desirable analytic properties, including an explicit normalizing constant and closed formulae when conditioning on Gaussian data. However, in practice GFs have two main caveats. First, it is crucial and non-trivial to find flexible covariance functions with few but interpretable parameters that can be learned from data. Second, inference of these parameters from Gaussian data of size \( n \) —or sampling the field at \( n \) locations— involves factorizing a kernel matrix \( \Sigma \in \mathbb{R}^{n \times n} \), leading to a \( \mathcal{O}(n^3) \) computational cost and \( \mathcal{O}(n^2) \) memory cost unless further structure is assumed or imposed on the covariance model. For this reason, many recent works have investigated novel ways to deal with large datasets, some of which are reviewed in [47].

The SPDE approach tackles the big \( n \) problem by replacing the GF with a GMRF approximation. A GMRF is a discretely indexed GF \( u_n(i), i \in \{1, \ldots, n\} \), such that the full conditional at each site \( 1 \leq i \leq n \) depends only on a (small) set of neighbors \( \partial i \) to site \( i \). This conditional independence structure is fully encoded in the precision matrix \( Q \) of the multivariate Gaussian distribution.
of $u_n \in \mathbb{R}^n$: it holds that $Q_{ij} \neq 0$ iff $i \in \partial i \cup \partial j$. Computationally, the main advantage comes from using numerical linear algebra techniques and Markov chain Monte Carlo algorithms that exploit, respectively, the sparsity of $Q$ and the characterization of the GMRF in terms of its full conditionals. The speed-up can be dramatic, with a typical computational cost $\mathcal{O}(n)$, $\mathcal{O}(n^{3/2})$, and $\mathcal{O}(n^2)$ for GMRFs in time, space, and space-time in two spatial dimensions, see [72]. In addition to alleviating the computational burden of GF methods, the SPDE approach also alleviates the modeling challenges by suggesting nonstationary generalizations of Matérn fields and extensions beyond Euclidean settings.

In this paper we employ graph-based discretizations of SPDEs to represent stationary and nonstationary Matérn models. With few exceptions e.g. [36, 12, 40, 46], previous work stemming from the SPDE approach considered representations based on finite element or finite difference discretizations [59, 17, 19, 20, 71, 95]. Graph representations provide an indirect way to define Matérn models in applications where only similarity relationships between abstract features may be available. Moreover, in contrast to finite elements, graph representations require minimal pre-processing cost: there is no need to compute triangulations and finite element basis or to define ghost domains as in [59]. This is an essential advantage when interpolating manifold data living in a high dimensional ambient space, particularly so when the underlying manifold or its dimension are unknown. Finally, a wide range of problems in Bayesian inversion, spatial statistics and graph-based machine learning can be formulated as latent Gaussian models, and using graph representations of Matérn fields as priors allows us to unify and contribute to the exchange of ideas across these disciplines.

A disadvantage of the graph-based approach is that error guarantees are weaker than for finite element or finite difference representations. Our belief is that this is not due to an intrinsic limitation of the graph-based approach, but rather to the underdevelopment of existing theory. Here we provide an up-to-date perspective of spectral convergence of graph Laplacians which overviews and generalizes some of the recent literature [23, 38, 39] and further show how these results can be used to establish the convergence of GMRFs to GFs.

1.1 Literature Review

The ubiquity of GFs in statistics, applied mathematics and machine learning has led, unsurprisingly, to the reinvention and relabeling of many algorithms and ideas. GFs play a central role in spatial statistics [41, 47], especially in the subfield of geostatistics [85], where they are used to interpolate data in a procedure called kriging and as a building block of modern hierarchical spatial models [5]. In machine learning, GFs are called Gaussian processes and kriging is known as Gaussian process regression [97]. Gaussian processes are one of the main tools in Bayesian non-parametric inference [96, 91, 40] and are an alternative to neural networks for supervised and semi-supervised regression [62, 40]. They are also related to, or used within, other machine learning algorithms including splines, support vector machines and Bayesian optimization [82, 77, 21, 31]. GFs are standard prior models for statistical Bayesian inverse problems [52, 25, 86, 76] with applications in medical imaging, remote sensing and ground prospecting [7, 30, 83, 29, 35]. Within Bayesian inversion, GFs are also employed as surrogates for the likelihood function [87]. GFs have found numerous applications, allowing for uncertainty quantification [88] in astrophysics [6], biology [89, 84], calibration of computer models [53, 63], data-driven learning of partial differential equations [69, 68], geophysics [51, 22], hydrology [75], image processing and medical imaging [28, 83, 70], meteorology [18, 59] and probabilistic
The emphasis of this paper is on Matérn models [64] and generalizations thereof. Matérn models are widely used in spatial statistics [85, 41], machine learning [97] and uncertainty quantification [88], with applications in various scientific fields [45, 26]. The SPDE approach to construct GMRF approximations to GFs was proposed in the seminal paper [59] and was further popularized through the software R-INLA [4]. GMRFs in statistics were pioneered by Besag [13, 14] and their computational benefits and applications are overviewed in the monograph [72].

In an independent line of work, the desire to define positive semi-definite kernels using only similarity relationships between features motivated the introduction of diffusion kernels [57] which can be interpreted as limiting cases of Matérn models. The main idea underlying the construction of diffusion kernels is to exploit that graph Laplacians [27, 92] and their powers satisfy the positive semi-definiteness requirement. This observation has permeated the construction of graph-based regularizations in manifold learning and machine learning applications, as well as the design of model reduction techniques e.g. [99, 67, 58, 61, 11, 9, 8]. Our work aims to demonstrate that a wide family of graph-based kernels in machine learning may be interpreted, in a rigorous way, as discrete approximations of standard GF models in spatial statistics.

Large sample limits of graph Laplacians have been widely studied. Most results concern either pointwise convergence [49, 9, 42, 48, 80, 90] or variational and spectral convergence [10, 81, 78, 23, 39], with [24] reconciling both perspectives to obtained improved rates. This paper builds on and generalizes spectral convergence theory —that is, convergence of eigenvalues and eigenfunctions of the graph-based operators to those defined in the continuum— to study GMRF approximations of GFs. Unsurprisingly, we shall see that optimal transport ideas are key to linking discrete and continuum objects; we will use a probabilistic extension of the $\mathcal{T}_L^2$ metric [37] to compare random discrete and continuum functions, in the spirit of [36, 40], giving a self-contained and digestible introduction to these concepts.

1.2 Main Contributions and Outline

Further to providing a unified narrative of existing literature, this paper contains some original contributions. We introduce GMRF approximations of nonstationary GFs defined on manifolds through graph representations of the corresponding SPDEs and generalize the constructions to arbitrary point clouds. Our main theoretical result, Theorem 4.1, covers nonstationary models and, to our knowledge, is the first to give rates of convergence of graph-based representations of GFs, suggesting a suitable topology in which to formalize the results. We also demonstrate through numerical examples that the mathematical unity that comes from viewing graph-based methods as discretizations of continuum ones facilitates the transfer of methodology and theory across Bayesian inverse problems, spatial statistics and graph-based machine learning. In particular, we introduce nonstationary models for graph-based classification problems, which to our best knowledge has not been considered before, and empirically observe an improvement of performance that deserves further research.

This paper is organized as follows. Section 2 introduces the SPDE formulation of the Matérn model and extends it to incorporate nonstationarity. Section 3 introduces the graph-based approach and constructs graph approximations of the Matérn fields. Section 4 presents the main result on the convergence of the graph Matérn model towards its continuum counterpart and discusses the ideas of the proof. Section 5 illustrates the application of graph Matérn models for three problems in
Bayesian inversion, spatial statistics and graph-based machine learning. Section 6 discusses further research directions. Our aim is to provide a digestible narrative and for this reason we postpone all proofs and most of the technical material to an appendix.

2 Matérn Models and the SPDE Approach

In this section we provide some background on GFs and the SPDE approach. We introduce the Matérn family in Subsection 2.1 and a nonstationary generalization in Subsection 2.2. All fields will be assumed to be centered and we focus our attention on their covariance structure.

2.1 Stationary Matérn Models

Recall that a GF in $\mathbb{R}^m$ belongs to the Matérn class if its covariance function can be written in the form

$$c_{\sigma,\nu,\ell}(x, y) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{|x - y|}{\ell}\right)^\nu K_\nu \left(\frac{|x - y|}{\ell}\right), \quad x, y \in \mathbb{R}^m,$$

(2.1)

where $|\cdot|$ is the Euclidean distance in $\mathbb{R}^m$, $\Gamma$ denotes the Gamma function and $K_\nu$ denotes the modified Bessel function of the second kind. The parameters $\sigma, \nu$ and $\ell$ control, respectively, the marginal variance (magnitude), regularity and correlation length scale of the field. While being defined in terms of three interpretable parameters, the modeling flexibility afforded by the Matérn covariance (2.1) is limited by its stationarity (the value of the covariance function depends only on the difference between its arguments) and isotropy (it depends only on their Euclidean distance).

An important characterization by Whittle [93, 94] is that Matérn fields can be defined as the solution to certain fractional order stochastic partial differential equation (SPDE). Precisely, setting $\tau := \ell^2, s := \nu + \frac{m}{2}$, a Gaussian field with covariance function (2.1) is the unique stationary solution to the SPDE

$$(\tau I - \Delta)^{\frac{s}{2}} u(x) = \mathcal{W}(x), \quad x \in \mathbb{R}^m,$$

(2.2)

where the marginal variance of $u$ is

$$\sigma^2 = \frac{\Gamma(s - \frac{m}{2})}{(4\pi)^{\frac{s}{2}} \Gamma(s) \tau^{s - \frac{m}{2}}}.$$  

(2.3)

Throughout this paper, fractional power operators such as $(\tau I - \Delta)^{\frac{s}{2}}$ will be defined spectrally [60] and $\mathcal{W}$ denotes spatial Gaussian white noise with unit variance.

As discussed in [59], the SPDE formulation of Matérn GFs has several advantages. First, it allows to approximate the solution to (2.2) by a GMRF and thereby to reduce the computational cost of inference and sampling [72, 79]. Second, it suggests natural nonstationary and anisotropic generalizations of the Matérn model by letting $\tau$ depend on the spatial variable [71] or by replacing the Laplacian with an elliptic operator with spatially varying coefficients [32, 33]. Third, it allows to define Matérn models in manifolds and in bounded spatial, temporal and spatio-temporal domains by using modifications of the SPDE (2.2), possibly supplemented with appropriate boundary conditions [55]. In order to gain theoretical understanding, in subsequent sections we will work under a manifold assumption and analyze the convergence of graph representations of Matérn fields defined on manifolds. This setting is motivated by manifold learning theory [11, 39] and will allow us to build on the rich literature on GFs on manifolds [2].
In more mathematical terms, the SPDE characterization shifts attention from the covariance function (or spectral density) description of Gaussian measures to the covariance (or precision) operator description [16]: keeping only the \( \tau \) term in the marginal variance given by equation (2.3), we see that the law of the field \( u(x) \) defined by equation (2.2) is — up to a scaling factor independent of \( \tau \) that we drop in what follows — the Gaussian measure \( \mathcal{N}(0, \mathcal{C}) \) with \( \mathcal{C} = \tau^s \frac{m}{2} (\tau I - \Delta)^{-s} \). Thus, the field admits a Karhunen-Loéve expansion

\[
  u(x) = \tau^{\frac{s}{2} - \frac{m}{4}} \sum_{i=1}^{\infty} \left[ \tau + \lambda^{(i)} \right]^{-\frac{s}{2}} \xi^{(i)}(x),
\]

where \( \{\xi^{(i)}\}_{i=1}^{\infty} \) is a sequence of independent standard normal random variables and \( \{\lambda^{(i)}, \psi^{(i)}\}_{i=1}^{\infty} \) are the eigenpairs of \( -\Delta \). Equivalently, we can view the above characterization as the Gaussian measure \( \mathcal{N}(0, (\tau I - \Delta)^{-s}) \) normalized by \( \tau^{\frac{s}{2} - \frac{m}{4}} \). This observation is important as it motivates the definition of the nonstationary Matérn field in Subsection 2.2, which facilitates the theory.

### 2.2 Nonstationary Matérn Models

In this subsection we introduce a family of nonstationary Matérn fields by modifying the SPDE (2.2). We consider a manifold setting which does not hinder the understanding of the modeling and will later allow us to frame the analysis in a concrete setting of applied significance. To that end, we let \( \mathcal{M} \) be an \( m \)-dimensional smooth, connected, compact Riemannian manifold without boundary that is embedded in \( \mathbb{R}^d \). We will let \( \tau \) depend on the spatial variable and replace the Laplacian by an elliptic operator \( \nabla \cdot (\kappa(x) \nabla) \), where differentiation is defined on \( \mathcal{M} \). More precisely, we consider the SPDE

\[
  \left[ \tau(x) I - \nabla \cdot (\kappa(x) \nabla) \right]^{\frac{s}{2}} u(x) = \mathcal{W}(x), \quad x \in \mathcal{M},
\]

where \( \mathcal{W} \) is a spatial white noise with unit variance on \( \mathcal{M} \). The additional \( \kappa \) acts as a change of coordinate \( \tilde{x} = \sqrt{\kappa(x)} x \) and introduces a factor of \( \kappa(x)^{-\frac{m}{2}} \) for the marginal variance, whence the field \( u(x) \) in equation (2.5) has marginal variance proportional to \( \tau(x)^{\frac{s}{2} - s} \kappa(x)^{-\frac{m}{2}} \) at each location. This motivates defining a nonstationary Matérn field through the following Karhunen-Loéve expansion, analogous to (2.4),

\[
  u(x) := \tau(x)^{\frac{s}{2} - \frac{m}{4}} \kappa(x)^{\frac{m}{4}} \sum_{i=1}^{\infty} \left[ \lambda^{(i)} \right]^{-\frac{s}{2}} \xi^{(i)}(x),
\]

where \( \{\xi^{(i)}\}_{i=1}^{\infty} \) is a sequence of independent standard normal random variables and \( \{\lambda^{(i)}, \psi^{(i)}\}_{i=1}^{\infty} \) are the eigenpairs of \( \mathcal{L}^r := \tau I - \nabla \cdot (\kappa \nabla) \). Indeed, \( \mathcal{L}^r \) is self-adjoint with respect to the \( L^2(\mathcal{M}) \) inner product and admits an eigenbasis. Again (2.6) should be interpreted as a sample from the Gaussian measure \( \mathcal{N}(0, [\mathcal{L}^r]^{-s}) \), normalized by the marginal variance at each point. For the theory outlined in Section 4 we will assume that \( \tau \) is Lipschitz, \( \kappa \) is continuously differentiable and both are bounded from below by a positive constant. The idea of viewing the functions \( \tau \) or \( \kappa \) as hyperparameters and learning them from data has been investigated in [32, 71, 66, 33, 95] and has motivated the need to penalize the complexity of priors [34]. We note that other approaches to introduce nonstationarity that do not stem directly from the SPDE formulation have been considered in the literature (e.g. [3, 44, 56, 65, 74]).
Remark 2.1. The normalizing factors $\tau(x)^{2} - \frac{m}{2} \kappa(x)^{2}$ are crucial in that they balance the marginal variances at different locations. To gain more intuition on the powers, consider the case where both $\tau$ and $\kappa$ are constant. Weyl's law then implies that the eigenvalues of $\mathcal{L}_{\tau,\kappa}$ satisfy

$$\lambda^{(i)} \asymp \tau + C \kappa \frac{i}{m},$$

and therefore

$$E \left\| \sum_{i=1}^{\infty} \left( \lambda^{(i)} \right)^{-\frac{s}{2}} \xi^{(i)} \psi^{(i)} \right\|_{L^2(M)}^2 \asymp \sum_{i=1}^{\infty} \left[ \tau + C \kappa \frac{i}{m} \right]^{-s} \times \sum_{i; \tau \geq \kappa \frac{i}{m}} \tau^{-s} + \sum_{i; \tau \leq \kappa \frac{i}{m}} \kappa^{-s} \frac{i^2}{m} \times \tau^{-s} \left( \frac{\tau}{\kappa} \right)^{-\frac{m}{2}} + \kappa^{-s} \int_{\left( \frac{\tau}{\kappa} \right)^{-\frac{m}{2}}}^{\infty} \frac{2i}{m} \, dx \times \tau^{-\frac{m}{2}} \kappa^{-\frac{m}{2}}.$$

Remark 2.2. Both parameters $\tau$ and $\kappa$ control the local length scales of the sample paths. To see this, notice that in the Karhunen-Loéve expansion for the stationary case (2.4), $\tau$ acts as a threshold on the essential frequencies of the samples. Only those frequencies with corresponding eigenvalue on the same order of $\tau$ have effective contributions. Hence a large $\tau$ incorporates higher frequencies and gives sample paths with small length scale. When $\tau$ depends on $x$ it induces a different length scale at different locations.

To see the effect of $\kappa$, notice that the coordinate transformation $\sqrt{\kappa(x)}I$ rescales the original distances by $1/\sqrt{\kappa(x)}$ and the effective distances to have the same correlations as before are scaled by $\sqrt{\kappa(x)}$ correspondingly. Hence a large $\kappa$ implies larger effective distances, which results in smaller local variations and larger length scales. Therefore $\tau$ and $\kappa$ play the opposite role, as demonstrated in Figure 1.

Figure 1 Draws from nonstationary GFs; left: $\kappa = 0.01; \tau = \exp(\cos(x))$; right: $\kappa = \exp(\cos(x)), \tau = 100.$
3 GMRF Approximation with Graph Representations of SPDEs

In this section we study GMRF approximations of the Matérn models introduced in Section 2. Since the work [59], a burgeoning literature has been devoted to linking GFs and GMRFs, doing the modeling with the former and computations with the latter [4]. The main idea of [59] is to introduce a stochastic weak formulation of the SPDE (2.2) and then construct a finite element (FEM) representation of the solution

$$u(x) = \sum_{k=1}^{n} w_k \varphi_k(x),$$

where $n$ is the number of vertices in the triangulation, $\{\varphi_k\}$ are interpolating piecewise linear hat functions and $\{w_k\}$ are Gaussian distributed weights. Importantly, these finite dimensional representations allow to obtain a GMRF precision matrix with computational cost $O(n)$. The convergence of the FEM representation to the GF has been studied in [59] and in more generality in [17, 19, 20].

The FEM representation requires triangulation of the domain, possibly adding artificial nodes to obtain a suitable mesh, and in practice it is rarely implementable in dimension higher than 3. However for many applications e.g. in machine learning, interest lies in interpolating or classifying input data in high dimensional ambient space with moderate but unknown intrinsic dimension, making FEM representations of GFs impractical. Graph Laplacians, discussed next, provide a canonical way to construct GMRF approximations in the given point cloud.

3.1 Graph Matérn Models

Let $(X, W)$ be a geometric graph with $X = \{x_1, \ldots, x_n\}$ a collection of $n$ distinct points (the graph nodes) and $W \in \mathbb{R}^{n \times n}$ a symmetric weight matrix whose entries $W_{ij} \geq 0$ prescribe the closeness between points. In applications including classification and regression, each graph node will represent either a feature or an auxiliary point used to improve the accuracy of the GMRF approximations described in this subsection.

Several definitions of graph Laplacians co-exist in the literature. Defining $D := \text{diag}(d_1, \ldots, d_n)$ the degree matrix with $d_i := \sum_{j=1}^{n} W_{ij}$, three popular choices are unnormalized $\Delta_n^{un} := D - W$, symmetric $\Delta_n^{sym} := D^{-1/2} \Delta_n^{un} D^{-1/2}$ and random-walk $\Delta_n^{rw} := D^{-1} \Delta_n^{un}$ graph Laplacians, see [92]. To streamline the presentation, we use $\Delta_n \in \mathbb{R}^{n \times n}$ as placeholder for a graph Laplacian with $n$ data points; its choice will be made explicit whenever it is relevant to the problem at hand.

To gain some intuition, let us consider the unnormalized graph Laplacian, whose positive semi-definiteness is verified by the relation

$$u_n^T (D - W) u_n = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} W_{ij} |u_n(i) - u_n(j)|^2 \geq 0. \quad (3.1)$$

Here $u_n = [u_n(1), \ldots, u_n(n)]^T \in \mathbb{R}^n$ is an arbitrary vector in $\mathbb{R}^n$, interpreted as a function on $X$ with the identification $u_n(x_i) \equiv u_n(i)$. Note that $\Delta_n^{un} = D - W$ annihilates constant vectors (in agreement with the intuition that the Laplacian annihilates constant functions) and 0 is always an eigenvalue. For a fully connected graph, one can see that the eigenvalue 0 has multiplicity 1, with the constant vectors as its only eigenspace. If we consider $N(0, \Delta_n^{-1})$ as a degenerate Gaussian
distribution in $\mathbb{R}^n$ with support on the orthogonal complement of the constant vectors, then (3.1) is the negative log-density of this distribution, which suggests that functions that take similar values on close nodes are favored, with closeness quantified by the weight matrix $W$. Moreover, it can be shown that the second eigenvector $\psi_n^{(2)}$ of $\Delta_n$ solves a relaxed graph cut problem \cite{92} so that $\psi_n^{(2)}$ encodes crucial information about partition of the points $x_i$’s. Hence $N(0, \Delta_n^{-1})$ naturally serves as a prior for clustering and classification \cite{12}. Various choices of the weight matrix have been considered in the literature, including $\varepsilon$-graphs and $k$-NN graphs. Both of them introduce sparsity in the weight matrix, which is inherited by the graph Laplacian. Under such circumstances, the graph Laplacian can be viewed as a sparse precision matrix, which gives rise to a GMRF.

It is important to note that the preceding discussion makes no assumption on the points $x_i$ or how their closeness is defined. For instance, the points may represent books and their closeness may be based on a reader’s perception of similarity between them. However, an important example in which we will frame our theoretical investigations arises from making a manifold assumption.

**Assumption 3.1 (Manifold Assumption).** The points $x_i$ are independently sampled from the uniform distribution $\gamma$ on an $m$-dimensional smooth, connected, compact manifold $M$ without boundary that is embedded in Euclidean space $\mathbb{R}^d$, with bounded sectional curvature and Riemannian metric inherited from $\mathbb{R}^d$.

To emphasize the stronger structure imposed by the manifold assumption we denote the point cloud by $X \equiv M_n = \{x_1, \ldots, x_n\} \subset M$. For many applications, the manifold assumption is an idealization of the fact that the point cloud has low dimensional structure despite living in a high dimensional ambient space, e.g., the MNIST dataset that we will study in Subsection 5.4. From a theoretical viewpoint, Assumption 3.1 allows us to establish a precise link between graph Laplacians and their continuum counterparts, as we now describe heuristically. Define the weight matrix $W$ on $M_n$ by

$$W_{ij} := \frac{2(m+2)}{m \nu_m h_n^{m+2}} \mathbf{1}\{|x_i - x_j| < h_n\},$$

where $|\cdot|$ is the Euclidean distance in $\mathbb{R}^d$, $h_n$ is the graph connectivity and $\nu_m$ is the volume of the $m$-dimensional unit ball. Then the unnormalized graph Laplacian $\Delta_n \text{un}$ is a discrete approximation of the Laplace-Beltrami operator $-\Delta$ on $M$.

Indeed, for a smooth function $f : \mathbb{R}^m \to \mathbb{R}$ we have by Taylor expansion

$$\int_{B_h(x)} [f(y) - f(x)] dy \approx \int_{B_h(x)} \nabla f(x)^T (y - x) dy + \frac{1}{2} \int_{B_h(x)} (y - x)^T \nabla^2 f(x) (y - x) dy.$$  

By symmetry, the first integral is zero and the second integral reduces to

$$\frac{1}{2} \sum_{i=1}^{m} \frac{\partial^2 f}{\partial x_i^2}(x) \int_{B_h(0)} z_i^2 = \frac{\nu_m h_n^{m+2}}{2(m+2)} \Delta f(x).$$

This gives

$$-\Delta f(x_i) \approx \frac{2(m+2)}{\nu_m h_n^{m+2}} \int_{B_h(x_i)} [f(x_i) - f(y)] dy \approx \sum_{j=1}^{n} W_{ij} [f(x_i) - f(x_j)],$$

(3.2)
which is exactly the way $\Delta_n$ is defined. Since $\mathcal{M}$ is locally homeomorphic to $\mathbb{R}^m$ and the geodesic distance between any two points is well approximated by the Euclidean distance, the heuristic argument above can be formalized to show point-wise convergence of $\Delta_n$ to $-\Delta$ in the manifold case. A rigorous result on spectral convergence will be given in more generality in Section 4.

The previous discussion suggests to introduce the following discrete analog to equation (2.2)

$$ (\tau I_n + \Delta_n)^\frac{1}{2} u_n = \mathcal{W}_n, $$

where $\mathcal{W}_n$ is an $n$-dimensional standard random variable and the marginal variance is set to be $\tau^2 q^{-s}$, which in the covariance operator form is $\mathcal{N}(0, \tau^{s-\frac{1}{2}}(\tau I + \Delta_n)^{-s})$. From here we define a stationary graph Matérn field through the Karhunen-Loève expansion

$$ u_n := \tau^\frac{s}{2} - \frac{D}{q} \sum_{i=1}^n \left[ \tau + \lambda_n^{(i)} \right]^{-\frac{s}{2}} \xi_n^{(i)} f_n^{(i)}, $$

(3.3)

where $\{\xi_n^{(i)}\}_{i=1}^n$ are independent standard normal random variables and $\{(\lambda_n^{(i)}, \phi_n^{(i)})\}_{i=1}^n$ are eigenpairs of $\Delta_n$. Equation (3.3) is a natural finite dimensional approximation of (2.4) and one should expect that spectral convergence of $\Delta_n$ towards $-\Delta$ will translate into convergence of (3.3) towards (2.4) in the large $n$ limit. This will be rigorously shown in Section 4.

**Remark 3.2.** The above construction can be adapted when the points $x_i$ are distributed according to a Lipschitz density $q$ that is bounded below and above by positive constants. In this case, (3.2) should take the form

$$ -\Delta f(x_i) \approx \sum_{j=1}^n W_{ij}[f(x_i) - f(x_j)] q(x_j)^{-1} \approx \frac{1}{2} \sum_{j=1}^n W_{ij}[f(x_i) - f(x_j)] [q(x_i)^{-1} + q(x_j)^{-1}], $$

where the last step follows from the Lipschitzness of $q$ and the fact that $q^{-1}$ is bounded away from 0 and is needed to ensure symmetry of the new weights. Setting $f = q$ in (3.2) we have

$$ q(x_i) \approx \frac{1}{\nu_m h_m^m} \int_{B_{h_n}(x_i)} q(y) dy - h_n^2 \Delta q(x_i) \approx \frac{1}{n \nu_m h_n^m} \sum_{j=1}^n 1\{|x_i - x_j| < h_n\} := q_{h_n}(x_i) $$

where we have dropped $h_n^2 \Delta q$ since it is of lower order. Hence the new weights should be adjusted as

$$ W_{ij} = \frac{m + 2}{m \nu_m h_n^{m+2}} 1\{|x_i - x_j| < h_n\} [q_{h_n}(x_i)^{-1} + q_{h_n}(x_j)^{-1}]. $$

### 3.2 Nonstationary Graph Matérn Models

Now we are ready to construct nonstationary graph Matérn fields that approximate the nonstationary Matérn field in Section 2.2. In analogy with the previous subsection, the crucial step is to obtain a graph discretization of the operator $\mathcal{L}^{\tau, \kappa} = \tau I - \nabla \cdot (\kappa \nabla)$ with spatially varying $\tau$ and $\kappa$. Notice that we have

$$ \nabla \cdot (\kappa \nabla f) = \sqrt{\kappa} \Delta (\sqrt{\kappa} f) - f \Delta \sqrt{\kappa}. $$
Applying (3.2) to $\Delta(\sqrt{\kappa}f)$ and $f\Delta\sqrt{\kappa}$ gives

$$-\nabla \cdot (\kappa \nabla f) \approx \int_{B(x)} \sqrt{\kappa(x)\kappa(y)} \left[ f(x) - f(y) \right] \approx \sum_{i=1}^{n} W_{ij} \sqrt{\kappa(x_i)\kappa(x_j)} \left[ f(x_i) - f(x_j) \right].$$

Hence $-\nabla \cdot (\kappa \nabla \cdot)$ can be approximated by $\Delta_n^\kappa = \tilde{D} - \tilde{W}$, where

$$\tilde{W}_{ij} = W_{ij} \sqrt{\kappa(x_i)\kappa(x_j)} = \frac{2(m + 2)}{mn\varepsilon_n} \left\{ \frac{1}{2} \left[ |x_i - x_j| < \varepsilon_n \right] \right\} \sqrt{\kappa(x_i)\kappa(x_j)}, \quad (3.4)$$

$$\tilde{D}_{ii} = \sum_{j=1}^{n} \tilde{W}_{ij}. \quad (3.5)$$

Now we can define the discrete analog of equation (2.5) as

$$(\tau_n + \Delta_n^\kappa)^{1/2} u_n = W_n,$$

where $\tau_n = \text{diag}(\tau(x_1), \ldots, \tau(x_n))$ and the marginal variance is set to be $\tau(x_i)^{2-s} \kappa(x_i)^{-\frac{m}{2}}$ at each point. Denoting $\kappa_n = \text{diag}(\kappa(x_1), \ldots, \kappa(x_n))$, we define —similarly as in Subsection 2.2— the nonstationary graph Matérn field through the Karhunen-Loéve expansion

$$u_n := \tau_n^{s/2} \kappa_n^{-\frac{m}{2}} \sum_{i=1}^{n} \left[ \lambda_n^{(i)} \right]^{-s} \xi(i) \psi_n^{(i)}, \quad (3.6)$$

where $\{\xi(i)\}_{i=1}^{n}$ are independent standard normal random variables and $\{\lambda_n^{(i)}, \psi_n^{(i)}\}_{i=1}^{n}$ are eigenpairs of $L_n^{\tau,\kappa} := \tau_n + \Delta_n^\kappa$. In the covariance operator view, $u_n$ follows a Gaussian distribution $N(0, C_n^{\tau,\kappa})$ with

$$C_n^{\tau,\kappa} := \tau_n^{s/2 - \frac{m}{4}} \kappa_n^{-\frac{m}{2}} \left[ L_n^{\tau,\kappa} \right]^{s-2} \kappa_n^{-\frac{m}{2}} \tau_n^{s-\frac{m}{4}}. \quad (3.7)$$

The representation (3.7) is useful for implementation in that, when $s \in \mathbb{N}$, one only needs to do Cholesky decomposition on $L_n^{\tau,\kappa}$ to generate samples from $N(0, \left[ L_n^{\tau,\kappa} \right]^{-s})$ and then multiply by the diagonal matrix $\tau_n^{s/2 - \frac{m}{4}} \kappa_n^{-\frac{m}{4}}$. Moreover, the covariance matrix for general $s$ is computable by performing a spectral decomposition on $L_n^{\tau,\kappa}$, extending the $s \in \mathbb{N}$ restriction in [59]. The case of fractional smoothness is also studied in [17] where a rational approximation is employed, giving a GMRF approximation.

**Remark 3.3.** As discussed in Remark 2.2, both $\tau_n$ and $\kappa_n$ control the local length scale. For many applications e.g. in machine learning, we shall focus on the modeling choice with $\tau_n$ only, because the operator $\nabla \cdot (\kappa \nabla)$ is less motivated for general $x_i$’s that do not come from a manifold. In such cases, one can construct a nonstationary Matérn field similarly as above, by using a graph Laplacian built with the $x_i$’s, e.g. with a $k$-NN graph. Indeed, the only key step is to normalize properly the marginal variances, which are largely determined by the growth of the spectrum as in Remark 2.1. Hence one can find an integer $m$ so that the first several $\lambda_n^{(i)}$’s grow roughly as $\frac{i^2}{m}$ and use $m$ as an effective dimension of the problem for normalization. Moreover, both the $k$-NN and $\varepsilon$-graphs result in sparsity in $\Delta_n$, and numerical linear algebra techniques can be employed to attain speed-up. □
4 Convergence of Graph Representations of Matérn Models

In this section we study the convergence of graph representations of GFs under Assumption 3.1. The analysis will generalize existing literature to cover the nonstationary models introduced in Subsection 3.2, obtaining new rates of convergence and suggesting a suitable topology in which to formalize the results.

4.1 Setup and Main Result

Recall from (2.6) and (3.6) that draws from the continuum and graph Matérn fields have Karhunen-Loève expansions

\begin{align}
    u &= \tau^{\frac{d}{2}} \frac{m}{\kappa} \sum_{i=1}^{n} \left[ \lambda(i) \right]^2 \xi(i) \psi(i), \\
    u_n &= \tau_n^{\frac{d}{2}} \frac{m}{\kappa} \sum_{i=1}^{n} \left[ \lambda_n(i) \right]^2 \xi(i) \psi(i).
\end{align}

We seek to establish convergence of \( u_n \) towards \( u \). First we need to find a suitable metric. Since \( u \) has continuum domain \( \mathcal{M} \) and \( u_n \) has discrete domain \( \mathcal{M}_n \), it is natural to relate them by a transport map, using ideas from optimal transport.

We work under Assumption 3.1 that the \( x_i \)'s are independent samples from the uniform distribution \( \gamma \) on \( \mathcal{M} \) and let \( \gamma_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \) be the empirical distribution of \( \mathcal{M}_n = \{ x_1, \ldots, x_n \} \). A transport map \( T : \mathcal{M} \to \mathcal{M}_n \) is a measurable transformation so that \( T\gamma = \gamma_n \), i.e., \( \gamma_n \) equals the push-forward of \( \gamma \) under \( T \) and so \( \gamma(T^{-1}(U)) = \gamma_n(U) \) for all measurable \( U \). If we let \( U_i = T^{-1}(\{x_i\}) \), then the \( U_i \)'s form a partition of \( \mathcal{M} \) and \( u_n \circ T \) is a piecewise constant interpolation of \( u_n \) so that it is now a function on \( \mathcal{M} \). Intuitively, if \( \gamma_n \) is close to \( \gamma \) and the transport map \( T \) allocates points in \( \mathcal{M} \) to \( \mathcal{M}_n \) properly, then \( u_n \circ T \) will be close to \( u \) in \( L^2(\gamma) \). This motivates the choice of \( TL^2 \) metric proposed by [37]. The idea is to view the functions \( u \) and \( u_n \) as points in the \( TL^2 \) space, defined as

\[ TL^2 := \{ (\mu, f) : \mu \in \mathcal{P}(\mathcal{M}), f \in L^2(\mu) \}, \]

endowed with the metric

\[ d_{TL^2}(\mu_1, \mu_2) := \inf_{\omega \in \mathcal{C}(\mu_1, \mu_2)} \left[ \int_{\mathcal{M}} \int_{\mathcal{M}} \left( d_\mathcal{M}(x, y)^2 + |f_1(x) - f_2(y)|^2 \right) d\omega(x, y) \right]^\frac{1}{2}, \]

where \( \mathcal{C} \) is the set of couplings between \( \mu_1 \) and \( \mu_2 \) and \( d_\mathcal{M} \) is the geodesic distance on \( \mathcal{M} \). In particular, we will study the \( TL^2 \) distance between the pairs \((\gamma_n, u_n)\) and \((\gamma, u)\). Given a transport map \( T : \mathcal{M} \to \mathcal{M}_n \), we can associate it with a coupling defined as \( \omega_T := (I \times T)^* \gamma \), the push-forward of \( \gamma \) under \( I \times T : \mathcal{M} \to \mathcal{M} \times \mathcal{M}_n \), where \( (I \times T)(x) = (x, T(x)) \). Hence we see that

\[ d_{TL^2}(\gamma_n, u_n, \gamma, u) \leq \inf_{T : T\gamma = \gamma_n} \left[ \int_{\mathcal{M}} \left( d_\mathcal{M}(x, T(x))^2 + |u_n(T(x)) - u(x)|^2 \right) d\gamma(x) \right]^\frac{1}{2}, \]

which makes precise the connection with the transport maps that we mentioned above. Moreover, if we restrict attention to measures that are absolutely continuous with respect to the volume form on \( \mathcal{M} \), then the right-hand side of (4.3) defines a metric on the corresponding subset of \( TL^2 \) and
generates the same topology as $d_{TL}^2$ [37]. Before stating our main result, we recall that the $\infty$-OT distance between $\gamma_n$ and $\gamma$ is defined by

$$\varepsilon_n = d_{\infty}(\gamma_n, \gamma) := \min_{T: T\gamma = \gamma_n} \text{ess sup}_{x \in \mathcal{M}} d_{\mathcal{M}}(x, T(x)).$$

Intuitively $\varepsilon_n$ quantifies how well the point cloud $\mathcal{M}_n$ approximates $\mathcal{M}$ and represents the smallest scale of variations that the point cloud can resolve. With the above setup, we have the following result.

**Theorem 4.1.** Suppose $\tau$ is Lipschitz, $\kappa \in C^1(\mathcal{M})$ and both are bounded below by positive constants. Suppose further $s > 2m$ and the graph connectivity $h_n$ satisfies

$$\frac{(\log n)^{c_m}}{n^{1/m}} \ll h_n \ll \frac{1}{n^{1/s}},$$

where $c_m = 3/4$ if $m = 2$ and $c_m = 1/m$ otherwise. Then with probability one

$$\mathbb{E}[d_{TL}^2((\gamma_n, u_n), (\gamma, u))] \leq C_{M, \tau, \kappa, s} \left[ \sqrt{n k_n^{-\frac{s}{m}}} + k_n^{-\frac{s}{m}} + \varepsilon_n + \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{-\frac{1}{m}} \right)^{\frac{1}{2}} \right],$$

where $k_n$ is chosen so that $n^{m/s} \ll k_n \ll h_n^{-m}$. 

**Remark 4.2.** The almost sure nature of Theorem 4.1 stems from Proposition 4.3 below which guarantees that, in a precise sense, the sequence $\{x_n\}_{n=1}^\infty$ approximates $\mathcal{M}$ accurately with probability 1. Note that $k_n$ is well defined by the upper bound in (4.4).

### 4.2 Outline of Proof

From the Karhunen-Loéve expansions (4.1) and (4.2) it is clear that the fundamental step in analyzing the convergence of the graph representations is to obtain bounds for both the eigenvalue and eigenfunction approximations. Appropriate choice of the graph connectivity $h_n$ is essential. Intuitively, we need $h_n \to 0$ so that finer scales are resolved as the sample size $n$ grows, but $h_n$ should not decrease too quickly. By [38][Theorem 2] and Borel-Cantelli, we have the following

**Proposition 4.3.** There is a constant $C$ such that, with probability one, there exists a sequence of transport maps $T_n : \mathcal{M} \to \mathcal{M}_n$ so that $\gamma_n = T_n \gamma$ and

$$\limsup_{n \to \infty} \frac{n^{1/m}}{(\log n)^{c_m}} \sup_{x \in \mathcal{M}} d(x, T_n(x)) \leq C,$$

where $c_m = 3/4$ if $m = 2$ and $c_m = 1/m$ otherwise.

Proposition 4.3 guarantees that $\varepsilon_n \lesssim \frac{(\log n)^{c_m}}{n^{1/m}}$. Since $\varepsilon_n$ represents the finest scale on the point cloud, the graph connectivity should be much larger than $\varepsilon_n$ to capture the local geometry, which explains the lower bound for $h_n$ in Theorem 4.1. The upper bound on $h_n$ is so that higher frequencies of $L_n^{\tau, \kappa}$ do not accumulate in the large $n$ limit. Denote $\{(\lambda^{(i)}_n, \psi^{(i)}_n)\}_{i=1}^n$ and $\{(\lambda^{(i)}, \psi^{(i)})\}_{i=1}^\infty$ as the eigenpairs of $L_n^{\tau, \kappa}$ and $L^{\tau, \kappa}$ with increasing eigenvalues, as both of them are self-adjoint and positive definite. We have the following results on spectral approximations:
Theorem 4.4 (Eigenvalue Approximation). Suppose \( k := k_n \) is such that \( h_n \sqrt{\lambda(k_n)} \ll 1 \) for \( n \) large. Then
\[
\left| \frac{\lambda_n^{(k)} - \lambda(k)}{\lambda(k)} \right| \leq C_{\mathcal{M}, \tau, \kappa} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)} \right),
\]
where \( C_{\mathcal{M}, \tau, \kappa} \) is a constant depending on \( \mathcal{M}, \tau, \kappa \).

Theorem 4.5 (Eigenfunction Approximation). Let \( \lambda \) be an eigenvalue of \( L^{\tau, \kappa} \) with multiplicity \( \ell \), i.e.,
\[
\lambda^{(k_n-1)} < \lambda(k_n) = \lambda = \ldots = \lambda(k_n+\ell-1) < \lambda(k_n+\ell).
\]

Suppose that \( h_n \sqrt{\lambda(k_n)} \ll 1 \) for \( n \) large. Let \( \psi_n^{(k_n)}, \ldots, \psi_n^{(k_n+\ell-1)} \) be orthonormal eigenvectors of \( L_n^{\tau, \kappa} \) associated with eigenvalues \( \lambda_n^{(k_n)}, \ldots, \lambda_n^{(k_n+\ell-1)} \). Then there exists orthonormal eigenfunctions \( \psi(k_n), \ldots, \psi(k_n+\ell-1) \) of \( L^{\tau, \kappa} \) so that, for \( j = k_n, \ldots, k_n + \ell - 1 \),
\[
\| \psi_n^{(j)} \circ T_n - \psi^{(j)} \|_{L^2}^2 \leq C_{\mathcal{M}, \tau, \kappa} j^3 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(j)} \right),
\]
where \( \{T_n\}_{n=1}^\infty \) is a sequence of transport maps as in Proposition 4.3.

Remark 4.6. The assumption that \( h_n \sqrt{\lambda(k_n)} \ll 1 \) for \( n \) large is crucial in that the spectral approximations are only provably accurate up to the \( k_n \)-th eigenvalue and eigenfunction. By Weyl’s law and the assumptions on \( \tau \) and \( \kappa \), we have by the minimax principle that \( \lambda(i) \asymp i^{2/3} \), which motivates the choice that \( k_n \ll h_n^{-m} \). The paper [40] proposed an alternative approach to obtain consistency where, by definition, graph-based frequencies beyond the \( k_n \)-th level are discarded.

Theorems 4.4 and 4.5 are proved in Appendix B and C respectively. The proofs follow the arguments in [23] and [38]. Theorem 4.4 is proved by showing a lower and an upper bound. The idea for proving the lower (upper) bound is to introduce an interpolation (projection) map that is almost an isometry and does not increase the corresponding Dirichlet energies. More precisely, we will introduce an interpolation map \( \mathcal{I} : L^2(\gamma_n) \rightarrow L^2(\gamma) \) so that for \( \psi_n \in V := \text{span}\{\psi_n^{(1)}, \ldots, \psi_n^{(k)}\} \), the span of the first \( k \) eigenfunctions of \( L_n^{\tau, \kappa} \),
\[
\| \mathcal{I}\psi_n \|_{L^2}^2 \geq (1 - \sigma_1 \sqrt{\lambda(k)}) \| \psi_n \|_{L^2}^2,
\]
\[
\langle \mathcal{I}\psi_n, L_n^{\tau, \kappa} \mathcal{I}\psi_n \rangle_{L^2} \leq (1 + \sigma_2) \langle \psi_n, L_n^{\tau, \kappa} \psi_n \rangle_{L^2},
\]
where \( \sigma_1 \) and \( \sigma_2 \) are small quantities depending on \( \varepsilon_n \) and \( h_n \). For an appropriately chosen \( k \), \( \mathcal{I} \) is injective when \( n \) is large and \( V = \mathcal{I}(V) \) has dimension \( k \). Hence the minimax principle implies
\[
\lambda(k) \leq \max_{f \in V \setminus 0} \frac{\langle f, L_n^{\tau, \kappa} f \rangle_{L^2}}{\| f \|_{L^2}^2} = \max_{\psi_n \in V \setminus 0} \frac{\langle \mathcal{I}\psi_n, L_n^{\tau, \kappa} \mathcal{I}\psi_n \rangle_{L^2}}{\| \mathcal{I}\psi_n \|_{L^2}^2} \leq \left( \frac{1 + \sigma_2}{1 - \sigma_1 \sqrt{\lambda(k)}} \right) \max_{\psi_n \in V \setminus 0} \frac{\langle \psi_n, L_n^{\tau, \kappa} \psi_n \rangle_{L^2}}{\| \psi_n \|_{L^2}^2} = \left( \frac{1 + \sigma_2}{1 - \sigma_1 \sqrt{\lambda(k)}} \right) \lambda(k).
\]
The upper bound for \( \lambda_n^{(k)} \) is proved similarly with a projection map.
For Theorem 4.5 the idea is to bound for $\psi_n^{(k)}$ a $\lambda_n^{(k)}$-eigenfunction of $L_{n,\kappa}^{\tau}$ the term

$$\|\mathcal{I}\psi_n^{(k)} - \mathbb{P}_{(\lambda^{(k)}-c,\lambda^{(k)}+a)}^\tau\psi_n^{(k)}\|,$$

where $\mathbb{P}_{(\lambda^{(k)}-c,\lambda^{(k)}+a)}^\tau$ is the orthogonal projection onto the space spanned by eigenfunctions of $L_{n,\kappa}^{\tau}$ associated with eigenvalues in the interval $(\lambda^{(k)} - c, \lambda^{(k)} + a]$. The numbers $a$ and $c$ are chosen so that the interval $(\lambda^{(k)} - c, \lambda^{(k)} + a]$ only contains $\lambda^{(k)}$ and hence $\mathbb{P}_{(\lambda^{(k)}-c,\lambda^{(k)}+a)}^\tau\psi_n^{(k)}$ is a $\lambda^{(k)}$-eigenfunction of $L_{n,\kappa}^{\tau}$. Then we apply a Gram-Schmidt orthogonalization and use the fact that $\mathcal{I}\psi_n^{(k)}$ will be close to $\psi_n^{(k)} \circ T_n$ to get the desired result.

With Theorem 4.4 and 4.5, Theorem 4.1 is proved by exploiting the Karhunen-Loéve expansions (4.1) and (4.2) and the triangle inequality. The detailed proof is in Appendix D.

5 Numerical Examples

In this section we demonstrate the use of the graph Matérn models introduced in Section 3 by considering applications in Bayesian inverse problems, spatial statistics, and graph-based machine learning.

For the three examples we employ graph Matérn models as priors within the general framework of latent Gaussian models, briefly overviewed in Subsection 5.1. Subsection 5.2 studies a toy Bayesian inverse problem on a manifold setting. Our aim is to compare the modeling of length scale through $\tau_n$ and $\kappa_n$; we further show that the accuracy of the reconstruction with the graph-based approach is satisfactory and that adding nonstationarity may help to overcome the poor performance of more naive hierarchical approaches in large noise regimes. In Subsection 5.3 we investigate the use of graph Matérn fields for interpolating U.S. county-level precipitation data. The graph-based approach has the benefit of not requiring additional nodes and to avoid the pre-processing cost of finite element representations. In addition, it can be directly applied when only pairwise distances between counties are available, without the need of performing multidimensional scaling to reconstruct the configuration of the point cloud. We also compare the performance of stationary and nonstationary graph Matérn models. In Subsection 5.4, a semi-supervised classification problem in machine learning is studied, where the low dimensional structure of the data naturally motivates the graph-based approach; we further show that nonstationary models may improve the classification accuracy over stationary ones.

5.1 A General Framework: Latent Gaussian Models

Latent Gaussian models are a flexible subclass of structured additive regression models defined in terms of a likelihood function, a latent process and hyperparameters. Let $\{x_i\}_{i=1}^n$ be a collection of features that we identify with graph nodes. The observation variable $y$ is modeled as a (possibly noisy) transformation of the latent process $u_n := [u_n(x_1), \ldots, u_n(x_n)]^T$, which conditioned on the hyperparameters follows a Gaussian distribution. Finally, a prior is placed on the hyperparameters. More precisely, we have

$$y|u_n, \mu \sim \pi(y|u_n, \mu),$$

$$u_n|\theta \sim \mathcal{N}(0, Q(\theta)^{-1}),$$

$$\langle \mu, \theta \rangle \sim \pi(\mu, \theta),$$

where
where $Q(\theta)$ is the precision matrix of the latent process and $\mu, \theta$ are hyperparameters. Markov Chain Monte Carlo inference methods are standard in Bayesian inverse problems with complex likelihood functions, but less computationally expensive deterministic approximations are often preferred in other applications. In particular, the integrated nested Laplace approximations proposed by \cite{73} and the corresponding R-INLA package has greatly facilitated inference of such models.

The sparsity of the precision matrix $Q(\theta)$ is crucial for efficient likelihood evaluations and sampling of the latent process. For the problems that we consider, the latent process will be modeled as a graph Matérn field, i.e.,

$$u_n|\tau_n \sim \mathcal{N}\left(0, Q(\tau_n, s)^{-1}\right), \quad Q(\tau_n, s) = \tau_n^{\frac{m}{2}} (\tau_n + \Delta_n)^{\frac{m}{2}},$$  \quad (5.1)\]

where $\Delta_n$ is a graph Laplacian constructed with the $x_i$'s and $\tau_n$ is a diagonal matrix modeling the length scale at each node. We note that the graph Laplacian is often sparse and its sparsity is inherited by $Q(\tau_n, s)$ for integer $s$.

A constant length scale graph Matérn field hyperprior is then placed on $\log(\tau_n)$:

$$\log \tau_n \sim \mathcal{N}\left(0, \nu^{s_0} \tau^{\frac{m}{2}} (\nu I + \Delta_n)^{-s_0}\right),$$  \quad (5.2)\]

where $\nu$ and $s_0$ are chosen by prior belief on the length scale. However, when $n$ is large, learning $\tau_n$ as an $n$-dimensional vector is computationally demanding. We instead adopt a truncated Karhunen-Loéve approximation for $\tau_n$. Recall that $\log(\tau_n)$ has the characterization

$$\log \tau_n = \nu^{s_0} \tau^{\frac{m}{2}} \sum_{i=1}^{n} \left[\nu + \lambda_n^{(i)}\right]^{-s_0} \xi^{(i)} \psi_n^{(i)},$$

where $\xi^{(i)} \sim i.i.d. \mathcal{N}(0, 1)$ and $\{(\lambda_n^{(i)}, \psi_n^{(i)})\}_{i=1}^{n_0}$ are the eigenpairs for $\Delta_n$. Since the $\lambda_n^{(i)}$'s are increasing, the contribution of the higher frequencies is less significant. Hence we consider a truncated expansion and model $\log(\tau_n)$ as

$$\log \tau_n = \nu^{s_0} \tau^{\frac{m}{2}} \sum_{i=1}^{n_0} \left[\nu + \lambda_n^{(i)}\right]^{-s_0} \theta^{(i)} \psi_n^{(i)},$$

where $n_0 \ll n$ is chosen based on the spectral growth and prior belief on $\tau_n$. Now the hyperparameters are the $\theta_i$'s, which are only $n_0$-dimensional, and the hyperprior for each is naturally taken to be the standard normal. Therefore a complete model of our interest in the following sections can be summarized as

$$y|u, \mu \sim \pi(y|u, \mu),$$

$$u|\theta, s \sim \mathcal{N}\left(0, Q(\theta, s)^{-1}\right),$$

\quad (5.3)\]

$$\mu, s \sim \mathcal{N}(0, I_{n_0}),$$

\quad (5.4)\]

where

$$Q(\theta, s) = [\tau_n(\theta)]^{\frac{m}{2}} [\tau_n(\theta) + \Delta_n]^{\frac{m}{2}} [\tau_n(\theta)]^{\frac{m}{2}},$$

\quad (5.5)\]

$$\log \tau_n(\theta) = \nu^{s_0} \tau^{\frac{m}{2}} \sum_{i=1}^{n_0} \left[\nu + \lambda_n^{(i)}\right]^{-s_0} \theta^{(i)} \psi_n^{(i)},$$

\quad (5.6)\]
Remark 5.1. Suppose for illustration that we are interested in the simple regression problem of inferring a Matérn field $u(x)$ based on data $y$ comprising Gaussian measurement of $u$ at given locations/features $x_1, \ldots, x_n$. As noted in the introduction, the computation cost scales as $\mathcal{O}(n^3)$. However, by modeling $u_n$ using a graph Matérn model we obtain a GMRF approximation, with sparse precision matrix, dramatically reducing the computational cost. Thus, one could introduce further auxiliary nodes $x_{n+1}, \ldots, x_N$ with $N \gg n$ to improve the prior GMRF approximation of the original Matérn model and still reduce the computational cost over formulations based on GF priors. Such ideas arise naturally in semi-supervised applications in machine learning where most features are unlabeled, but can also be of interest in applications in spatial statistics, as discussed in [72][Chapter 5] and grant further investigation in Bayesian inverse problems.

Remark 5.2. There should be an additional parameter controlling the marginal variance of the latent process $u_n$ as in (5.3), but this parameter can be tuned and fixed easily by matching the scales of $u_n$ and the data $y$. Indeed, the normalizing factors $\tau_n^{m/4-s/2}$ guarantee that $\mathbb{E}|u_n|^2$ are roughly the same for different $\tau_n$’s. Hence one can for instance estimate $\mathbb{E}|u_n|^2$ by setting $\tau_n \equiv 1$ and normalize the observations $y$ by $\sqrt{\mathbb{E}|u_n|^2}/|y|^2$.

Similarly, we need to tune for the marginal variance of the hyperparameters as in (5.2). As $\tau_n$ essentially acts as a cut off on the significant frequencies, this can be done by matching the scale of $\tau_n$ with the eigenvalues of $\Delta_n$ based on one’s prior belief.

5.2 Application in Bayesian Inverse Problems

In this subsection we investigate the use of nonstationary graph Matérn models to define prior distributions in Bayesian inverse problems. For simplicity of exposition and to avoid distraction from our main purpose of illustrating the modeling of the nonstationarity, we consider a toy example taken from the inverse problem literature [71]. The ideas presented here apply immediately to Bayesian inverse problems with more involved likelihood functions, defined for instance in terms of the solution operator of a differential equation [46, 15].

We study the reconstruction of a signal function given noisy but direct point-wise observations. The domain of the problem is taken to be the unit circle, where the hidden signal $u^\dagger$ is parametrized by $t \in [0, 2\pi)$ as

$$u^\dagger(t) = \begin{cases} 
\exp\left(4 - \frac{\pi^2}{t(\pi-t)}\right), & t \in (0, \pi), \\
1, & t \in [\pi + 0.5, 1.5\pi], \\
-1, & t \in (1.5\pi, 2\pi - 0.5], \\
0, & \text{otherwise}.
\end{cases}$$

Hence if $x = (\cos(t), \sin(t))$ for $t \in [0, 2\pi)$, then $u^\dagger(x)$ is understood as $u^\dagger(t)$. Such signal is considered in [71] for its varying length scale, where the domain is the interval $[0, 10] \subset \mathbb{R}$ and a uniform grid finite difference discretization is used to define a Matérn prior following the SPDE approach. Here we suppose instead to have only indirect access to the domain through $n = 1000$ points $x_i$’s that are drawn independently from the uniform distribution on the circle, and use a graph Matérn model.

We assume to be given noisy observations of the signal at $J = n/2$ points:

$$y(x_i) = u^\dagger(x_i) + \eta_i, \quad \eta_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \ldots, J,$$  \hspace{1cm} (5.7)
where σ is set to be 0.1 and we have observations at every other node. To recover the signal function at the nodes \( x_i \)'s, we adopt a hierarchical Bayesian approach which we cast into the framework of latent Gaussian models. More precisely, the observation equation (5.7) gives the likelihood model

\[
y|u_n \sim \mathcal{N}(Su_n, \sigma^2 I_J),
\]

where \( S \in \mathbb{R}^{J \times n} \) is a matrix of 0 and 1's that indicates the location of the observations. The latent process \( u_n := [u^*(x_1), \ldots, u^*(x_n)]^T \) and the hyperparameters are modeled as in Section 5.1, where the smoothness is fixed as \( s = 2 \) and the other parameters are chosen as \( s = 2, s_0 = 1, \nu = 1, n_0 = 21 \).

We note that by setting \( s_0 = 1 \), the hyperprior is actually an approximation of a zero-mean Gaussian process with exponential covariance function, where the sample paths can undergo sudden changes. The choice \( n_0 = 21 \) is motivated by the fact that the Laplacian on the circle has spectrum \( \{i^2\}_{i=0}^\infty \), where any non-zero eigenvalue has multiplicity 2. Together with the choices \( s_0 = 1, \nu = 10 \) we see that the coefficients in the expansion (5.6) have decreased by a factor of 10 after the \( n_0 \)-th eigenfunction, and therefore higher frequencies are not very consequential. The graph Laplacian is constructed as in Section 3.1 with connectivity \( \varepsilon_n = 4 \times n^{-1/8} \).

**Algorithm 5.1** Posterior sampling \( u, \tau | y \)

Initialize \( u_0^n, \theta^0 \) and set step size \( \beta_0 \).

for \( i = 1, \ldots, M \) do

(a) Generate \( \xi \sim \mathcal{N}(0, I_{J+n}) \) and update

\[
u^n = \left[ \begin{array}{c} \sigma^{-1} S \\ L(\theta_{i-1}) \end{array} \right]^\dagger \left( \begin{array}{c} \sigma^{-1} y \\ 0 \end{array} \right) + \xi,
\]

where \( L(\theta) \) is the Cholesky factor of \( Q(\theta) \) and \( \dagger \) denotes the matrix pseudoinverse.

(b) for \( j = 1, \ldots, n_0 \) do

(i) Generate \( \xi^{(j)} \sim \mathcal{N}(0, 1) \) and propose \( \tilde{\theta}^{i,(j)} = \theta^{i-1,(j)} + \beta_0 \xi^{(j)} \).

(ii) Denote \( \tilde{\theta}^{i,(-j)} = (\tilde{\theta}^{i,(1)}, \ldots, \tilde{\theta}^{i,(j-1)}, \theta^{i-1,(j+1)}, \ldots, \theta^{i-1,(n_0)}) \). Accept \( \tilde{\theta}^{i,(j)} \) with probability

\[
p = \min \left\{ 1, \frac{\pi(\tilde{\theta}^{i,(j)}, \tilde{\theta}^{i,(-j)} | u^n, y)}{\pi(\tilde{\theta}^{i-1,(j)}, \tilde{\theta}^{i,(-j)} | u^n, y)} \right\},
\]

where \( \pi(\theta | u_n, y) \) is given in (5.8).

end for

end for

We will follow a similar MCMC sampling as in [71] detailed in Algorithm 5.1 for inferring the signal function \( u_n \) together with the length scale \( \tau_n \). To illustrate the idea, we notice that the observation equation and the graph Matérn model for \( u_n \) translate into the equations

\[
s^{-1} Su_n = \sigma^{-1} y + \xi_1,
\]

\[
L(\theta)u_n = \xi_2,
\]
where $L(\theta)$ is the Cholesky factor of $Q(\theta)$ and $\xi_1 \sim \mathcal{N}(0, I_J), \xi_2 \sim \mathcal{N}(0, I_n)$. The above pair of equations motivate the update for $u_n$ as

$$
\begin{bmatrix}
\sigma^{-1}S \\
L(\theta)
\end{bmatrix}^\dagger \begin{bmatrix}
\sigma^{-1}y \\
0
\end{bmatrix} + \xi,
$$

where $\xi \sim \mathcal{N}(0, I_{J+n})$. The hyperparameters $\theta$ are updated with a Metropolis-within-Gibbs sampling scheme, where the full posterior $\theta|u_n, y$ has the form

$$
\pi(\theta|u_n, y) \propto \sqrt{\det(Q(\theta))} \exp\left(-\frac{1}{2}u_n^TQ(\theta)u_n - \frac{1}{2}|\theta|^2\right).
$$

(5.8)

In Figure 2a&2b we plot the posterior means of $u_n$ and $\tau_n$ and 95% credible intervals for each of their coordinates. The oscillatory paths of the reconstructions are due to the graph approximation, where the eigenfunctions $\psi_n^{(i)}$ of the graph Laplacian are in general very ragged. We notice that $\tau_n$ varies rapidly in the region where the signal is piecewise constant, indicating a change of length scale. Moreover, the sudden jump of the signal from 1 to -1 suggests a small local length scale which leads to a larger $\tau_n$, as predicted in Remark 2.2.

To further understand the effect of modeling the length scale through $\kappa_n$, we choose a different prior for the latent process by setting

$$
Q(\theta) = \kappa_n(\theta)^{-\frac{m}{4}}(I + \Delta_n^\kappa)^s \kappa_n(\theta)^{-\frac{m}{4}},
$$

$$
\log \kappa_n(\theta) = \nu \frac{m}{2} - \frac{m}{4} \sum_{i=1}^{m_0} \left[\nu + \lambda_n^{(i)}\right]^{-\frac{m}{4}} \theta^{(i)}\psi_n^{(i)},
$$

so that the length scale is controlled by $\kappa_n$ instead. Here $\Delta_n^\kappa$ is the discrete approximation of $\nabla \cdot (\kappa \nabla)$ introduced in Section 3.2 and we adopt the same hyperparameter modeling as for $\tau_n$. In Figure 3a&3b, we plot the posterior means and 95% credible intervals for each coordinate of $u_n$ and $\kappa_n$, as a comparison with their counterparts for $\tau_n$. The figures show that the two approaches give similar reconstructions for the signal and, in agreement with the intuition given in Remark 2.2, $\tau_n$ and $\kappa_n$ are almost inversely proportional to each other.

![Figure 2](image)

**Figure 2** Posterior means and 95% credible intervals for (a) signal from nonstationary model; (b) length scale of nonstationary model; (c) signal from stationary model (constant $\tau_n$) when length scale is modeled through $\tau_n$. 
Figure 3 Posterior means and 95% credible intervals for (a) signal from nonstationary model; (b) length scale of nonstationary model; (c) signal from stationary model constant \( \kappa_n \), when length scale is modeled through \( \kappa_n \).

Remark 5.3. As noted in [46][Section 4.5], the hierarchical approach performs poorly if the noise in the observations is large and the latent process is modeled with a constant length scale; the single length scale is blurred by the noise and the model essentially fits the noisy observations, as can be seen from the oscillatory reconstructions in Figures 2c and 3c. An important observation stemming from the above example is that adding nonstationarity into the length scale may help alleviate such issue.

5.3 Application in Spatial Statistics

In this subsection we consider interpolation of county-level precipitation data in the U.S. for January 1981, available from https://www.ncdc.noaa.gov/cag/county/mapping. Similar problems have been studied in [33, 17] using the SPDE formulation and finite element representations, adding nodes for triangulation of the space. Here we shall assume that only pairwise distances between counties are available and we will perform inference without adding artificial nodes. The inter-county distances are available as great circle distances from https://data.nber.org/data/county-distance-database.html and are only recorded for each pair of counties that are closer than a certain threshold distance apart, which naturally suggests a graph representation. Let \( \{x_i\}_{i=1}^{n=3107} \) denote the \( n \) counties (excluding Alaska, Hawaii and several other counties that we do not have precipitation data for). We model the precipitation \( y \) with a latent Gaussian model, where the \( J \) observations are given as noisy perturbations of the latent process \( u_n \):

\[
y|u, \sigma \sim \mathcal{N}(Su, \sigma^2 I_J),
\]

where \( S \in \mathbb{R}^{J \times n} \) is a matrix of 0 and 1’s that specifies the observation locations. Notice that we have included the noise size \( \sigma \) as a hyperparameter to be inferred. The latent process \( u_n \) will be modeled in four different ways for comparison purposes as in [17]. The idea is to consider a graph Matérn prior for \( u_n \), where

\[
u_n|\theta, s \sim \mathcal{N}(0, Q(\theta, s)^{-1}), \quad Q(\theta, s) = \tau_n(\theta)\frac{\tau_n(\theta) + \Delta_n}{\tau_n(\theta) + \Delta_n} s^2 \tau_n(\theta)\frac{\tau_n(\theta) + \Delta_n}{\tau_n(\theta) + \Delta_n} s^2, \quad m = 2,
\]

and consider \( s \) to be possibly a hyperparameter, while at the same time allow \( \tau_n \) be to identically equal to a constant. In other words, we will model \( u_n \) as a stationary/nonstationary graph Matérn
field with possibly fractional smoothness parameter. In the most general case, the length scale parameter $\tau_n$ is modeled as in (5.6), where the parameters are chosen as $s_0 = 2, \nu = 0.1, n_0 = 10$ and the hyperpriors for $\sigma, s$ are chosen as

$$
\log \sigma \sim \mathcal{N}(\log(0.01), 1), \quad \log s \sim \mathcal{N}(\log 2, 1).
$$

The marginal variance of $\tau_n$ is then tuned to be on the same order as the 10th eigenvalue of $\Delta_n$.

For the stationary case, the modeling for the latent process simplifies to

$$
u_n|\tau, s \sim \mathcal{N}(0, Q(\tau, s)^{-1}), \quad Q(\tau, s) = \tau^{\frac{m}{2} - s}(\tau I_n + \Delta_n)^s,
$$

and a log-normal hyperprior is placed on $\tau$.

For this problem $\Delta_n$ is an unnormalized graph Laplacian $D - W$, with weights

$$
W_{ij} = \begin{cases} 
\exp\left(-\frac{d_{ij}^2}{2\bar{d}^2}\right), & \text{if } d_{ij} \text{ is recorded}, \\
0, & \text{otherwise,}
\end{cases}
$$

where $d_{ij}$ is the distance between two counties and $\bar{d}$ is the mean of all the pairwise distances. As mentioned above, the pairwise distances are only recorded for counties that are less than 100 miles apart, which implies that $W$ is sparse. Instead of using an MCMC sampling scheme, we adopt an evidence maximization approach, where we first compute the optimal hyperparameter $(\sigma^*, s^*, \theta^*)$ (for the most general case) by maximizing the marginal posterior $(\sigma, s, \theta)|y$, and then compute the posterior $u_n|y, \sigma^*, s^*, \theta^*$. For the most general case, the marginal posterior of $(\sigma, s, \theta)$ is equal up to a constant to

$$
\log \pi(\sigma, s, \theta|y) = \log \pi(\sigma, s, \theta) - J \log \sigma + \frac{1}{2\sigma^4} y^T S\tilde{Q}(\sigma, s)^{-1} S^T y - \frac{||y||^2}{2\sigma^2} + \frac{1}{2} \log \left[\det(Q(\theta, s)) - \det(\tilde{Q}(\sigma, s, \theta))\right],
$$

where $\tilde{Q}(\sigma, \theta, s) = \sigma^{-2} S^T S + Q(\theta, s)$ and the posterior $u_n|y, \sigma^*, s^*, \theta^*$ is a Gaussian $\mathcal{N}(\mu, \Sigma)$, where

$$
\mu = [\sigma^*]^{-2} \tilde{Q}(\sigma^*, \theta^*, s^*)^{-1} S^T y, \quad \Sigma = \tilde{Q}(\sigma^*, \theta^*, s^*)^{-1}.
$$

The predictive distribution is then the restriction of $\mathcal{N}(\mu, \Sigma)$ to the unobserved nodes, denoted as $\pi_{\text{pred}}$, and techniques for computing partial inverse of a sparse matrix can be applied. We numerically optimize $\log \pi(\sigma, s, \theta|y)$ with the fminunc function in Matlab.

To perform inference, we first normalize the data $y$ as described in Remark 5.2 so that it has mean-zero and has magnitude at the same level of $u_n$ from the graph Matérn field, in which case we are only interested in the variations of $u_n$. We then adopt a pseudo-crossvalidation by randomly selecting 90% of the data as observations and make predictions for the remaining ones. The process is repeated 20 times and we evaluate the predictions through the root mean square error (RMSE), the continuous rank probability score (CRPS), and the logarithmic scoring rule (LS) as shown in
Table 5.1 Comparison of the four models through RMSE, CRPS and LS.

|                              | RMSE | CRPS | LS   |
|------------------------------|------|------|------|
| Stationary & $s = 2$        | 0.0394 | 0.0199 | -578.9 |
| Stationary & Inferred $s$    | 0.0399 | 0.0201 | -521.7 |
| Nonstationary & $s = 2$      | 0.0408 | 0.0185 | -648.5 |
| Nonstationary & Inferred $s$ | 0.0414 | 0.0186 | -644.6 |

Table 5.1. The three criteria are considered in [33, 17] for similar comparisons, with each defined as

$$
\text{RMSE} := \frac{\| y_{\text{test}} - \mathbb{E} \pi_{\text{pred}} \|_2}{\sqrt{n_{\text{test}}}}
$$

$$
\text{CRPS} := \frac{1}{n_{\text{test}}} \sum_{i=1}^{n_{\text{test}}} \text{crps}(\pi_{\text{pred}}^{(i)}, y_{\text{test}}^{(i)})
$$

$$
= \frac{1}{n_{\text{test}}} \sum_{i=1}^{n_{\text{test}}} \int_{-\infty}^{\infty} \left[ \pi_{\text{pred}}(y_{\text{test}}^{(i)}) - 1 \{ y_{\text{test}}^{(i)} \leq t \} \right]^2 dt
$$

$$
\text{LS} := -\log \pi_{\text{pred}}(y_{\text{test}}),
$$

where $y_{\text{test}}$ is the test data with size $n_{\text{test}}$ and $\pi_{\text{pred}}^{(i)}$ is the marginal distribution for each unobserved node. Since $\pi_{\text{pred}}$ is Gaussian (and hence its marginals), the above quantities are computable, and the CRPS can be calculated with its representation for Gaussians [43]:

$$
\text{crps}(\mathcal{N}(a, b^2), y) = b \left\{ \frac{y - a}{b} \left[ 2\Phi \left( \frac{y - a}{b} \right) - 1 \right] + 2\varphi \left( \frac{y - a}{b} \right) - \frac{1}{\sqrt{\pi}} \right\},
$$

where $\Phi$ and $\varphi$ are the c.d.f. and p.d.f. of the standard normal respectively.

We notice in Table 5.1 that the nonstationary model improves CRPS and LS but not RMSE over the stationary one, as was observed in [33, 17] using finite element representations of GFs. This suggests that adding nonstationarity improves the prediction in a distribution sense. However, inferring the smoothness $s$ from data appears not to improve the predictions, in contrast to the results in [17]. We believe this is due to the different formulations that we are taking, where [17] adopts an SPDE approach and a rational approximation for fractional smoothness. It is also possible that this is in general a feature of the graph representation as similar observations are made in Subsection 5.4. We shall leave more in-depth investigations for future studies.

5.4 Application in Machine Learning

In this subsection we illustrate the use of graph Matérn priors in a Bayesian formulation of semi-supervised binary classification [12]. We seek to classify images $\{ x_i \}_{i=1}^J$ of two different digits of the MNIST dataset given $J \ll n$ noisy labels. Similarly as above, the problem is cast into a latent Gaussian model, where the labels are assumed to be a probit transform of the latent process $u_n$:

$$
y_i = \text{sign} \left( u_n(x_i) + \eta_i \right), \quad i = 1, \ldots, J,
$$
where \( \eta_i \sim N(0, \sigma^2) \). The likelihood model associated with the above equation is

\[
\pi(y|u_n, \sigma) = \sum_{i=1}^{J} \Phi\left(\frac{y_i - u_n(x_i)}{\sigma}\right),
\]

where \( \Phi \) is the c.d.f. of the standard normal. As in Subsection 5.3, the latent process \( u_n \) will be modeled as a graph Matérn field in four different ways, by considering stationary/nonstationary length scale and fixed/inferred smoothness \( s \). For the most general case, the latent process is modeled as

\[
u_n|\theta, s \sim N(0, Q(\theta, s)^{-1}), \quad Q(\theta, s) = \tau_n(\theta) \frac{m}{4} - \frac{\Delta_n}{2} \tau_n(\theta) \frac{m}{4} - \frac{s}{2},
\]

and \( \tau_n \) is modeled as in (5.6):

\[
\log \tau_n(\theta) = \nu \frac{m}{4} - \frac{n_0}{4} \sum_{i=1}^{n_0} \left( \nu + \lambda_n(i) \right) - \frac{n_0}{2} \theta^{(i)} \psi_n^{(i)}
\]

with standard normal hyperprior on each of the \( \theta_i \)'s and a log-normal prior for \( s \). As in Remark 3.3, the effective dimension \( m \) is about 4 and the other parameters are chosen as \( s_0 = 4, \nu = 0.1, n_0 = 10 \), with marginal variance of \( \tau_n \) tuned empirically. For this problem \( \Delta_n \) is taken to be a symmetric \( k \)-nearest neighbor graph Laplacian \( \Delta_n = I - D^{-1/2}W D^{-1/2} \), with self-tuning weights proposed by [98]:

\[
W_{ij} = \exp\left(-\frac{|x_i - x_j|^2}{2\delta(i)\delta(j)}\right),
\]

where the images \( x_i \)'s are viewed as vectors in \( \mathbb{R}^{784} \) and \( \delta(i) \) is the Euclidean distance between \( x_i \) and its \( k \)-th nearest neighbor. The sparsity of \( \Delta_n \) follows from the \( k \)-nearest neighbor construction.

Similarly as in Subsection 5.3, we adopt an evidence maximization approach for inferring the optimal hyperparameters, which are then used to find the MAP estimator for \( u_n \). However, since the likelihood is non Gaussian, there is no closed form formula for the marginal posterior of the hyperparameters \( \pi(\sigma, \theta, s|y) \), and we then apply a Laplace approximation [73]. More precisely, denoting \( z \) as all the hyperparameters, \( \pi(z|y) \) is approximated by

\[
\pi(z|y) \propto \pi(u_n, z, y) \pi(u_n|z, y)_{u_n = u_n^*} \approx \pi(u_n, z, y)_{u_n = u_n^*}, \tag{5.10}
\]

where \( u_n^* \) is the mode of \( \pi(u_n|z, y) \) and \( \tilde{\pi}(u_n|z, y) \) is its Laplace approximation at \( u_n^* \). The log density for \( u_n|z, y \) has form

\[
\log \pi(u_n|z, y) \propto \sum_{i=1}^{J} \Phi\left(\frac{y_i - u_n(x_i)}{\sigma}\right) - \frac{1}{2} u_n^T Q(\theta, s) u_n, \tag{5.11}
\]

and the mode \( u_n^* \) is found numerically with the Newton’s method, where the gradient and Hessian of (5.11) are available analytically. The logarithm of the last expression in (5.10) is equal up to a constant to

\[
\log \pi(\sigma, \theta, s) - \frac{1}{2} [u_n^*]^T Q(\theta, s) u_n^* + \frac{1}{2} \log \left| \det(Q(\theta, s)) \right| - \log(Q(\sigma, \theta, s)) + \sum_{i=1}^{J} \log \frac{\Phi\left(\frac{y_i u_n^*(x_i)}{\sigma}\right)}{\Phi\left(\frac{y_i u_n(x_i)}{\sigma}\right)},
\]
where \( \tilde{Q}(\theta, s) = Q(\sigma, \theta, s) + H \) and \( H \) is diagonal with entries

\[
H_{ii} = \frac{y_i u_n^*(x_i) \phi(\sigma^{-1} u_n^*(x_i))}{\sigma^2 \Phi(\sigma^{-1} y_i u_n^*(x_i))} + \left[ \frac{\phi(\sigma^{-1} u_n^*(x_i))}{\sigma \Phi(\sigma^{-1} y_i u_n^*(x_i))} \right]^2, \quad i = 1, \ldots, J,
\]

and zero otherwise. The priors on \( \sigma \) and \( s \) are taken to be

\[
\log \sigma \sim \mathcal{N}(\log(0.1), 1), \\
\log s \sim \mathcal{N}(\log(4), 1).
\]

Table 5.2 shows the classification error rates of the four different models for four pairs of digits, with \( n = 1000 \) and \( J = 20 \), where each experiment is repeated 100 times. We see that the nonstationary model improves slightly the performance while the model with inferred smoothness does the opposite. We believe this may be due to the fact that \( s = 4 \) is already a near optimal choice for this problem, or it may also be an intrinsic characteristic of the graph representations as mentioned in Subsection 5.3. Table 5.3 shows the classification error rates for the inferred \( s \) case when the prior is taken to be narrower:

\[
\log s \sim \mathcal{N}(\log 4, 0.01),
\]

in which case the nonstationary model with inferred \( s \) also improves the prediction.

**Table 5.2** Classification error rates with 2% labeled data for different pairs of digits with hyperprior \( \log s \sim \mathcal{N}(\log 4, 1) \).

|                 | 3&8  | 5&8  | 4&9  | 7&9  |
|-----------------|------|------|------|------|
| Stationary & s = 4 | 8.90% | 8.64% | 17.67% | 10.13% |
| Stationary & Inferred s | 9.61% | 9.51% | 18.33% | 11.00% |
| Nonstationary & s = 4 | 8.44% | 7.23% | 17.38% | 9.37% |
| Nonstationary & Inferred s | 8.77% | 8.12% | 19.92% | 10.70% |

**Table 5.3** Classification error rates with 2% labeled data for different pairs of digits with hyperprior \( \log s \sim \mathcal{N}(\log 4, 0.01) \).

|                 | 3&8  | 5&8  | 4&9  | 7&9  |
|-----------------|------|------|------|------|
| Stationary & Inferred s | 8.91% | 8.66% | 17.69% | 10.14% |
| Nonstationary & Inferred s | 8.67% | 7.06% | 17.54% | 9.71% |

6 Conclusions and Open Directions

This paper introduces a graph representation of the Matérn fields motivated by its SPDE formulation of GFs and extends the construction to arbitrary point clouds. The resulting graph Matérn fields constitute GMRF approximations of the GFs, for which numerical linear algebra techniques can be applied to gain speed up by exploiting sparsity. We have shown through rigorous analysis the convergence of the graph Matérn fields towards their continuum counterparts with an explicit rate
under a manifold assumption. The analysis builds on and generalizes existing literature on spectral convergence of graph Laplacians.

Numerical examples demonstrate the application of graph Matérn fields in Bayesian inverse problems, spatial statistics and graph-based machine learning, aiming at bridging these fields and transfer ideas among them. The graph Matérn models can be directly implemented on the given point cloud, without any additional pre-processing such as adding nodes for triangulation for FEM methods. We demonstrate through comparisons certain benefits of the nonstationary models, where in particular nonstationary models improves classification accuracy. We believe adding nonstationarity for graph-based learning problems has not been considered before and our empirical observations open doors for future research.

The nonstationarity introduced through $\tau$ is well-studied while not much has been said about $\kappa$. We hope to investigate its modeling effects beyond the role as a length scale parameter as in Remark 2.2 and to consider anisotropic models where the Laplacian is replaced by $\nabla \cdot (H(x)\nabla)$ and the graph discretizations thereof. The case where $H$ is independent of the spatial variable can be easily dealt with by introducing a coordinate transform by $H^{-1/2}$. However the general case is more involved and further research is needed.

Another possible future direction is to further investigate the case where the points are distributed according to a non-uniform density. As in Remark 3.2, we normalize the weights to remove the effects of the density, aiming at recovering the Laplacian. A more interesting question is whether the density can be incorporated as part of the continuum operator that will lead to meaningful Matérn type field. Especially for the machine learning applications, we wonder if the density of the point cloud can shed light on constructing priors for these problems.

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In this Appendix we prove the main theorems in Section 4. Section A makes precise our setup and assumptions, defines several quantities of interest and presents other necessary preliminaries. Sections B and C contain proofs for the spectral convergence of $L_n^{\tau, \kappa}$ towards $L^{\tau, \kappa}$. Finally Section D gives the proof of Theorem 4.1.

A Preliminaries

Suppose $\mathcal{M}$ is an $m$-dimensional smooth, connected, compact manifold without boundary embedded in $\mathbb{R}^d$, with the absolute value of sectional curvature bounded by $K$ and Riemannian metric inherited from $\mathbb{R}^d$. Let $\{x_n\}_{n=1}^\infty$ be a sequence of independent samples from the uniform distribution $\gamma$ on $\mathcal{M}$. Denote $\mathcal{M}_n := \{x_1, \ldots, x_n\}$ and let $\gamma_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ be the empirical distribution of the point cloud $\mathcal{M}_n$. Throughout $\tau$ and $\kappa$ will denote Lipschitz continuous functions on $\mathcal{M}$ with $\kappa \in C^1(\mathcal{M})$. We assume that both functions are bounded from below by positive constants, so there exist $\alpha, \beta > 0$ with $\frac{1}{\beta} \leq \tau \leq \beta$, $\frac{1}{\alpha} \leq \kappa \leq \alpha$. We will analyze the spectral convergence of $L_n^{\tau, \kappa}$ towards $L^{\tau, \kappa}$, where

\[
L_n^{\tau, \kappa} := \tau I - \nabla \cdot (\kappa \nabla),
\]

\[
L_n^{\tau, \kappa} =: \tau_n + \Delta_n^\kappa,
\]

with $\tau_n := \text{diag}(\tau(1), \ldots, \tau(n))$. Here $\Delta_n^\kappa = D - W \in \mathbb{R}^{n \times n}$ and the entries of $D$ and $W$ are given by

\[
W_{ij} := \frac{2(m+2)}{n \nu_m h_n^m + 2} \mathbf{1}\{d_\mathcal{M}(x_i, x_j) < h_n\} \sqrt{\kappa(x_i) \kappa(x_j)},
\]

\[
D_{ii} := \sum_{j=1}^n W_{ij},
\]

where $\nu_m$ is the volume of the $m-$dimensional unit ball and $d_\mathcal{M}$ is the geodesic distance on $\mathcal{M}$.

Remark A.1. We remark that this is slightly different from (3.4) for the reason that in practice we would have no knowledge on the geodesic distances. However, the two distances are roughly the same in a small local neighborhood and going one from the other only introduces an error of higher order than our interest [38]. Hence to streamline our presentation we use the geodesic distance in the following.

As discussed in Section 4, the scaling of $h_n$ will be chosen so that

\[
\frac{(\log n)^{c_m}}{n^{1/m}} \ll h_n \ll \frac{1}{n^{1/s}}, \quad (A.1)
\]

where $c_m = 3/4$ if $m = 2$ and $c_m = 1/m$ otherwise. We recall that the scaling of $h_n$ in (A.1) implies that the $\infty$-OT distance between $\gamma_n$ and $\gamma$ satisfies $\varepsilon_n = d_\infty(\gamma_n, \gamma) \ll h_n$. In what follows we assume that we are in a realization where the conclusion of Proposition 4.3 holds and we let $\{T_n\}_{n=1}^\infty$ be a sequence of transport maps satisfying the bound (4.5).

We will use the following inner products and induced norms on continuum and discrete spaces

\[
\langle f, g \rangle_{L^2} := \int f(x)g(x)d\gamma(x), \quad \langle f, g \rangle_\tau := \int f(x)g(x)\tau(x)d\gamma(x), \quad \langle f, g \rangle_\kappa := \int f(x)g(x)\kappa(x)d\gamma(x),
\]

\[
\langle v, w \rangle_2 := \frac{1}{n} \sum_{i=1}^n v(x_i)w(x_i), \quad \langle v, w \rangle_\tau := \frac{1}{n} \sum_{i=1}^n v(x_i)w(x_i)\tau(x_i), \quad \langle v, w \rangle_\kappa := \frac{1}{n} \sum_{i=1}^n v(x_i)w(x_i)\kappa(x_i).
\]
Notice that $\mathcal{L}^{\tau,\kappa} : \mathcal{D}(\mathcal{L}^{\tau,\kappa}) \subset L^2(\gamma) \to L^2(\gamma)$ is self-adjoint with respect to the $\langle \cdot, \cdot \rangle_{L^2}$ inner-product and has a compact resolvent; we will denote by $\{\lambda^{(k)}\}_{k=1}^\infty$ and $\{\psi^{(k)}\}_{k=1}^\infty$ its eigenvalues and eigenfunctions and recall that from standard theory

$$\mathcal{D}(\mathcal{L}^{\tau,\kappa}) = \{ f \in L^2(\gamma) : \sum_{k=1}^\infty |\lambda^{(k)}|^2 \langle f, \psi^{(k)} \rangle_{L^2}^2 < \infty \}.$$ 

Similarly, $L_n^{\tau,\kappa}$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_2$. By the minimax principle we can characterize the $k$-th smallest eigenvalues of $\mathcal{L}^{\tau,\kappa}$ and $L_n^{\tau,\kappa}$ by

$$\lambda^{(k)} = \min_{V} \max_{f \in V \setminus 0} \frac{\langle f, \mathcal{L}^{\tau,\kappa} f \rangle_{L^2}}{\langle f, f \rangle_{L^2}},$$

$$\lambda_n^{(k)} = \min_{V} \max_{v \in V \setminus 0} \frac{\langle v, L_n^{\tau,\kappa} v \rangle_2}{\langle v, v \rangle_2},$$

where the minimum is taken over all subspaces $V$ (or $V$) of dimension $k$. We define the continuum and discrete the Dirichlet energies

$$D[f] := \langle f, \mathcal{L}^{\tau,\kappa} f \rangle_{L^2} = \int \tau(x) f(x)^2 + \int \kappa(x) |\nabla f|^2 = \|f\|_V^2 + \|\nabla f\|_V^2 := D^0[f] + D^1[f],$$

$$D_{h_n}[v] := \langle v, L_n^{\tau,\kappa} v \rangle_2 = \frac{1}{n} \sum_{i=1}^{n} \tau(x_i)v(x_i)^2 + \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} W_{ij}|v(x_i) - v(x_j)|^2 =: D^0_{h_n}[v] + D^1_{h_n}[v].$$

For the lemmas and theorems below, we shall denote $C_M, C_{M,\tau,\kappa}$ etc. as constants that depend on the corresponding subscripts.

## B Convergence of Spectrum with Rate

In this section we prove Theorem 4.4 by establishing a lower and an upper bound on the eigenvalues of $L_n^{\tau,\kappa}$ in terms of those of $\mathcal{L}^{\tau,\kappa}$. With the above definitions of the Dirichlet energies, the eigenvalues have the characterizations

$$\lambda^{(k)} = \min_{V} \max_{f \in V \setminus 0} \frac{D[f]}{\|f\|_{L^2}^2}, \quad \lambda_n^{(k)} = \min_{V} \max_{v \in V \setminus 0} \frac{D_{h_n}[v]}{\|v\|_2^2}.$$ 

In order to compare the Dirichlet energies as in (4.6), we need an intermediate quantity defined by

$$E_r[f] := \int_M \int_{B_r(x)} |f(x) - f(y)|^2 \sqrt{\tau(x)\kappa(x)} d\gamma(y) d\gamma(x).$$

Notice that $D^1_{h_n}$ can be seen as a finite sample approximation of $E_{h_n}$ up to a multiplicative constant. The following lemma, which can be proved with the same argument as [38][Lemma 5], connects $E_{h_n}$ with $D^1$.

**Lemma B.1.** For $f \in L^2(\gamma)$ and $r < 2h_n$,

$$E_r[f] \leq (1 + C_{M,\kappa} h_n) \frac{\nu_m r^{m+2}}{m+2} D^1[f].$$
B.1 Upper Bound

To start with, define the projection map $P : L^2(\gamma) \to L^2(\gamma_n)$ by

$$ Pf(x_i) := n \int_{U_i} f(x) d\gamma(x), $$

where $U_i = T_n^{-1}(\{x_i\})$ and $\{T_n\}_{n=1}^\infty$ is a sequence of transportation maps as in Proposition 4.3. The $U_i$’s are called transportation cells.

**Lemma B.2 (Discrete Dirichlet Energy Upper Bound).** Let $f \in H^1(\gamma)$.

1. $\|Pf\|_2 - \|f\|_{L^2} \leq C_M \|\nabla f\|_{L^2}$.

2. $D_{h_n}[Pf] \leq \left[1 + C_{M, \tau, n} \left(h_n + \frac{\epsilon_n}{h_n}\right)\right] D[f]$.

**Proof.** The first statement is proved in [23][Lemma 4.3(1)]. The second statement will be proved by combining upper bounds for $D_{h_n}^0[Pf]$ and $D_{h_n}^1[Pf]$. First, by Hölder’s inequality and the fact that $\text{vol}(U_i) = 1/n$,

$$ D_{h_n}^0[Pf] = \frac{1}{n} \sum_{i=1}^n \tau(x_i) Pf(x_i)^2 = \frac{1}{n} \sum_{i=1}^n \tau(x_i) n^2 \left| \int_{U_i} f(x) d\gamma(x) \right|^2 
\leq \sum_{i=1}^n \tau(x_i) \int_{U_i} f(x)^2 d\gamma(x) 
\leq \left[1 + \text{Lip}(\tau) \alpha \epsilon_n\right] \sum_{i=1}^n \int_{U_i} \tau(x) f(x)^2 d\gamma(x) 
= \left[1 + \text{Lip}(\tau) \alpha \epsilon_n\right] D^0[f]. \tag{B.1} $$

For the upper bound on $D_{h_n}^1[Pf]$, observe that

$$ Pf(x_i) - Pf(x_j) = n^2 \int_{U_i} \int_{U_j} f(y) - f(x) d\gamma(y) d\gamma(x), $$

which implies

$$ |Pf(x_i) - Pf(x_j)|^2 \leq n^2 \int_{U_i} \int_{U_j} |f(y) - f(x)|^2 d\gamma(y) d\gamma(x). $$

Therefore by Lipschitz continuity of $\kappa$,

$$ D_{h_n}^1[Pf] = \frac{m + 2}{n^2 \nu_M h_n^{m+2}} \sum_{i=1}^n \sum_{j=1}^n \sqrt{\kappa(x_i) \kappa(x_j)} \left| \left\{ d_M(x_i, x_j) < h_n \right\} \right| |Pf(x_i) - Pf(x_j)|^2 
\leq \frac{m + 2}{\nu_M h_n^{m+2}} \sum_{i=1}^n \sum_{j=1}^n \sqrt{\kappa(x_i) \kappa(x_j)} \left| \left\{ d_M(x_i, x_j) < h_n \right\} \right| \int_{U_i} \int_{U_j} |f(y) - f(x)|^2 d\gamma(y) d\gamma(x) 
\leq [1 + \text{Lip}(\kappa) \alpha \epsilon_n] \frac{m + 2}{\nu_M h_n^{m+2}} \sum_{i=1}^n \sum_{j=1}^n \left\{ d_M(x_i, x_j) < h_n \right\} \int_{U_i} \int_{U_j} |f(y) - f(x)|^2 \sqrt{\kappa(x) \kappa(y)} d\gamma(y) d\gamma(x) 
\leq [1 + \text{Lip}(\kappa) \alpha \epsilon_n] \frac{m + 2}{\nu_M h_n^{m+2}} \int_{V(x)} |f(y) - f(x)|^2 \sqrt{\kappa(x) \kappa(y)} d\gamma(y) d\gamma(x). $$
where if \( x \in U \), then \( V(x) = \bigcup_{j: j < i} U_j \). Notice that \( V(x) \subset B_{h_n + 2\varepsilon_n}(x) \) and hence

\[
D_{h_n}^1[Pf] \leq [1 + \text{Lip}(\kappa)\alpha\varepsilon_n] \frac{m + 2}{\nu_m h_n^{m+2}} \int_{\mathcal{M}} \int_{B_{h_n + 2\varepsilon_n}(x)} |f(y) - f(x)|^2 \sqrt{\kappa(x)\kappa(y)} d\gamma(y) d\gamma(x) = [1 + \text{Lip}(\kappa)\alpha\varepsilon_n] \frac{m + 2}{\nu_m h_n^{m+2}} E_{h_n + 2\varepsilon_n}[f] \leq \left[1 + C_{M,\kappa}(h_n + 2\varepsilon_n)\right] \left(\frac{h_n + 2\varepsilon_n}{h_n}\right)^{m+2} D^1[f] \leq \left[1 + C_{M,\kappa}\left(h_n + \frac{\varepsilon_n}{h_n}\right)\right] D^1[f],
\]

(B.2)

where we have used Lemma B.1 and the assumption that \( \varepsilon_n \ll h_n \). The result follows by combining (B.1) and (B.2).

\[ \square \]

**Corollary B.3** (Upper Bound). Suppose \( k := k_n \) is such that \( \varepsilon_n \sqrt{\lambda(k_n)} \ll 1 \) for \( n \) large. Then

\[
\lambda_n^{(k)} \leq \left[1 + C_{M,\tau,\kappa}\left(h_n + \frac{\varepsilon_n}{h_n} + \sqrt{\lambda(k)}\varepsilon_n\right)\right] \lambda^{(k)}.
\]

**Proof.** Let \( \mathcal{V} \) be the span of eigenfunctions \( f_1, \ldots, f_k \) of \( L_{\tau,\kappa}^r \) associated with eigenvalues \( \lambda_1, \ldots, \lambda^{(k)} \). For \( f \in \mathcal{V} \), we have

\[
\|\nabla f\|_{L^2} \leq \sqrt{\alpha} \|\nabla f\|_{\kappa} \leq \sqrt{\alpha} \sqrt{D[f]} \leq \sqrt{\alpha} \lambda^{(k)} \|f\|_{L^2}.
\]

Lemma B.2 (1) then implies that

\[
\|Pf\|_2 \geq \|f\|_{L^2} - C_M \varepsilon_n \|\nabla f\|_{L^2} \geq \|f\|_{L^2} - C_M \varepsilon_n \sqrt{\lambda^{(k)}} \|f\|_{L^2}.
\]

Therefore, the assumption that \( \varepsilon_n \sqrt{\lambda^{(k)}} \ll 1 \) implies that \( P|\mathcal{V} \) is injective and \( V = P(\mathcal{V}) \) has dimension \( k \). By Lemma B.2 (2) we have

\[
\lambda_n^{(k)} \leq \max_{u \in \mathcal{V} \setminus 0} \frac{D_h[u]}{\|u\|_2^2} = \max_{f \in \mathcal{V} \setminus 0} \frac{D_h[f]}{\|f\|_2^2} \leq \max_{f \in \mathcal{V} \setminus 0} \frac{\left[1 + C_{M,\tau,\kappa}\left(h_n + \frac{\varepsilon_n}{h_n}\right)\right] D[f]}{\left(1 - C_{M,\tau,\kappa}\varepsilon_n \sqrt{\lambda^{(k)}}\right) \|f\|_2^2} = \frac{\left[1 + C_{M,\tau,\kappa}\left(h_n + \frac{\varepsilon_n}{h_n}\right)\right] \lambda^{(k)}}{1 - C_{M,\tau,\kappa}\varepsilon_n \sqrt{\lambda^{(k)}}} \leq \left[1 + C_{M,\tau,\kappa}\left(h_n + \frac{\varepsilon_n}{h_n} + \sqrt{\lambda^{(k)}}\varepsilon_n\right)\right] \lambda^{(k)}.
\]

\[ \square \]

### B.2 Lower Bound

Define \( P^* : L^2(\gamma_n) \to L^2(\gamma) \) by

\[
P^* v := \sum_{i=1}^{n} v(x_i) 1_{U_i},
\]
where $U_i$’s are the transportation cells as in the definition of $P$. We note that $P^*$ defines a piecewise constant interpolation map; for the subsequent analysis we need to introduce a smoothing operator $\Lambda$ so that the map $\mathcal{I} := \Lambda \circ P^*$ satisfies $\mathcal{I}v \in H^1(\gamma)$. We now detail the construction of the smoothness operator. Let

$$\psi(t) := \begin{cases} 
\frac{m+2}{2m}(1 - t^2), & 0 \leq t \leq 1, \\
0, & t > 1.
\end{cases}$$

Consider for $r < 2h_n$ the kernel

$$k_r(x, y) := r^{-m} \psi \left( \frac{d_M(x, y)}{r} \right)$$

and the associated integral operator

$$\Lambda^0_r f = \int_M k_r(x, y) f(y) d\gamma(y).$$

Let $\theta(x) := \Lambda^0_r 1_M = \int_M k_r(x, y) d\gamma(y)$ and then define

$$\Lambda_r f := \theta^{-1} \Lambda^0_r f,$$

so that $\Lambda_r$ preserves constant functions. Finally we define the interpolation operator $\mathcal{I} : L^2(\gamma_n) \to L^2(\gamma)$ by

$$\mathcal{I}v := \Lambda_{h_n - 2r} P^* v.$$

We next present some auxiliary bounds that will be needed later.

**Lemma B.4 (Auxiliary Bounds).** For $f \in L^2(\gamma)$, we have

$$\|\Lambda_r f\|_r^2 \leq [1 + \text{Lip}(r)\beta r][1 + C m K r^2] \|f\|_r^2,$$  \hfill (B.3)

$$\|\Lambda_r f - f\|_r^2 \leq [1 + \text{Lip}(\kappa)\alpha r] \frac{C m}{\nu_m r m} E_r[f],$$  \hfill (B.4)

$$\|\nabla (\Lambda_r f)\|_r^2 \leq [1 + \text{Lip}(\kappa)\alpha r] [1 + C m^2 K r^2] \frac{m+2}{\nu_m r m+2} E_r[f].$$  \hfill (B.5)

**Proof.** The above results are proved in the same way as in [23][Lemma 5.3, 5.4, 5.5] with little adjustments and the main differences are the additional factors $1 + \text{Lip}(\tau)\beta r$ or $1 + \text{Lip}(\kappa)\alpha r$. To illustrate the idea, we will prove (B.3) and the generalizations for (B.4) and (B.5) are similar. First by [23][Lemma 5.1], we have for each $x \in M$,

$$(1 + C m K r^2)^{-1} \leq \theta(x) \leq (1 + C m K r^2),$$  \hfill (B.6)

where recall that $K$ is an upper bound on the absolute value of the sectional curvature. Then we have

$$|\Lambda_r f|^2 = \theta^{-2} \left| \int_M k_r(x, y) f(y) \right|^2 \leq \theta^{-2} \int_M k_r(x, y) d\gamma(y) \int_M k_r(x, y) |f(y)|^2 d\gamma(y)$$

$$= \theta^{-1} \int_M k_r(x, y) |f(y)|^2 d\gamma(y)$$

$$\leq [1 + C m K r^2] \int_M k_r(x, y) |f(y)|^2 d\gamma(y).$$
Noticing that \( k_r(x, y) \) is zero when \( d_M(x, y) > r \) and \( \tau \) is Lipschitz, we have

\[
\|\Lambda rf\|_r^2 \leq [1 + CmK] \int_M \int_M k_r(x, y)|f(y)|^2 \tau(x) d\gamma(x) d\gamma(y)
\]

\[
\quad = [1 + CmK] \int_M |f(y)|^2 \left[ \int_{B_r(y)} k_r(x, y) \tau(x) d\gamma(x) \right] d\gamma(y)
\]

\[
\quad \leq [1 + \text{Lip}(\tau) r \beta] [1 + CmK] \int_M |f(y)|^2 \left[ \int_{B_r(y)} k_r(x, y) \tau(y) d\gamma(x) \right] d\gamma(y)
\]

\[
\quad = [1 + \text{Lip}(\tau) r \beta] [1 + CmK] \int_M k_r(x, y) \tau(y) d\gamma(x) \int_M |f(y)|^2 \tau(y) d\gamma(y)
\]

\[
\quad = [1 + \text{Lip}(\tau) r \beta] [1 + CmK]^2 \|f\|_r^2.
\]

\[\square\]

**Lemma B.5 (Discrete Dirichlet Energy Lower Bound).** For each \( v \in L^2(\gamma_n) \),

1. \( \|\mathbb{I}v\|_{L^2} - \|v\|_2 \leq C_e h_n \sqrt{D_{h_n}[v]} \).

2. \( D[\mathbb{I}v] \leq \left[1 + C_{M, \tau, \kappa} \left(h_n + \frac{\varepsilon_n}{h_n}\right)\right] D_{h_n}[v] \).

**Proof.** 1. By equation (6.4) in the proof of [23][Lemma 6.2(1)],

\[
\|\mathbb{I}v - P^*v\|_{L^2} \leq C h_n \|\delta v\|,
\]

where

\[
\|\delta v\| = \frac{m + 2}{\nu_m n^2 h_n^{m+2}} \sum_{i=1}^n \sum_{j=1}^n 1\{d_M(x_i, x_j) < h_n\} \|v(x_i) - v(x_j)\|^2.
\]

The result follows by noticing that \( \|\delta v\| \leq \sqrt{\alpha D_{h_n}[v]} \) and

\[
\|\mathbb{I}v\|_{L^2} - \|v\|_2 = \|\mathbb{I}v\|_{L^2} - \|P^*v\|_{L^2} \leq \|\mathbb{I}v - P^*v\|_{L^2}.
\]

2. The second statement will be proved by combining lower bounds for \( D_{h_n}^0[\mathbb{I}v] \) and \( D_{h_n}^1[\mathbb{I}v] \).

For the lower bound on \( D_{h_n}^0[\mathbb{I}v] \), we have by (B.3),

\[
D^0[\mathbb{I}v] = \|\Lambda_{h_n - 2\varepsilon_n} P^*v(x)\|_r^2 \leq \left[1 + \text{Lip}(\tau) \beta(h_n - 2\varepsilon_n)\right] \left[1 + CmK(h_n - 2\varepsilon_n)^2\right] \int \tau(x)|P^*v(x)|^2 d\gamma(x).
\]

We also have

\[
\int \tau(x)|P^*v(x)|^2 d\gamma(x) = \sum_{i=1}^n \int_{U_i} \tau(x)|v(x_i)|^2 d\gamma(x)
\]

\[
\quad \leq [1 + \text{Lip}(\tau) \beta \varepsilon_n] \sum_{i=1}^n \int_{U_i} \tau(x_i)v(x_i)|^2 d\gamma(x) = [1 + \text{Lip}(\tau) \beta \varepsilon_n] D_{h_n}^0[v].
\]
Therefore
\[
D^0[\mathcal{I}v] \leq (1 + C_{\mathcal{M}, \tau} h_n) D^0_{h_n}[v]. \tag{B.9}
\]

Next we seek a lower bound for \( D^1_{h_n}[\mathcal{I}v] \). We have
\[
D^1_{h_n}[v] = \frac{m + 2}{n^2 \nu_m h_n^{m+2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \sqrt{\kappa(x_i) \kappa(x_j)} \mathbf{1}\{d_M(x_i, x_j) < h_n\} |v(x_i) - v(x_j)|^2
\]
\[
= \frac{m + 2}{n^2 \nu_m h_n^{m+2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \sqrt{\kappa(x_i) \kappa(x_j)} \mathbf{1}\{d_M(x_i, x_j) < h_n\} \int_{U_i} \int_{U_j} |P^* v(x) - P^* v(y)|^2 d\gamma(y) d\gamma(x)
\]
\[
\geq [1 - \text{Lip}(\kappa)\alpha \varepsilon_n] \frac{m + 2}{\nu_m h_n^{m+2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbf{1}\{d_M(x_i, x_j) < h_n\} \int_{U_i} \int_{U_j} |P^* v(x) - P^* v(y)|^2 \sqrt{\kappa(x) \kappa(y)} d\gamma(y) d\gamma(x)
\]
\[
= [1 - \text{Lip}(\kappa)\alpha \varepsilon_n] \frac{m + 2}{\nu_m h_n^{m+2}} \int_{\mathcal{M}} \int_{V(x)} |P^* v(x) - P^* v(y)|^2 \sqrt{\kappa(x) \kappa(y)} d\gamma(y) d\gamma(x),
\]
where if \( x \in U_i \) then \( V(x) = \bigcup_{j: j \sim i} U_j \). Notice that \( V(x) \supset B_{h_n - 2\varepsilon_n}(x) \) and hence,
\[
D^1_{h_n}[v] \geq [1 - \text{Lip}(\kappa)\alpha \varepsilon_n] \frac{m + 2}{\nu_m h_n^{m+2}} \int_{\mathcal{M}} \int_{B_{h_n - 2\varepsilon_n}} |P^* v(x) - P^* v(y)|^2 \sqrt{\kappa(x) \kappa(y)} d\gamma(y) d\gamma(x) \tag{B.10}
\]
\[
= [1 - \text{Lip}(\kappa)\alpha \varepsilon_n] \frac{m + 2}{\nu_m h_n^{m+2}} E_{h_n - 2\varepsilon_n}[P^* v]. \tag{B.11}
\]

Combining inequality (B.5) with (B.11) gives
\[
D^1[\mathcal{I}v] = \|\nabla(\mathcal{I}v)\|_h^2
\]
\[
= \|\nabla(\Lambda_{h_n - 2\varepsilon_n} P^* v)\|_h^2
\]
\[
\leq [1 + \text{Lip}(\kappa)\alpha(h_n - 2\varepsilon_n)] \left[ 1 + C m^2 K(h_n - 2\varepsilon_n)^2 \right]^2 \frac{m + 2}{\nu_m (h_n - \varepsilon_n)^{m+2}} E_{h_n - 2\varepsilon_n}[P^* v]
\]
\[
\leq [1 + \text{Lip}(\kappa)\alpha(h_n - 2\varepsilon_n)] \left[ 1 + C m^2 K(h_n - 2\varepsilon_n)^2 \right]^2 \left( \frac{h_n}{h_n - 2\varepsilon_n} \right)^{m+2} [1 - \text{Lip}(\kappa)\alpha \varepsilon_n]^{-1} D^1_{h}[v]
\]
\[
\leq \left[ 1 + C_{\mathcal{M}, \kappa}(h_n + \varepsilon_n) \right] D^1_{h}[v], \tag{B.13}
\]
where we have used Lemma B.1 and the fact that \( \varepsilon_n \ll h_n \). The second statement follows by combining (B.9) and (B.13). \( \square \)

**Corollary B.6** (Lower Bound). Suppose \( k := k_n \) is such that \( h_n \sqrt{k_n} \ll 1 \) for \( n \) large. Then
\[
\lambda_n^{(k)} \geq \left[ 1 - C_{\mathcal{M}, \tau, \kappa} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{k} \right) \right] \lambda^{(k)}.
\]
Proof. Since we are interested in proving lower bounds for $\lambda_n^{(k)}$, we can assume WLOG that $\lambda_k^{(n)} < \lambda^{(k)}$. Let $V$ be the span of eigenvectors $v_1, \ldots, v_k$ of $L_n^{\tau,k}$ associated with eigenvalues $\lambda_1^{(n)}, \ldots, \lambda_k^{(n)}$. Lemma B.5(1) implies for $v \in V$

$$\|Iv\|_{L^2} \geq \left[1 - C_{\mathcal{M},\tau,k} h_n \sqrt{D_{h_n}(v)}\right]\|v\|_2 \geq \left[1 - C_{\mathcal{M},\tau,k} h_n \sqrt{\lambda^{(k)}_n}\right]\|v\|_2 \geq \left[1 - C_{\mathcal{M},\tau,k} h_n \sqrt{\lambda(k)}\right]\|v\|_2.$$  

Therefore, the assumption that $h_n \sqrt{\lambda(k)} \ll 1$ implies that $I|_V$ is injective and $V = I(V)$ has dimension $k$. Lemma B.5 then gives

$$\lambda^{(k)} \leq \max_{f \in V} \frac{D[f]}{\|f\|_{L^2}^2} = \max_{v \in V} \frac{D[Iv]}{\|Iv\|_{L^2}^2} \leq \max_{v \in V} \frac{\left[1 + C_{\mathcal{M},\tau,k} \left(h_n + \frac{\varepsilon_n}{h_n}\right)\right] D_{h_n}[u]}{\left(1 - C_{\mathcal{M},\tau,k} h_n \sqrt{\lambda(k)}\right)^2 \|u\|_2} \leq \max_{v \in V} \frac{\left[1 + C_{\mathcal{M},\tau,k} \left(h_n + \frac{\varepsilon_n}{h_n}\right)\right] \lambda^{(k)}_n}{\left(1 - C_{\mathcal{M},\tau,k} h_n \sqrt{\lambda(k)}\right)^2} \lambda^{(k)}_n \leq \left[1 + C_{\mathcal{M},\tau,k} \left(\frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)}\right)\right] \lambda^{(k)}.$$  

Therefore

$$\lambda^{(k)}_n \geq \left[1 + C_{\mathcal{M},\tau,k} \left(\frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)}\right)\right]^{-1} \lambda^{(k)} \geq \left[1 - C_{\mathcal{M},\tau,k} \left(\frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)}\right)\right] \lambda^{(k)}.$$  

Combining Lemma B.2 and B.5 we have:

**Theorem B.7.** Suppose $k := k_n$ is such that $h_n \sqrt{\lambda(k_n)} \ll 1$ for $n$ large. Then

$$\frac{|\lambda^{(k)}_n - \lambda^{(k)}|}{\lambda^{(k)}} \leq C_{\mathcal{M},\tau,k} \left[\frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)}\right],$$  

where $C_{\mathcal{M},\tau,k}$ is a constant depending on $\mathcal{M}, \tau, \kappa$.

### C Convergence of Eigenfunctions with Rate

In this section we prove Theorem 4.5. Before we proceed, we introduce some additional notations. For any interval $J$ of $\mathbb{R}$, denote $H_J(\gamma)$ the subspace of $H^1(\gamma)$ that is spanned by eigenfunctions of $L^{\tau,k}$ associated with eigenvalues in $J$ and $\mathbb{P}_J(\gamma)$ the orthogonal projection from $L^2(\gamma)$ onto $H_J(\gamma)$. Similarly we use the notation $H_J(\gamma_n)$ and $\mathbb{P}_J(\gamma_n)$ for $L_n^{\tau,k}$. To ease notation, we will denote $H_{(-\infty,\lambda)}(\gamma_n)$ and $H_{(-\infty,\lambda)}(\gamma_n)$ as $H_{\lambda}(\gamma)$ and $H_{\lambda}(\gamma_n)$, respectively. We shall also denote both projections as $\mathbb{P}_J$ when no confusion arises.

To start with, we need several auxiliary results.

**Lemma C.1.** Let $u \in H_{\lambda}(\gamma_n)$.

1. $\|P_I v - u\|_2 \leq C_{\kappa} h_n \sqrt{D_{h_n}(v)}$.  


2. \( D[IV] \geq \left[ 1 - C_{M, \tau, \kappa} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda} \right) \right] D_{h_n}[v]. \)

Proof. 1. By \([23][\text{Lemma 6.4(2)}],\)

\[
\|PTv - v\|_2 \leq C h_n \|\delta v\|,
\]

where \(\|\delta v\|\) is defined in (B.8) The result follows by noticing that \(\|\delta v\| \leq \sqrt{\alpha D_{h_n}[v]}\).

2. We first bound \(D_{h_n}[PTv]\) in terms of \(D_{h_n}[v]\). Denoting \(PTv\) as \(w\), we have

\[
D_{h_n}[w] = \langle w, L_n^{\tau, \kappa}w \rangle_2 = \langle w - P\lambda w + P\lambda w, L_n^{\tau, \kappa}(w - P\lambda w + P\lambda w) \rangle_2 \\
= \langle w - P\lambda w, L_n^{\tau, \kappa}(w - P\lambda w) \rangle_2 + \langle P\lambda w, L_n^{\tau, \kappa}P\lambda w \rangle_2 + \langle w - P\lambda w, L_n^{\tau, \kappa}P\lambda w \rangle_2 \\
\geq \langle P\lambda w, L_n^{\tau, \kappa}P\lambda w \rangle_2,
\]

where we have used that \(P\lambda w\) and \(L_n^{\tau, \kappa}P\lambda w \in H_\lambda(\gamma_n)\) are orthogonal to \(w - P\lambda w\). Since \(L_n^{\tau, \kappa}\) is nonsingular, \(\langle \cdot, L_n^{\tau, \kappa} \rangle_2\) defines an inner product and the triangle inequality implies

\[
\sqrt{D_{h_n}[w]} \geq \sqrt{\langle P\lambda w, L_n^{\tau, \kappa}P\lambda w \rangle_2} \geq \sqrt{\langle v, L_n^{\tau, \kappa}v \rangle_2} - \sqrt{\langle v - P\lambda w, L_n^{\tau, \kappa}(v - P\lambda w) \rangle_2}.
\]

Now we bound the second term above. Since \(v \in H_\lambda\), we have \(v = P\lambda v\) and

\[
\langle v - P\lambda w, L_n^{\tau, \kappa}(v - P\lambda w) \rangle_2 = \langle P\lambda(v - w), L_n^{\tau, \kappa}P\lambda(v - w) \rangle_2 \\
\leq \lambda \|P\lambda(v - w)\|_2^2 \leq \lambda \|v - w\|_2^2 \leq C_\kappa \lambda h_n^2 D_{h_n}[v],
\]

where the last step follows from (C.1). Hence

\[
\sqrt{D_{h_n}[PTv]} \geq \left[ 1 - C_\kappa \sqrt{\lambda h_n} \right] \sqrt{D_{h_n}[v]},
\]

and the result follows from Lemma B.2, which says

\[
D_{h_n}[PTv] \leq \left[ 1 + C_{M, \tau, \kappa} \left( h_n + \frac{\varepsilon_n}{h_n} \right) \right] D[IV].
\]

\[\square\]

We fix orthonormal eigenfunctions \(\{v_k\}_{k=1}^n\) and \(\{f_j\}_{j=1}^\infty\) for \(L_n^{\tau, \kappa}\) and \(L^{\tau, \kappa}\). The following lemma bounds the projection error when \(J\) is a half-interval.

**Lemma C.2.** Suppose \(k := k_n\) is such that \(h_n \sqrt{\lambda^{(k_n)}} \ll 1\). Then, for any \(a > 0\),

\[
\|IV_k - P\lambda^{(k)} + a IV_k\|_2^2 \leq C_{M, \tau, \kappa} a^{-1} k \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right),
\]

\[
D[IV_k - P\lambda^{(k)} + a IV_k] \leq C_{M, \tau, \kappa} a^{-1} (\lambda^{(k)} + a) k \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right).
\]
Proof. Let $V$ be the span of $v_1, \ldots, v_k$ and $\mathcal{V} = \mathcal{I}(V)$. Since $h_n \sqrt{\lambda^{(k)}} \ll 1$, Theorem 4.4 implies $\lambda_n^{(k)} \leq C \lambda^{(k)}$ and then by Lemma B.5, for any $v \in V$,

\[
\|\mathcal{I}v\|_{L^2} \geq \left[ 1 - C_{\mathcal{M}, \tau, n} h_n \sqrt{\lambda^{(k)}} \right] \|v\|_2 \geq \left[ 1 - C_{\mathcal{M}, \tau, n} h_n \sqrt{\lambda^{(k)}} \right] \|v\|_2
\]

\[
D[\mathcal{I}v] \leq \left[ 1 + C_{\mathcal{M}, \tau, n} \left( h_n + \frac{\varepsilon_n}{h_n} \right) \right] D[h_n[v]].
\]

The assumption $h_n \sqrt{\lambda^{(k)}} \ll 1$ also implies that $\mathcal{I}|\mathcal{V}$ is injective and $\mathcal{V}$ is $k$-dimensional. Let $\lambda_V^{(1)}, \ldots, \lambda_V^{(k)}$ be the eigenvalues of $A := \mathcal{L}^{\tau, \kappa}|V$. The minimax principle implies that, for $j \leq k$,

\[
\lambda_V^{(j)} \leq \left[ 1 + C_{\mathcal{M}, \tau, n} \left( h_n + \frac{\varepsilon_n}{h_n} \right) \right] \lambda_n^{(j)} \leq \lambda_n^{(j)} + C_{\mathcal{M}, \tau, n} \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right).
\]

(C.2)

Define another operator $\tilde{\mathcal{L}}^{\tau, \kappa}$ by

\[
\tilde{\mathcal{L}}^{\tau, \kappa} f = \mathcal{L}^{\tau, \kappa} \mathbb{P}_{\lambda^{(k)} + a} f + \lambda^{(k)}(f - \mathbb{P}_{\lambda^{(k)} + a} f).
\]

Let $\{f_i\}$'s be the eigenvectors of $\mathcal{L}^{\tau, \kappa}$ associated with eigenvalues $\{\lambda^{(i)}\}$. We observe that $\tilde{\mathcal{L}}^{\tau, \kappa}$ is self-adjoint with respect to the $L^2(\gamma)$ inner product and shares the same eigenvectors with corresponding eigenvalues $\lambda^{(1)}, \ldots, \lambda^{(k)}, \lambda^{(k)}, \ldots$. Let $\tilde{A} := \tilde{\mathcal{L}}^{\tau, \kappa}|\mathcal{V}$ and $\tilde{\lambda}_V^{(1)}, \ldots, \tilde{\lambda}_V^{(k)}$ be its eigenvalues. Let $f \in \mathcal{V}$ and $g = f - \mathbb{P}_{\lambda^{(k)} + a} f$. Since $\mathcal{L}^{\tau, \kappa} \mathbb{P}_{\lambda^{(k)} + a} f = \tilde{\mathcal{L}}^{\tau, \kappa} \mathbb{P}_{\lambda^{(k)} + a} f$, we have by orthogonality

\[
\langle f, \mathcal{L}^{\tau, \kappa} f \rangle_{L^2} - \langle f, \tilde{\mathcal{L}}^{\tau, \kappa} f \rangle_{L^2} = \langle g, \mathcal{L}^{\tau, \kappa} g \rangle_{L^2} - \langle g, \tilde{\mathcal{L}}^{\tau, \kappa} g \rangle_{L^2}
\]

\[
= \langle g, \mathcal{L}^{\tau, \kappa} g \rangle_{L^2} - \lambda^{(k)} \|g\|_{L^2}^2 \geq \frac{a}{\lambda^{(k)} + a} \langle g, \mathcal{L}^{\tau, \kappa} g \rangle_{L^2},
\]

(C.3)

where the last inequality follows from the fact that $\langle g, \mathcal{L}^{\tau, \kappa} g \rangle_{L^2} \geq (\lambda^{(k)} + a) \|g\|_{L^2}^2$. By the minimax principle, we have $\tilde{\lambda}_V^{(j)} \geq \lambda^{(j)}$ for $j \leq k$ and by Theorem 4.4 we have

\[
\tilde{\lambda}_V^{(j)} \geq \lambda_n^{(j)} - C_{\mathcal{M}, \tau, n} \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right).
\]

Together with (C.2), we get

\[
\lambda_V^{(j)} - \tilde{\lambda}_V^{(j)} \leq C_{\mathcal{M}, \tau, n} \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right),
\]

and by (23)[Lemma 7.2], for any $f \in \mathcal{V}$,

\[
\langle f, \mathcal{L}^{\tau, \kappa} f \rangle_{L^2} - \langle f, \tilde{\mathcal{L}}^{\tau, \kappa} f \rangle_{L^2} = \langle f, A f \rangle_{L^2} - \langle f, \tilde{A} f \rangle_{L^2} \leq k \max_{1 \leq j \leq k} \{ \lambda_V^{(j)} - \tilde{\lambda}_V^{(j)} \} \leq C_{\mathcal{M}, \tau, n} k \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right),
\]

where we have used the fact that $A \geq \tilde{A}$ from (C.3). Hence (C.3) implies

\[
D[g] = \langle g, \mathcal{L}^{\tau, \kappa} g \rangle_{L^2} \leq C_{\mathcal{M}, \tau, n} a^{-1}(\lambda^{(k)} + a) k \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right),
\]

\[
\|g\|_{L^2}^2 \leq C_{\mathcal{M}, \tau, n} a^{-1} k \lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right).
\]
The next lemma bounds the projection error when \( J \) is a finite interval.

**Lemma C.3.** Suppose \( k := k_n \) is such that \( h_n \sqrt{\lambda(k_n)} \ll 1 \). Let \( a \leq b \leq c \leq \lambda(k) \) be constants so that the interval \((\lambda(k) + a, \lambda(k) + b)\) does not contain any eigenvalue of \( L_{\tau, \nu} \). Then

\[
\|\mathcal{I}v_k - \mathbb{P}_{(\lambda(k) - c, \lambda(k) + a)}\mathcal{I}v_k\|_{L^2}^2 \leq C_{M, \tau, \nu} C^{-1} b^{-1} k \left[ \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)} \right]^2 + c^{-1} a.
\]

**Proof.** Let \( f = \mathcal{I}v_k \) and decompose it as

\[
f = \mathbb{P}_{(\lambda(k) - c, \lambda(k) + a)} f + \mathbb{P}_{(-\infty, \lambda(k) - c]} f + \mathbb{P}_{(\lambda(k) + a, \infty)} f =: f_0 + f_- + f_+.
\]

Orthogonality implies

\[
\langle f, L_{\tau, \nu} f \rangle_{L^2} = \langle f_0, L_{\tau, \nu} f_0 \rangle_{L^2} + \langle f_-, L_{\tau, \nu} f_- \rangle_{L^2} + \langle f_+, L_{\tau, \nu} f_+ \rangle_{L^2},
\]

and we have by assumption that \( f_+ = \mathbb{P}_{[\lambda(k) + a, \infty)} f \). By Lemma C.2, we have

\[
\|f_+\|_{L^2}^2 \leq C_{M, \tau, \nu} b^{-1} k \lambda(k) \left[ \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)} \right],
\]

\[
\langle f_+, L_{\tau, \nu} f_+ \rangle_{L^2} \leq C_{M, \tau, \nu} b^{-1} k \lambda(k) \left[ \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)} \right].
\]

By Lemma C.1 (2), we have

\[
\langle f, L_{\tau, \nu} f \rangle_{L^2} = D[\mathcal{I}v_k] \geq \left[ 1 - C_{M, \tau, \nu} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)} \right) \right] D_{h_n} [v_k] = \left[ 1 - C_{M, \tau, \nu} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)} \right) \right] \lambda_n^{(k)}.
\]

Then

\[
\langle f_0, L_{\tau, \nu} f_0 \rangle_{L^2} + \langle f_-, L_{\tau, \nu} f_- \rangle_{L^2} = \langle f, L_{\tau, \nu} f \rangle_{L^2} - \langle f_+, L_{\tau, \nu} f_+ \rangle_{L^2} \geq \lambda_n^{(k)} - C_{M, \tau, \nu} b^{-1} (\lambda(k) + b) k \lambda(k) \left[ \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda(k)} \right].
\]

We also have

\[
\langle f_0, L_{\tau, \nu} f_0 \rangle_{L^2} \leq (\lambda(k) + a) \|f_0\|_{L^2},
\]

\[
\langle f_-, L_{\tau, \nu} f_- \rangle_{L^2} \leq (\lambda(k) - c) \|f_-\|_{L^2},
\]

which implies

\[
\langle f_0, L_{\tau, \nu} f_0 \rangle_{L^2} + \langle f_-, L_{\tau, \nu} f_- \rangle_{L^2} \leq \lambda(k) (\|f_0\|^2_{L^2} + \|f_-\|^2_{L^2}) + a \|f_0\|^2_{L^2} - c \|f_-\|^2_{L^2} \leq \lambda(k) \|f\|^2_{L^2} + a \|f\|^2_{L^2} - c \|f_-\|^2_{L^2}.
\]

By Lemma B.5(1), we have

\[
\|f\|_{L^2} = \|\mathcal{I}v_k\|_{L^2} \leq \left[ 1 + C_{\nu} h_n \sqrt{\lambda_n^{(k)}} \right] \|v_k\|_2 \leq 1 + C_{\nu} h_n \sqrt{\lambda(k)},
\]
which gives
\[ \langle f_0, L^\tau \chi f_0 \rangle_{L^2} + \langle f_-, L^\tau \chi f_- \rangle_{L^2} \leq (\lambda^{(k)} + a)(1 + C_n h_n^2 \lambda^{(k)}) - c\|f_-\|_{L^2}^2. \]

Combining with (C.5) we have
\[ (\lambda^{(k)} + a)(1 + C_n h_n^2 \lambda^{(k)}) - c\|f_-\|_{L^2}^2 \geq \lambda^{(k)} - C_{M, \tau, n} b^{-1}(\lambda^{(k)} + b)k\lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right), \]

and then
\[ \|f_-\|_{L^2}^2 \leq C_{M, \tau, n} c^{-1} b^{-1}(\lambda^{(k)} + b)k\lambda^{(k)} \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right) + c^{-1} a + c^{-1} \lambda^{(k)} - \lambda^{(k)} \]
\[ \leq C_{M, \tau, n} c^{-1} b^{-1} k(\lambda^{(k)})^2 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(k)}} \right) + c^{-1} a, \]

(C.6)

where the assumption \( b \leq \lambda^{(k)} \) is used in the last step. The result then follows by combining (C.4) and (C.6) and noticing that \( \|\mathcal{I}v_k - P_{(\lambda^{(k)} - c, \lambda^{(k)} + a)}\mathcal{I}v_k\|_{L^2}^2 = \|f_+\|_{L^2}^2 + \|f_-\|_{L^2}^2. \)

Now we are ready to prove Theorem 4.5.

**Theorem C.4 (Eigenfunction Approximation).** Let \( \lambda \) be an eigenvalue of \( L^\tau \chi \) with multiplicity \( \ell \), i.e.,
\[ \lambda^{(k_n-1)} < \lambda^{(k_n)} = \lambda = \ldots = \lambda^{(k_n+\ell-1)} < \lambda^{(k_n+\ell)}. \]

Suppose that \( h_n \sqrt{\lambda^{(k_n)}} \ll 1 \) for \( n \) large. Let \( \psi^{(k_n)}_n, \ldots, \psi^{(k_n+\ell-1)}_n \) be orthonormal eigenvectors of \( L^\tau \chi \) associated with eigenvalues \( \lambda^{(k_n)}, \ldots, \lambda^{(k_n+\ell-1)} \). Then there exists orthonormal eigenfunctions \( \tilde{\psi}^{(k_n)}, \ldots, \tilde{\psi}^{(k_n+\ell-1)} \) of \( L^\tau \chi \) so that for \( j = k_n, \ldots, k_n + \ell - 1 \)
\[ \|\psi^{(j)} - \tilde{\psi}^{(j)}\|_{L^2}^2 \leq C_{M, \tau, n} \delta j^2 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(j)}} \right), \]

where \( \{T_n\}_{n=1}^\infty \) is a sequence of transport maps in Proposition 4.3.

**Proof.** For each \( j = k, \ldots, k + \ell - 1 \), let \( a = (\varepsilon_n/h_n + h_n \sqrt{\lambda^{(j)}}) \) and \( b = c = \frac{\delta j}{2} \), where
\[ \delta \lambda = \min\{\lambda^{(k_n)} - \lambda^{(k_n-1)}, \lambda^{(k_n+\ell)} - \lambda^{(k_n+\ell-1)}\} \]
so that the assumptions of Lemma C.3 are satisfied. Indeed, \( a \leq b \leq c \leq \lambda^{(k)} \) and the interval \( (\lambda^{(j)} + a, \lambda^{(j)} + b) \) does not contain any eigenvalue of \( L^\tau \chi \) and \( P_{(\lambda^{(j)} - c, \lambda^{(j)} + a)} = P_{(\lambda^{(j)})} \). Hence we obtain
\[ \|\mathcal{I} \psi^{(j)}_n - \tilde{\psi}^{(j)}\|_{L^2} \leq C_{M, \tau, n} \delta j^2 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(j)}} \right), \]
where \( \tilde{\psi}^{(j)} = P_{(\lambda)} \mathcal{I} \psi^{(j)}_n \) is a \( \lambda \)-eigenfunction of \( L^\tau \chi \). Lemma B.5(1) implies that \( \mathcal{I} \) is almost an isometry on the span of \( \psi^{(k)}_n, \ldots, \psi^{(k+\ell-1)}_n \) and by the polarization identity we get that the
The $I\psi_n^{(j)}$'s are almost orthonormal up to $C_{M,\tau,\kappa} h_n \sqrt{\lambda^{(j)}}$. This implies the $\tilde{\psi}^{(j)}$'s are almost orthonormal up to $C_{M,\tau,\kappa} \delta_\lambda^{-2} j [\lambda^{(j)}]^2 (\varepsilon_n/h_n + h_n \sqrt{\lambda^{(j)}})$. Hence letting $\{\psi_j^{(j)}\}_{j=1}^{k+\ell-1}$ be the Gram-Schmidt orthogonalization of $\{\tilde{\psi}^{(j)}\}_{j=1}^{k+\ell-1}$, we get

$$\|I \psi_n^{(j)} - \psi^{(j)}\|_L^2 \leq C_{M,\tau,\kappa} \delta_\lambda^{-2} j [\lambda^{(j)}]^2 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(j)}} \right).$$

Using (B.7) that $\|Iv - P^*v\|_L^2 \leq Ch_n^2 D_n[u]$ gives

$$\|P^* \psi_n^{(j)} - \psi^{(j)}\|_L^2 \leq C_{M,\tau,\kappa} \delta_\lambda^{-2} j [\lambda^{(j)}]^2 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(j)}} \right).$$

By Weyl's law that $\lambda^{(j)} \asymp j^{\frac{2}{m}}$ and hence $\delta_\lambda \asymp j^{\frac{2}{m}-1} \asymp j^{-1} \lambda^{(j)}$, we conclude that

$$\|P^* \psi_n^{(j)} - \psi^{(j)}\|_L^2 \leq C_{M,\tau,\kappa} j^3 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(j)}} \right).$$

The result follows by observing that $P^* \psi_n^{(j)} = \psi^{(j)} \circ T_n$.

\section{Convergence of Gaussian Matérn Field}

Now we are ready to prove Theorem 4.1.

\textbf{Theorem D.1.} Suppose $s > 2m$ and $h_n$ satisfies

$$\frac{\log n}{n^{1/m}} \ll h_n \ll \frac{1}{n^{1/s}},$$

where $c_m = 3/4$ if $m = 2$ and $c_m = 1/m$ otherwise. Let $u$ and $u_n$ be defined by (4.1) and (4.2). Then with probability 1,

$$\mathbb{E} \left[ d_{TL^2} \left( (\gamma_n, u_n), (\gamma, u) \right) \right] \leq C_{M,\tau,\kappa, s} \left[ \sqrt{n k_n^{-\frac{m}{2}}} + k_n^{\frac{3}{2}} - m + \varepsilon_n + \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{-\frac{1}{2}} \right)^{\frac{1}{2}} \right],$$

where $k_n$ is chosen so that $n^{m/s} \ll k_n \ll h_n^{-m}$.

\textbf{Proof.} Suppose we are in a realization where the conclusion of Proposition 4.3 holds and let $\{T_n\}_{n=1}^\infty$ be a sequence of transport maps satisfying the bound (4.5). By Weyl's law that $\lambda^{(k)} \asymp k^{\frac{2}{m}}$, we see that the choice of $k_n$ ensures that $h_n \sqrt{\lambda^{(k_n)}} \ll 1$ and the assumption of Theorem C.4 is satisfied. Hence we can fix orthonormal eigenfunctions $\{\psi^{(i)}\}_{i=1}^\infty$ of $\mathcal{L}^{\tau,\kappa}$ and $\{\psi^{(n)}_i\}_{i=1}^n$ of $\mathcal{L}^{\tau,\kappa}$ for each $n$ so that

$$\|\psi_n^{(i)} \circ T_n - \psi^{(i)}\|_L^2 \leq C_{M,\tau,\kappa} j^3 \left( \frac{\varepsilon_n}{h_n} + h_n \sqrt{\lambda^{(i)}} \right),$$

for $i = 1, \ldots, k_n$. Recall $u_n$ and $u$ have the following representations

$$u_n := \tau^{\frac{3}{2}} - m \frac{m}{k_n} \sum_{i=1}^n \left[ \lambda^{(i)} \right]^{-\frac{3}{2}} \xi^{(i)} \psi^{(i)}_n,$$

$$u = \tau^{\frac{3}{2}} - m \frac{m}{k_n} \sum_{i=1}^\infty \left[ \lambda^{(i)} \right]^{-\frac{3}{2}} \xi^{(i)} \psi^{(i)}.$$
To bound the $TL^2$ distance between them, we introduce four intermediate functions.

$$u_{kn}^k := \tau_n^{\frac{s}{2} - \frac{m}{4}} \kappa_n^m \sum_{i=1}^{k_n} \lambda_n^{(i)} - \frac{s}{2} \xi_n^{(i)} \psi_n^{(i)},$$

$$\bar{u}_{kn}^k := \tau_n^{\frac{s}{2} - \frac{m}{4}} \kappa_n^m \sum_{i=1}^{k_n} \lambda_n^{(i)} - \frac{s}{2} \xi_n^{(i)} \psi_n^{(i)},$$

$$u_n^k := \tau_n^{\frac{s}{2} - \frac{m}{4}} \kappa_n^m \sum_{i=1}^{k_n} \lambda_n^{(i)} - \frac{s}{2} \xi_n^{(i)} \psi_n^{(i)}.$$

It then suffices to bound the difference between any two consecutive functions. For the following proof, we shall use the notation $a \lesssim b$ to denote $a \leq C_{M_2, \tau, \kappa, s} b$ and similarly for $\gtrsim$. By Theorem 4.4 and Weyl's law we have that $\lambda_n^{(k_n)} \gtrsim \lambda_n^{(k_n)} \gtrsim k_n^{2/m}$, which gives

$$\mathbb{E}\left[ d_{TL^2}( (\gamma_n, u_n), (\gamma, u_{kn}) ) \right] \lesssim \beta \tau_n^{m/4} \alpha (\sum_{i=k_n+1}^{n} \lambda_n^{(i)} - \frac{s}{2})^{\frac{1}{2}} \lesssim (n \lambda_n^{(k_n)} - \frac{s}{2})^{\frac{1}{2}} \lesssim \sqrt{n} k_n^{-\frac{s}{2m}}. \quad (D.2)$$

Similarly,

$$\mathbb{E}\left[ d_{TL^2}( (\gamma, u_n^k), (\gamma, u) ) \right] \lesssim \left( \sum_{i=k_n+1}^{\infty} \lambda_n^{(i)} - \frac{s}{2} \right)^{\frac{1}{2}} \lesssim \left( \sum_{i=k_n+1}^{\infty} i^{-\frac{2}{m}} \right)^{\frac{1}{2}} \lesssim \left( \int_{k_n}^{\infty} x^{-\frac{2a}{m}} \right)^{\frac{1}{2}} \lesssim k_n^{-\frac{s}{2m}}. \quad (D.3)$$

By Lipschitz continuity of $x^{-s/2}$ away from 0 we have, for $i = 1, \ldots, k_n$,

$$\left| \left[ \lambda_n^{(i)} \right] - \left[ \lambda^{(i)} \right] \right| \lesssim \left( \left[ \lambda_n^{(i)} \right] \wedge \left[ \lambda^{(i)} \right] \right)^{-\frac{s}{2}} |\lambda_n^{(i)} - \lambda^{(i)}| \lesssim \left[ \lambda^{(i)} \right]^{-\frac{s}{2}} \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{\frac{1}{m}} \right).$$

Hence

$$\mathbb{E}\left[ d_{TL^2}( (\gamma_n, u_n^{k_n}), (\gamma_n, \bar{u}_n^{k_n}) ) \right] \lesssim \left( \sum_{i=1}^{k_n} \left( \left[ \lambda_n^{(i)} \right] - \left[ \lambda^{(i)} \right] \right)^{\frac{1}{2}} \right)^{\frac{1}{2}}$$

$$\lesssim \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{\frac{1}{m}} \right)^{\frac{1}{2}} \lesssim \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{\frac{1}{m}} \right)^{\frac{1}{2}} \lesssim \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{\frac{1}{m}} \right), \quad (D.4)$$

where in the last step $s > 2m$ implies $\sum_{i=1}^{\infty} \left[ \lambda^{(i)} \right]^{-s} < \infty$. By Lipschitz continuity of $\tau$ and $\kappa$, and the fact that $d(x, T_n(x)) \leq \varepsilon_n$, we have

$$\left| \tau(T_n(x)) \frac{s}{2} - \frac{m}{2} \kappa(T_n(x)) \frac{m}{2} \tau(x) \frac{s}{2} - \frac{m}{2} \kappa(x) \frac{m}{2} \right| \lesssim \varepsilon_n.$$
Finally by (D.1), we have

\[
\mathbb{E}\left[ d_{TL}^2\left( (\gamma_n, \tilde{u}_n^k), (\gamma, u^k) \right) \right] \lesssim \sup_{x \in \mathcal{M}} \left| \tau(T_n(x)) \frac{1}{\sqrt{n}} \kappa(T_n(x)) \frac{1}{\sqrt{2}} - \tau(x) \frac{1}{\sqrt{2}} \kappa(x) \frac{1}{\sqrt{2}} \right| \left( \sum_{i=1}^{k_n} \left[ \lambda(i) \right]^{-s} \right)^{\frac{1}{2}} \\
+ \sum_{i=1}^{k_n} \left[ \lambda(i) \right]^{-\frac{3}{2}} \| \psi_n^{(i)} \circ T_n - \psi^{(i)} \|_{L^2} \\
\lesssim \varepsilon_n + \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{-\frac{1}{2}} \right)^{\frac{1}{2}} \left( \sum_{i=1}^{k_n} i^{-\frac{3}{2}} \left[ \lambda(i) \right]^{-s} \right)^{\frac{1}{2}} \\
\lesssim \varepsilon_n + \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{-\frac{1}{2}} \right)^{\frac{1}{2}}, \quad \text{(D.5)}
\]

where the assumption \( s > 2m \) implies \( \sum_{i=1}^{\infty} i^3 [\lambda(i)]^{-s} < \infty \). Hence combining (D.2), (D.3), (D.4), (D.5), we have

\[
\mathbb{E}\left[ d_{TL}^2\left( (\gamma_n, u_n), (\gamma, u) \right) \right] \leq C_{M, \tau, \kappa, s} \left[ \sqrt{n} k_n^{-\frac{m}{m}} + k_n^{-\frac{2m}{m}} + \varepsilon_n + \left( \frac{\varepsilon_n}{h_n} + h_n k_n^{-\frac{1}{2}} \right)^{\frac{1}{2}} \right].
\]

\( \square \)