# Lengthscale-informed sparse grids for kernel methods in high dimensions

Elliot J. Addy<sup>1</sup>, Jonas Latz<sup>2</sup>, Aretha L. Teckentrup<sup>1</sup>

<sup>1</sup>School of Mathematics and Maxwell Institute for Mathematical Sciences, University of Edinburgh, King's Buildings, Edinburgh, EH9 3FD, UK.

<sup>2</sup>Department of Mathematics, University of Manchester, Alan Turing Building, Oxford Road, Manchester, M13 9PL, UK.

Corresponding Author. E-mail: e.j.addy@sms.ed.ac.uk;

#### Abstract

Kernel interpolation, especially in the context of Gaussian process emulation, is a widely used technique in surrogate modelling, where the goal is to cheaply approximate an input-output map using a limited number of function evaluations. However, in high-dimensional settings, such methods typically suffer from the curse of dimensionality; the number of required evaluations to achieve a fixed approximation error grows exponentially with the input dimension. To overcome this, a common technique used in high-dimensional approximation methods, such as quasi-Monte Carlo and sparse grids, is to exploit functional anisotropy: the idea that some input dimensions are more 'sensitive' than others. In doing so, such methods can significantly reduce the dimension dependence in the error. In this work, we propose a generalisation of sparse grid methods that incorporates a form of anisotropy encoded by the lengthscale parameter in Matérn kernels. We derive error bounds and perform numerical experiments that show that our approach enables effective emulation over arbitrarily high dimensions for functions exhibiting sufficient anisotropy.

**Keywords:** Kernel methods, High-dimensional approximation, Sparse grids, Lengthscales, Gaussian processes. **Mathematics Subject Classification:** 41A25, 41A63, 62G08, 65B99, 65C20, 65D12, 65D15, 65D32, 65D40.

<sup>\*</sup>ORCID-IDs: 0009-0003-2667-8493, 0000-0002-4600-0247, 0000-0001-5089-0476.

#### 1 Introduction

Kernel methods are widely used in surrogate modelling, where the goal is to cheaply approximate an input-output map using a limited number of function evaluations. Due to their mesh-free nature, kernel methods are especially well-suited to the low-data regime, where data acquisition poses the primary computational bottleneck, as well as scattered data approximation, where the location of function evaluations may be very irregular. Kernel methods are well known in the numerical analysis community, for example through approximation with radial basis functions [1–5], as well as in the statistics community, where the Gaussian process framework for regression is well established [6–10].

In this work, we are interested in the accuracy of kernel methods as a function of the number of function evaluations (or training points) used to construct the approximation. More precisely, we consider the problem of interpolation, where we wish to approximate a function f from given evaluations  $\{(\mathbf{x}, f(\mathbf{x}))\}_{\mathbf{x} \in \mathcal{X}}$  at N distinct points. From a numerical analysis point of view, we then wish to bound the error  $||f - s_{\mathcal{X}, \varphi}(f)||$  between the true function f and its interpolant  $s_{\mathcal{X}, \varphi}(f)$  built using the evaluations at  $\mathcal{X}$  and kernel  $\varphi$ , in a suitably chosen norm. From a statistical point of view, the interpolant  $s_{\mathcal{X}, \varphi}(f)$  takes the role of the posterior mean in Gaussian process regression (see e.g. [11]), and the former error analysis hence enables us to conclude on convergence of the methodology also in this framework.

The form of the error bounds, and the tools used to derive them, depend heavily on the kernel  $\varphi$  employed in the approximation. Frequently used kernels in practice are the family of Matérn kernels [12, 13], since their parametric nature allows for flexibility to model various behaviours in terms of amplitude, length-scale and regularity. A further desirable feature of Matérn kernels is that the corresponding interpolants  $s_{\mathcal{X},\varphi}(f)$  lie in Sobolev spaces [14], enabling the derivation of error bounds in the widely used Sobolev framework [1, 3, 15]. In general, however, these error bounds unfortunately scale poorly with the number of inputs and suffer from the curse of dimensionality. The number of function evaluations required to maintain a fixed error  $\varepsilon$  grows exponentially with the input dimension, rendering the application of kernel methods to high-dimensional models notoriously challenging [7, 16, 17].

To combat the challenge posed by a high input dimension, a central idea in high-dimensional approximation is to take advantage of anisotropy in the target function f. If f is more difficult to approximate along certain axial directions than others, we can allocate computational effort preferentially to the more sensitive directions—placing fewer interpolation points in directions where f is relatively smooth and/or flat. Two well-known techniques in this direction are anisotropic sparse grids (for approximation and integration) and weighted quasi-Monte Carlo methods (for integration). To alleviate the dependence on the input dimension in the error bounds, anisotropic sparse grids require that the function f is more regular in certain inputs, or equivalently that approximations in these input dimensions decay at faster rates [18–20]. Weighted quasi-Monte Carlo methods, on the other hand, assume that the partial first (and possibly higher) derivative of f is much smaller in certain inputs, or equivalently that the variation of f is small in these input dimensions [21, 22]. Alternative approaches to kernel methods in high-dimensional input spaces are typically based on

low-dimensional approximations, including for example ANOVA-type decompositions [23, 24], sparsity assumptions [25] or projection-based dimension reduction [26].

In practice, the assumption that f is more regular in some of its inputs, as required by anisotropic sparse grids, is often not satisfied or difficult to verify. This motivates the development of alternative formulations of anisotropy for kernel methods for approximation with sparse grids. One natural candidate is the lengthscale parameter  $\lambda$  in Matérn kernels; larger values of  $\lambda$  correspond to flatter, more slowly varying interpolants, effectively assuming a reduced sensitivity to changes in the inputs. Lengthscale-anisotropic kernels, such as the anisotropic squared exponential kernel  $\varphi(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp^{-\sum_{j=1}^d (x_j - x_j')^2/2\lambda_j^2}$ , are commonly used in the spatial statistics and machine learning literature, see e.g. [27–29] and the references therein. The length-scales  $\{\lambda_j\}_{j=1}^d$  are typically estimated using the observed values  $\{(\mathbf{x}, f(\mathbf{x}))\}_{\mathbf{x} \in \mathcal{X}}$ , and, in the same spirit as in this work, the estimated lengthscales are then frequently used in an automatic relevance determination (ARD) framework [30–32] to assign varying levels of importance to the different inputs.

From a theoretical point of view, the effect of lengthscale adaptivity and/or anisotropy in Gaussian process regression has notably been studied in the works [28, 29, 33, 34] (see also the references therein). In [34], the author studies the effect of adapted (or estimated) length-scales  $\{\hat{\lambda}_j\}_{j=1}^d$ , dependent on the number of observed evaluations N, in Matérn kernels on error bounds for the posterior mean and covariance. The authors of [28] show that for a suitable hyper-prior defined on  $\lambda_j \equiv \lambda$ , Gaussian process regression with the squared exponential kernel can adapt to the smoothness of the target f and provide optimal convergence rates in a general setting. The effect of anisotropic lengthscales, again defined through a suitable hyper-prior, was studied in [29]. We note, however, that the faster convergence rates proved in [29] additionally rely on anisotropic regularity as was the case for anisotropic sparse grids discussed earlier. Finally, while the authors of [33] show that approximation with anisotropic squared exponential kernels can theoretically lead to dimension independent error bounds, their proof is not constructive and a choice of kernel function and observation points achieving these rates is to the best of our knowledge unknown.

In this work, our goal is to incorporate lengthscale-based anisotropy into the well-studied framework of kernel methods and sparse grid approximation. In particular, we investigate how directional sensitivity, encoded via the lengthscales of separable Matérn kernels, can be exploited to improve upon established error estimates and lead to convergence rates that exhibit dimension robust behaviour. To the best of our knowledge, this work is the first to develop a method with proven improved error bounds in the high-dimensional setting assuming only anisotropy in the lengthscales, not requiring anisotropic (or infinite) regularity. Furthermore, we would like to emphasise that our approach does not involve any form of dimension reduction or truncation; our method works in the full high-dimensional setting. Finally, we note that the use of structured designs such as the introduced lengthscale-informed sparse grids enables fast linear algebra routines (see e.g. [35, 36]), resulting in a method that scales well with the number of observed function evaluations as well as the input dimension.

#### Our contributions

This paper makes the following key contributions:

- 1. We introduce a novel sparse grid construction based on uniformly-spaced points, termed lengthscale-informed sparse grids (LISGs), designed to exploit lengthscale-anisotropy in target functions and resulting in sparse grids with controlled growth in the individual input dimensions. The construction is detailed in Definition 8.
- 2. We derive an error bound for lengthscale-anisotropic Matérn kernel interpolation using LISGs in terms of the sparse grid level L (see Theorem 2), demonstrating its superior performance in high-dimensional settings. We further include an explicit relationship between the sparse grid level L and the number of points in the corresponding LISG, see Theorem 3.
- 3. Using the relationship between kernel interpolation and Gaussian process emulation, we derive an analogous error bound to point 2. above for the posterior marginal variance in Proposition 8. (The convergence of the posterior mean follows directly from Theorem 2.)
- 4. We adapt the fast inference algorithm for isotropic sparse grids from [36] to LISGs in Algorithm 1, resulting in an algorithm with significantly lower computational cost in terms of the input dimension d. In terms of the sparse grid level L, the cost of inverting the largest matrix in Algorithm 1 is  $\mathcal{O}(L2^L)$ .
- 5. We demonstrate the dimension-robust performance of our method on test problems in up to 100 dimensions.

#### Paper structure

In Section 2, we provide the necessary background material and review relevant prior results. Sections 2.1 and 2.2 cover Gaussian process emulation and its connections to kernel interpolation. Sections 2.3 and 2.4 introduce the regularity and anisotropy assumptions required of the target function. In Section 3 we introduce lengthscale-informed sparse grids; defining their construction in Section 3.1 and in Sections 3.2 and 3.3 we present general error bounds for the approximation error and associated marginal variance, respectively. Full derivations of the main theorems are provided in Section 4. In Section 5 we derive an adapted algorithm for fast computations of interpolants, and in Section 6 we present numerical results exploring the performance of our method on a test problem in high-dimensional settings under different anisotropy conditions.

#### Notation

Notation	Description
f	Target function, later assumed to be in the Native space of interpolating kernels; $\mathcal{N}_{\varphi}(\Omega)$ .
d	Dimension of the input space of $f$ .

$\mathcal{X}, \Omega$	Arbitrary finite point set and compact set where $\mathcal{X} \subset \Omega \subset \mathbb{R}^d$ .
$h_{\mathcal{X},\Omega}$	The fill-distance of $\mathcal{X}$ in $\Omega$ ; $\sup_{\mathbf{x}\in\Omega}\inf_{\mathbf{x}'\in\mathcal{X}}\ \mathbf{x}-\mathbf{x}'\ _2$ .
$R_{\Omega}$	Restriction operator to $\Omega$ ; $R_{\Omega}(g) = g _{\Omega}$ .
$\varphi$	Arbitrary positive definite kernel function $\varphi : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ .
$m_{\mathcal{X}}^f,arphi_{\mathcal{X}}$	Posterior mean and covariance functions with data $D_{\mathcal{X}} = \{\mathbf{x}, f(\mathbf{x})\}_{x \in \mathcal{X}}$ . (See Section 2.1)
$s_{\mathcal{X},arphi}$	Kernel interpolation operator with interpolating kernel $\varphi$ and data $D_{\mathcal{X}} = \{\mathbf{x}, f(\mathbf{x})\}_{x \in \mathcal{X}}$ . Note $s_{\mathcal{X}, \varphi}(f) = m_{\mathcal{X}}^f$ . (See Definition 2)
$\mathcal{N}_{arphi}(\Omega)$	Native space, or reproducing kernel Hilbert space, of the kernel $\varphi$ , restricted to $\Omega$ . (See Definition 1)
$\phi_{\nu,\lambda},\Phi_{\nu,\lambda}$	Matérn and separable Matérn kernel functions. (See Definitions 3 and 4)
$\nu,  \alpha,  \beta$	Regularity parameters in Matérn kernels and Sobolev spaces.
$\lambda$ , $\lambda$	Lengthscale parameter in $\mathbb{R}_{\geq 0}$ and lengthscale vector in $\mathbb{R}^d_{\geq 0}$ for Matérn and separable Matérn kernels, respectively.
$\sigma$	Standard deviation parameter in Matérn kernels.
$\Gamma$ , $\Gamma_k$	The unit interval $(-1/2, 1/2)$ and the intervals $(-2^{-k-1}, 2^{-k-1})$ , respectively. Note $\Gamma_0 = \Gamma$ .
L	Level parameter for sparse grids in $\mathbb{N}_0$ .
$p, \mathbf{p}$	Penalty parameter in $\mathbb{N}_0$ , and penalty vector in $\mathbb{N}_0^d$ .
$\mathcal{I}_L^d$	Multi-index set $\{l \in \mathbb{N}_0^d :  l _1 \le L\}$ .
$\mathcal{X}_l,\mathcal{X}_l^p$	One dimensional uniformly spaced point sets and $p$ -penalised point sets in $\Gamma$ . Note $\mathcal{X}_l^0 = \mathcal{X}_l$ . (See Definitions 5 and 7)
$\mathcal{X}_{d,L}^{\otimes},\mathcal{X}_{d,L,\mathbf{p}}^{\otimes}$	Standard and lengthscale-informed sparse grid designs in $\Gamma^d$ . (See Definition 6)
$S_{L,\boldsymbol{ u}},P_{L,\boldsymbol{ u},\mathbf{p}}$	Standard and lengthscale-informed sparse grid kernel interpolation operators. Note $P_{L,\nu,0} = S_{L,\nu}$ . (See Definition 8)
$N_{d,\mathbf{p}}(L)$	Number of points in lengthscale-informed sparse grid; $ \mathcal{X}_{d,L,\mathbf{p}}^{\otimes} $ .
$\mathcal{S}_{\lambda},\mathcal{T}_{\lambda}$	Function- and point- stretching operators, respectively. (See Definition 10)
u, v	Subsets of $\{1,\ldots,d\}$ of size $0 \leq k \leq d$ , denoting a $k$ -dimensional subspace. For a given $\mathbf{c} \in \mathbb{R}^d$ , we define $\mathbf{c}_{\mathfrak{u}} := (c_{\mathfrak{u}_1},\ldots,c_{\mathfrak{u}_k}) \subset \mathbb{R}^k$ , where $\mathfrak{u}_j < \mathfrak{u}_{j+1}$ .
$\mathcal{P}_k^d$	Set of all subsets of $\{1, \ldots, d\}$ of size $k$ ; $\{\mathfrak{u} \subset \{1, \ldots, d\} :  \mathfrak{u}  = k\}$ .

# 2 Background

In this section, we provide the relevant background material to define lengthscale-informed sparse grids, including: The wider context of Gaussian process emulation

in Section 2.1, the connection to kernel interpolation in Section 2.2, sparse grids for kernel methods in Section 2.3 and finally our formulation of lengthscale-anisotropy in Section 2.4.

#### 2.1 Gaussian process emulation

The broad aim of emulation is to approximate a function  $f:\Omega\to\mathbb{R}$ , where  $\Omega\subset\mathbb{R}^d$  is compact with Lipschitz boundary and  $d\in\mathbb{N}$ , using only point-wise evaluations of f. Gaussian process emulation approaches this problem in a Bayesian framework: We begin by placing a prior distribution on the unknown function, f, modelling it as a Gaussian process,

$$f_0 \sim GP(0, \varphi),$$
 (1)

where  $\varphi: \Omega \times \Omega \to \mathbb{R}$  is the prior covariance kernel in which prior knowledge about f is encoded, and we have chosen a zero prior mean. The choice of zero prior mean is for ease of presentation only, and our error bound in Theorem 2 can be extended to suitable non-zero prior means (satisfying the same assumptions as f), as shown in Theorem 3.5, [34]. Given a set of function evaluations  $D_{\mathcal{X}} = \{(\mathbf{x}, f(\mathbf{x}))\}_{\mathbf{x} \in \mathcal{X}}$  at N distinct points,  $\mathcal{X} = \{\mathbf{x}_i\}_{1 \leq i \leq N} \subset \Omega$ , we update the prior distribution with Bayes' rule. The posterior distribution is also a Gaussian process (see e.g. [6]),

$$f_0|D_{\mathcal{X}} \sim \mathrm{GP}(m_{\mathcal{X}}^f, \varphi_{\mathcal{X}}),$$
 (2)

with closed form expressions for the posterior mean function,  $m_{\mathcal{X}}^f: \Omega \to \mathbb{R}$ , and posterior covariance kernel,  $\varphi_{\mathcal{X}}: \Omega \times \Omega \to \mathbb{R}$ , given by

$$m_{\mathcal{X}}^f(\mathbf{x}) = \varphi(\mathbf{x}, \mathcal{X})^T \varphi(\mathcal{X}, \mathcal{X})^{-1} f(\mathcal{X}),$$
 (3)

$$\varphi_{\mathcal{X}}(\mathbf{x}, \mathbf{x}') = \varphi(\mathbf{x}, \mathbf{x}') - \varphi(\mathbf{x}, \mathcal{X})^T \varphi(\mathcal{X}, \mathcal{X})^{-1} \varphi(\mathbf{x}', \mathcal{X}). \tag{4}$$

Here we define the vectors  $\varphi(\mathbf{x}, \mathcal{X}) := [\varphi(\mathbf{x}, \mathbf{x}_1), \dots, \varphi(\mathbf{x}, \mathbf{x}_N)] \in \mathbb{R}^N$  and  $f(\mathcal{X}) := [f(\mathbf{x}_1), \dots, f(\mathbf{x}_N)] \in \mathbb{R}^N$ , whereas  $\varphi(\mathcal{X}, \mathcal{X}) \in \mathbb{R}^{N \times N}$  is the covariance matrix such that  $\varphi(\mathcal{X}, \mathcal{X})_{ik} = \varphi(\mathbf{x}_i, \mathbf{x}_k)$ . In general, this procedure is  $\mathcal{O}(N^3)$  as a consequence of having to invert (or solve linear systems with)  $\varphi(\mathcal{X}, \mathcal{X})$ . The posterior mean function,  $m_{\mathcal{X}}^f$ , is often used in inference algorithms as an approximation for f, and the posterior covariance,  $\varphi_{\mathcal{X}}$ , can be considered a local measure of uncertainty in this approximation [37, 38]. Our focus is to provide error estimates for the posterior mean and covariance kernel that are insensitive to the input dimension, d, by a judicious choice of the design,  $\mathcal{X}$ , and covariance kernel,  $\varphi$ .

#### 2.2 Approximating with kernels

To measure the approximation error of the mean function to f, we draw from results in the scattered data approximation literature [1]. In particular, the posterior mean function of a Gaussian process,  $m_{\chi}^f$ , is a kernel interpolant of f, uniquely defined

as the function of minimum norm in the *Native space* of the covariance kernel that interpolates f at  $\mathcal{X} \subseteq \Omega$ .

**Definition 1** A Hilbert space H of functions  $f:\Omega\to\mathbb{R}$ , with  $\Omega\subset\mathbb{R}^d$ , is a *Native* or reproducing kernel Hilbert space if point evaluation is a continuous linear functional. Each Native space, H, is associated to a unique function,  $\varphi:\Omega\times\Omega\to\mathbb{R}$ , called the reproducing kernel of H, which satisfies the reproducing kernel property: For all  $f\in H$ ,  $x\in\Omega$ , we have  $\langle f,\varphi(\cdot,x)\rangle_H=f(x)$ . For a given kernel,  $\varphi$ , we denote the corresponding Native space by  $H=\mathcal{N}_{\varphi}(\Omega)$ , with induced norm  $\|f\|_{\mathcal{N}_{\varphi}(\Omega)}=\langle f,f\rangle_H^{1/2}$ .

**Definition 2** Let  $f: \Omega \to \mathbb{R}$  be bounded and let  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \Omega$  be a finite discrete set such that  $|\mathcal{X}| = N$ . Define a linear sampling operator by  $T_{\mathcal{X}}(f) = f(\mathcal{X}) := [f(\mathbf{x}_1), \dots, f(\mathbf{x}_N)]$ . The  $\varphi$ -kernel interpolant operator, applied to f, with respect to  $\mathcal{X}$ , denoted  $s_{\mathcal{X}, \varphi}(f) \in \mathcal{N}_{\varphi}(\Omega)$ , is given by

$$s_{\mathcal{X},\varphi}(f) := \underset{\substack{g \in \mathcal{N}_{\varphi}(\Omega) \\ T_{\mathcal{X}}(g) = T_{\mathcal{X}}(f)}}{\arg \min} \|g\|_{\mathcal{N}_{\varphi}(\Omega)}. \tag{5}$$

**Proposition 1** (Section 6.2, [27], Theorem 1, [39]) For all  $\mathbf{x} \in \Omega$ ,  $s_{\mathcal{X}, \varphi}(f)(\mathbf{x}) = m_{\mathcal{X}}^f(\mathbf{x})$ .

Proposition 2 (Chapter 10, [1]) The Native space norm of a kernel interpolant is given by

$$||s_{\mathcal{X},\varphi}(f)||_{\mathcal{N}_{\varphi}(\Omega)} = \mathbf{w}^T \varphi(\mathcal{X}, \mathcal{X}) \mathbf{w}, \tag{6}$$

where  $\mathbf{w} = \varphi(\mathcal{X}, \mathcal{X})^{-1} f(\mathcal{X}).$ 

We restrict ourselves to the case of Matérn kernels; a popular class of positive definite kernels whose Native spaces are known to be *Sobolev spaces*, see e.g.[1, 40].

**Definition 3** ([41]) Let  $d \in \mathbb{N}$ . A *Matérn covariance kernel* is a symmetric, positive-definite kernel  $\phi_{\nu,\lambda} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_{>0}$ , defined by

$$\phi_{\nu,\lambda}(\mathbf{x}, \mathbf{x}') := \sigma^2 \frac{2^{1-\nu_j}}{\Gamma(\nu)} \left( \sqrt{2\nu} \frac{\|\mathbf{x} - \mathbf{x}'\|_2}{\lambda} \right)^{\nu} K_{\nu} \left( \sqrt{2\nu} \frac{\|\mathbf{x} - \mathbf{x}'\|_2}{\lambda} \right), \tag{7}$$

for all  $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$ , where  $\nu, \lambda, \sigma > 0$  and  $K_{\nu}$  is the modified Bessel function of the second kind.

The three hyperparameters  $\nu$ ,  $\lambda$ , and  $\sigma$  represent the smoothness, lengthscale and standard deviation of the kernels, respectively. The posterior mean function of a Gaussian process with covariance kernel  $\phi_{\nu,\lambda}$  does not depend on the standard deviation,  $\sigma$ , and hence we suppress it in our notation, considering it a free parameter of concern only in the wider statistical framework. Definition 3 is much simplified for half-integer  $\nu$ , with notable examples including the exponential kernel,  $\phi_{1/2,\lambda}(\mathbf{x},\mathbf{x}') = \sigma^2 \exp(-\|\mathbf{x} - \mathbf{x}'\|_2/\lambda)$  and, by taking the limit  $\nu \to \infty$ , the Gaussian (or squared-exponential) kernel  $\phi_{\nu\to\infty,\lambda} = \sigma^2 \exp(-\|\mathbf{x} - \mathbf{x}'\|_2^2/2\lambda^2)$ .

**Proposition 3** (Corollary 10.13, [1]) The function spaces  $\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R}^d)$  and  $H^{\nu+d/2}(\mathbb{R}^d)$  are isomorphic, with equivalent norms. This further holds for restrictions to Lipschitz  $\Omega \subset \mathbb{R}^d$ , specifically  $\mathcal{N}_{\phi_{\nu,\lambda}|_{\Omega \times \Omega}}(\Omega) \cong H^{\nu+d/2}(\Omega)$ .

Remark 1 For ease of notation, we will denote  $\mathcal{N}_{\varphi}(\Omega) = \mathcal{N}_{\varphi|_{\Omega \times \Omega}}(\Omega)$  for kernels  $\varphi : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$  and domains  $\Omega \subset \mathbb{R}^d$ .

**Proposition 4** (Theorem 10.47, [1]) Let  $g \in \mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R}^d)$ . Then,  $R_{\Omega}(g) \in \mathcal{N}_{\phi_{\nu,\lambda}}(\Omega)$ , where  $R_{\Omega}(g)$  represents the usual restriction of functions  $g|_{\Omega}$ .

We note that the Sobolev spaces  $\mathcal{N}_{\phi_{\nu,\lambda}} = H^{\nu+1/2}$  depend only on the smoothness parameter,  $\nu$ . In particular, changing the lengthscale does not change the space. Upper bounds for the interpolation error in the Sobolev norm are then given in terms of the *fill-distance* of the point-set in the domain;

$$h_{\mathcal{X},\Omega} := \sup_{\mathbf{x} \in \Omega} \inf_{\mathbf{x}' \in \mathcal{X}} \|\mathbf{x} - \mathbf{x}'\|_{2}. \tag{8}$$

**Proposition 5** (Theorem 3.2, [5]) Let  $d \in \mathbb{N}$ ,  $\beta > d/2$  and  $0 \le \alpha \le \beta$ . Let  $\Omega \subset \mathbb{R}^d$  be bounded with Lipschitz boundary such that is satisfies an interior cone condition. For  $f \in H^{\beta}(\Omega)$ , and  $h_{\mathcal{X},\Omega}$  sufficiently small, there exists a constant C, independent of f and N, such that

$$\left\| I - R_{\Omega}(s_{\mathcal{X},\phi_{\nu,\lambda}}) \right\|_{H^{\beta}(\Omega) \to H^{\alpha}(\Omega)} \le C h_{\mathcal{X},\Omega}^{\beta-\alpha}. \tag{9}$$

We see that the error is governed by both the smoothness of f and the fill-distance, which can be thought of as the largest distance any point in  $\Omega$  can be from the points in  $\mathcal{X}$ , including the boundary of  $\Omega$ . In the best case, the fill-distance decays at a rate of  $N^{-1/d}$  in terms of the number of training points, see e.g. [34] and the references therein. Here we are immediately confronted with the so called 'curse of dimensionality;' if we increase the dimension, d, we require exponentially many more points in  $\mathcal{X}$  in order to retain the same fill-distance, and hence the same approximation error. Approximation schemes that aim to reduce this dimension dependence assume additional structure on f, with the general goals of (a), avoiding the d-dimensional 2-norm in the error bound, and (b), requiring fewer points in less 'sensitive' dimensions. To address these, we introduce spaces of dominating mixed smoothness and function anisotropy, respectively.

# 2.3 Sparse grids and Sobolev spaces of dominating mixed smoothness

It is common in the high-dimensional approximation literature to work with functions with bounded mixed derivatives, see e.g. [19, 22, 42]. Specifically, we will consider f

to be in a Sobolev space of dominating mixed smoothness,

$$H_{\min}^{\alpha}(\Omega) := H^{\alpha_1}(\Gamma^{(1)}) \otimes \cdots \otimes H^{\alpha_d}(\Gamma^{(d)}),$$
 (10)

where  $\alpha \in \mathbb{N}_0^d$  and  $\Omega = \prod_{j=1}^d \Gamma^{(j)}$ , with each  $\Gamma^{(j)}$  compact in  $\mathbb{R}$ . The theory can extend to higher dimensional component domains, however we consider only one-dimensional  $\Gamma^{(j)}$  for ease of notation. Sparse grid methods are an application of the Smolyak algorithm to function approximation problems in such spaces, [18, 43–45]. In the Gaussian process emulation setting, this is simply equivalent to employing product covariance kernels on sparse grid designs. For Matérn kernels, the corresponding product kernels are known as separable Matérn kernels.

**Definition 4** (See e.g. [34]) Define the hyperparameter vectors  $\boldsymbol{\nu} \coloneqq (\nu_1, \dots, \nu_d)$  and  $\boldsymbol{\lambda} \coloneqq (\lambda_1, \dots, \lambda_d)$ , and let  $\{\phi_{\nu_j, \lambda_j}\}_{1 \le j \le d}$  be a collection of d-many one dimensional Matérn kernels,  $\phi_{\nu_j, \lambda_j} : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_{>0}$ . We define the *separable Matérn kernel*,  $\Phi_{\boldsymbol{\nu}, \boldsymbol{\lambda}} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_{>0}$ , by the tensor product,  $\Phi_{\boldsymbol{\nu}, \boldsymbol{\lambda}} = \phi_{\nu_1, \lambda_1} \otimes \cdots \otimes \phi_{\nu_d, \lambda_d}$ .

**Proposition 6** (i) The Native spaces of separable Matérn kernels are the completion of the tensor product of the Native spaces of the constituent one-dimensional Matérn kernels,  $\mathcal{N}_{\Phi_{\nu,\lambda}}(\Omega) = \mathcal{N}_{\phi_{\nu_1,\lambda_1}}(\Gamma^{(1)}) \otimes \cdots \otimes \mathcal{N}_{\phi_{\nu_d,\lambda_d}}(\Gamma^{(d)})$ , under the induced norm,

$$\langle f_1 \otimes \cdots \otimes f_d, f_1 \otimes \cdots \otimes f_d \rangle_{\mathcal{N}_{\Phi_{\nu, \lambda}}(\Omega)}^{1/2} = \prod_{j=1}^d \langle f_j, f_j \rangle_{\mathcal{N}_{\phi_{\nu_j, \lambda_j}}(\Omega)}^{1/2},$$

for  $f_j \in \mathcal{N}_{\phi_{\nu_i,\lambda_i}}(\Omega)$ ,  $1 \leq j \leq d$ .

(ii) These spaces are isomorphic to Sobolev spaces with dominating mixed smoothness. In particular,

$$\mathcal{N}_{\Phi_{\nu,\lambda}}(\Omega) \cong H_{mix}^{\nu+1/2}(\Omega^d),$$

with equivalent norms.

*Proof* As shown in Proposition 2, [19], (i) follows from Theorem 1, Section 8, [46], and (ii) follows from Theorem 10.12 [1].

We define a sparse grid design in terms of Cartesian products of one-dimensional point sets. Since the error is driven by the fill-distance, a natural choice are uniformly-spaced designs. Without loss of generality, we consider all component dimensions to be the unit interval  $\Gamma^{(j)} = \Gamma := (-1/2, 1/2)$  for all  $1 \le j \le d$ , and consequently  $\Omega = \Gamma^d$ .

**Definition 5** Let  $l \in \mathbb{N}_0$  be given. We define  $\mathcal{X}_l$  to be the set of  $2^l - 1$  uniformly spaced points in  $\Gamma$ ;  $\mathcal{X}_l \coloneqq \left\{ n/2^{l+1} \in \Gamma : n \in \mathbb{Z} \right\}$ .

Remark 2 In order for the sparse grid approximation to also be an interpolant, and accordingly coincide with the posterior mean function of a Gaussian process, we require this sequence to be nested, i.e.,  $\mathcal{X}_l \subset \mathcal{X}_{l+1}$  for all  $l \in \mathbb{N}_0$ .

**Definition 6** (See e.g [43]) The sparse grid design,  $\mathcal{X}_{d,L}^{\otimes} \subset \Gamma^d$ , of construction level  $L \in \mathbb{N}_0$  is given by

$$\mathcal{X}_{d,L}^{\otimes} := \bigcup_{\boldsymbol{l} \in \mathcal{I}_{t}^{d}} \mathcal{X}_{l_{1}} \times \dots \times \mathcal{X}_{l_{d}}, \tag{11}$$

where  $\mathcal{I}_L^d := \{ \boldsymbol{l} \in \mathbb{N}_0^d : |\boldsymbol{l}|_1 \leq L \}.$ 

**Theorem 1** (Theorem 1, [19], Theorem 3.11, [34]) Let  $0 \le \alpha_j < \nu_j$  for all  $1 \le j \le d$  and define the standard sparse grid kernel interpolant operator by  $S_{L,\nu,\lambda} = s_{\chi_{d,L}^{\otimes},\Phi_{\nu,\lambda}}$ . For large enough  $L \in \mathbb{N}_0$ , there exists a constant  $C_1$ , independent of L, such that

$$\|I - S_{L,\nu,\lambda}\|_{H^{\nu+1/2}_{mix}(\Gamma^d) \to H^{\alpha+1/2}_{mix}(\Gamma^d)} \le C_1 N_{L,d}^{-b_{\min}} (\log N_{L,d})^{(1+b_{\min})(d-1)}, \qquad (12)$$
where  $N_{L,d} := |\mathcal{X}_{d,L}^{\otimes}| \text{ and } b_{\min} = \min_{1 \le j \le d} \nu_j - \alpha_j.$ 

In contrast to the general Sobolev setting shown in Proposition 5, the error in the number of training points exhibits dimension dependence only in the logarithmic factor, resulting in significantly improved scalability in high dimensions. Beyond  $d \approx 10$ , however, the logarithmic term becomes prohibitively large in many practical applications. As such, in order to apply these methods to arbitrarily high dimensional problems, we must assume additional structure on f.

## 2.4 Lengthscale anisotropy

In order to enforce lengthscale assumptions on f, we work directly in the Native space norm of separable Matérn kernels. We say that a function  $f \in H^{\nu+1/2}_{\text{mix}}(\Gamma^d)$  exhibits lengthscale anisotropy according to  $\lambda \in \mathbb{R}^d_{\geq 0}$  if it is bounded in the corresponding Native space norm,

$$||f||_{\mathcal{N}_{\Phi_{\nu,\lambda}}(\Gamma^d)} < C.$$

In particular, in the high-dimensional setting, we are interested in functions bounded independently of the dimension, d.

To fit within the sparse grid framework, we restrict ourselves to lengthscales on the form  $\lambda_j = 2^{p_j}$ , where  $p \in \mathbb{N}_0$  is the *penalty*. Therefore, a *penalty vector*,  $\mathbf{p} \in \mathbb{N}_0^d$ , completely specifies the lengthscale anisotropy of a given problem. The results presented in Section 3 assume exact knowledge of the lengthscales a *priori*, however numerical results in Figure 6, Section 6, suggest the method is robust to minor misspecifications of the penalties.

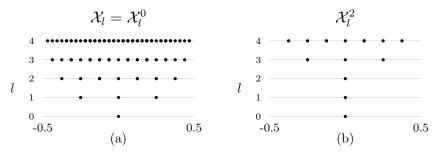
Without loss of generality, we will assume the input space to be ordered from most to least 'sensitive,' i.e.  $p_j \leq p_{j+1}$  for all  $1 \leq j \leq d-1$ . While our results apply to any degree of anisotropy, to emulate in arbitrarily high dimensions, we require the lengthscales to be at least 'eventually' increasing, i.e. if we consider the penalty a sequence  $\{p_j\}_{j\in\mathbb{N}}$ , then for all  $j\in\mathbb{N}$ , there must exist some  $m\in\mathbb{N}$  such that  $p_{j+m}>p_j$ . The difficulty of a given problem is then directly linked to the growth of these penalties. In Section 6 we consider test problems with both linearly and logarithmically growing penalties, corresponding to exponentially and linearly growing lengthscales, respectively.

# 3 Lengthscale-informed sparse grids for kernel interpolation

This section develops the theoretical foundations of our lengthscale-informed sparse grid interpolation framework. In Section 3.1, we formally introduce the construction of the interpolation operator. Section 3.2 presents approximation error bounds in the native space and  $L^{\infty}$ -norms, including a discussion of the theoretical and practical benefits of incorporating lengthscale information in comparison to standard isotropic sparse grids. Finally, in Section 3.3, we extend these results to bound the corresponding posterior marginal variance in the Gaussian process framework.

#### 3.1 Construction

The construction of lengthscale-informed sparse grids diverges from their isotropic counterparts only in that the onset of the growth of points in each axial direction,  $1 \leq j \leq d$ , is delayed by the corresponding penalty,  $p_i \in \mathbb{N}_0$ . In this way, we link the size of the sparse grid in each dimension to the lengthscale parameter,  $\lambda_i$ .

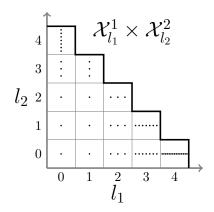


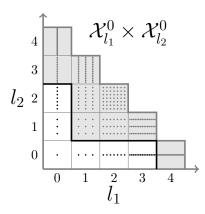
**Fig. 1**: The nested point-sets  $\mathcal{X}_l$ , (a), and  $\mathcal{X}_l^p$  with penalty p=2, (b), for different levels,  $l \in \mathbb{N}_0$ .

In contrast to the isotropic construction, the component one-dimensional point sets are now defined in terms of the penalty, depicted in Figure 1.

**Definition 7** Let 
$$l, p \in \mathbb{N}_0$$
 be given. We define the *p-penalised point-set*,  $\mathcal{X}_l^p \subset \Gamma$ , by 
$$\mathcal{X}_l^p := \begin{cases} \mathcal{X}_{l-p} & \text{for } l \geq p+1, \text{ and} \\ \mathcal{X}_0 = \{0\} & \text{for } 0 \leq l \leq p. \end{cases}$$
 (13)

We note that this sequence retains a nested structure  $\mathcal{X}_{l}^{p} \subset \mathcal{X}_{l+1}^{p}$ , and that, for the case p=0, we recover our original point set  $\mathcal{X}_l^0=\mathcal{X}_l$ . The lengthscale-informed sparse grid operator is defined in terms of tensor products of one dimensional interpolants defined over these designs, where the penalties are now described by a vector.





- (a) Lengthscale-informed sparse grid, L = 4,  $\mathbf{p} = (1, 2)$ .
- (b) Isotropic sparse grid (gray), L = 4,  $\mathbf{p} = (0,0)$ .

Fig. 2: Component diagrams for constructing two-dimensional sparse grids. A sparse grid is the union of all cartesian-product grids,  $\mathcal{X}_{l_1}^{p_1} \times \cdots \times \mathcal{X}_{l_d}^{p_d}$ , each corresponding to a multi-index  $\boldsymbol{l} \in \mathcal{I}_L^d$ . The highlighted components in (b) show the components of (a) mapped onto the isotropic component diagram.

**Definition 8** Let  $L \in \mathbb{N}_0$  and  $\mathbf{p} \in \mathbb{N}_0^d$ . We define the lengthscale-informed sparse grid interpolant operator,  $P_{L,\nu,\mathbf{p}}: \mathcal{N}_{\Phi_{\nu,2\mathbf{p}}}(\Gamma^d) \to \mathcal{N}_{\Phi_{\nu,2\mathbf{p}}}(\Gamma^d)$ , by

$$P_{L,\nu,\mathbf{p}} := \sum_{l \in \mathcal{I}_{t}^{d}} \bigotimes_{j=1}^{d} R_{\Gamma} \circ \left( s_{\mathcal{X}_{l_{j}}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} - s_{\mathcal{X}_{l_{j}-1}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} \right). \tag{14}$$

This operator maps a function  $f \in \mathcal{N}_{\Phi_{\nu,2P}}(\Gamma^d)$  to its  $\Phi_{\nu,2P}$ -kernel interpolant, with interpolation points arranged in a *lengthscale-informed sparse grid*; for all  $\mathbf{x} \in \Gamma^d$ ,

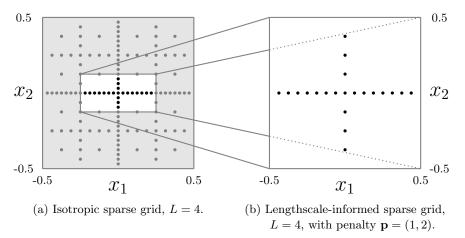
$$P_{L,\nu,\mathbf{p}}(f)(\mathbf{x}) = s_{\mathcal{X}_{L,\mathbf{p}}^{\otimes},\Phi_{\nu,2\mathbf{p}}}(f)(\mathbf{x}), \tag{15}$$

where

$$\mathcal{X}_{\mathbf{p},L}^{\otimes} = \bigcup_{\mathbf{l} \in \mathcal{I}_{t}^{d}} \mathcal{X}_{l_{1}}^{p_{1}} \times \dots \times \mathcal{X}_{l_{d}}^{p_{d}}.$$
 (16)

By Proposition 1, this also means that  $P_{L,\nu,\mathbf{p}}(f)$  is indeed the posterior mean function of a Gaussian process with zero prior mean, prior covariance kernel  $\Phi_{\nu,2\mathbf{p}}$ , and data in the form of evaluations of f at points in  $\mathcal{X}_{\mathbf{p},L}^{\otimes}$ . In the component diagrams shown in Figure 2, we see a two dimensional example of how the construction of lengthscale-informed sparse grids relate to their isotropic counterparts. Choosing a trivial penalty  $\mathbf{p} = \mathbf{0}$  recovers exactly the isotropic sparse grid construction in Definition 6. In this way, lengthscale-informed sparse grids can be viewed as a generalisation of sparse

grids to settings with lengthscale anisotropy. The resultant isotropic and lengthscale-informed sparse grid designs are illustrated in Figure 3.



**Fig. 3**: Here we can see how a lengthscale-informed sparse grid, (b), is simply an isotropic sparse grid, (a), of the same level, L, stretched by the penalty vector,  $\mathbf{p}$ , where points outside the domain are then excluded. Since  $p_2 > p_1$ , f is assumed to be more sensitive in  $x_1$ , and so more points are placed in the horizontal direction.

Remark 3 The theoretical results presented in Section 3.2 rely upon recursive properties of uniformly spaced points. Extending the analysis to other point sets, for example Clenshaw-Curtis abscissae, would require significant alterations to the theory. The numerical experiments presented in Section 6 nevertheless suggest that similar convergence behaviour may hold in practice.

#### 3.2 Bounding the error

We now state our main theoretical results. Theorem 2 establishes an upper bound for the approximation error for Matérn kernel interpolation on lengthscale-informed sparse grids in terms of L, the level of construction of the sparse grid. We measure the error in the corresponding Native space norm of the separable Matérn kernel, wherein any anisotropy in the lengthscale is encoded via the penalty vector  $\mathbf{p} \in \mathbb{N}_0^d$ . By Proposition 7, this also gives us an upper bound in  $L^{\infty}$ . Theorem 3 then links the number of abscissae in a lengthscale-informed sparse grid to L via an explicit expression. We compare both results directly with their isotropic counterparts and consequently exhibit how, for a fixed L, increased penalties correspond, in a sense, to lower dimensional problems, with respect to their computational complexity. Derivations of the two theorems are presented in Section 4.

**Definition 9** We define  $\mathcal{P}_k^d$  to be the set of all k-length subsets of  $\{1,\ldots,d\}$ , ordered such that, for a given  $\mathfrak{u} \in \mathcal{P}_k^d$ , we have  $\mathfrak{u}_i < \mathfrak{u}_{i+1}$ , for all  $1 \leq i \leq k-1$ . For a given  $\mathfrak{u} \in \mathcal{P}_k^d$ , and a given vector  $\mathbf{a} = [a_1,\ldots,a_d]$ , we define the subvector  $\mathbf{a}_{\mathfrak{u}} := [a_{\mathfrak{u}_1},\ldots,a_{\mathfrak{u}_k}]$ .

**Theorem 2** (Native space approximation error) Let  $\mathbf{p} \in \mathbb{N}_0^d$ ,  $L \in \mathbb{N}_0$ , be given, and let  $\boldsymbol{\nu}, \boldsymbol{\alpha} \in \mathbb{R}_{\geq 0}^d$  be such that  $\nu_j - \alpha_j = c \in \mathbb{R}_{\geq 0}$  for all  $1 \leq j \leq d$ . For constants  $C_4^{(\boldsymbol{\nu}, \boldsymbol{\alpha})}$  and  $C_5^{(\boldsymbol{\nu}_1, \boldsymbol{\alpha}_1)}$  independent of  $\mathbf{p}$ , the approximation error of the lengthscale-informed sparse grid interpolation operator is bounded by,

$$||I - P_{L, \boldsymbol{\nu}, \mathbf{p}}||_{\mathcal{N}_{\Phi_{\boldsymbol{\nu}, 2\mathbf{p}}}(\Gamma^d) \to \mathcal{N}_{\Phi_{\boldsymbol{\alpha}, 2\mathbf{p}}}(\Gamma^d)}$$

$$\leq C_4^{(\boldsymbol{\nu}, \boldsymbol{\alpha})} \sum_{k=1}^d 2^{-ck} \sum_{\mathfrak{u} \in \mathcal{P}_k^d} 2^{-c|\mathbf{p}_{\mathfrak{u}}|_1} \epsilon_{\boldsymbol{\nu}_{\mathfrak{u}}, \boldsymbol{\alpha}_{\mathfrak{u}}}^{(k)} (L - |\mathbf{p}_{\mathfrak{u}}|_1 - k),$$

$$(17)$$

where  $\epsilon_{\nu_u,\alpha_u}^{(k)}(L)$  is the corresponding approximation error bound for a k-dimensional isotropic sparse grid of level L, in the mixed Sobolev norm. That is,

$$||I - S_{L, \boldsymbol{\nu}_{\mathbf{u}}}||_{H_{mix}^{\boldsymbol{\nu}_{\mathbf{u}} + 1/2}(\Gamma^{k}) \to H_{mix}^{\boldsymbol{\alpha}_{\mathbf{u}} + 1/2}(\Gamma^{k})} \le C_{5}^{(\boldsymbol{\nu}_{\mathbf{u}}, \boldsymbol{\alpha}_{\mathbf{u}})} \sum_{\boldsymbol{l} \in \mathbb{N}_{0}^{k} \setminus \mathcal{I}_{L}^{k}} 2^{-c|\boldsymbol{l}|_{1}}$$
(18)

$$=: \epsilon_{\boldsymbol{\nu}_{\mathfrak{u}},\boldsymbol{\alpha}_{\mathfrak{u}}}^{(k)}(L). \tag{19}$$

For L < 0, we define  $\epsilon_{\boldsymbol{\nu}_{1},\boldsymbol{\alpha}_{1}}^{(k)}(L) := \epsilon_{\boldsymbol{\nu}_{1},\boldsymbol{\alpha}_{1}}^{(k)}(0)$ .

Proof See Section 4.1.  $\Box$ 

Remark 4 This result contrasts with those of Nobile, Tempone & Wolfers (2018) [19], where error bounds are established in more standard  $H_{\text{mix}}^{\otimes}$  norms. While the equivalence constants between these and the corresponding native space norms generally grow with the kernel lengthscales (see Proposition 13), the following results show that the  $L^{\infty}$ -error is nonetheless controlled by the Native space norm, independently of the lengthscale anisotropy.

**Proposition 7** For the Native space  $\mathcal{N}_{\varphi}(\Omega)$ , with reproducing kernel  $\varphi$ , we have, for any  $g \in \mathcal{N}_{\varphi}(\Omega)$ 

$$||g||_{L^{\infty}(\Omega)} \le ||\sqrt{\varphi(\cdot,\cdot)}||_{L^{\infty}(\Omega)}||g||_{\mathcal{N}_{\omega}(\Omega)}. \tag{20}$$

*Proof* Using the reproducing property of the kernel  $\varphi$  and the Cauchy-Schwarz inequality, we have, for any  $\mathbf{x} \in \Omega$ ,

$$g(\mathbf{x}) = \langle g(\cdot), \varphi(\cdot, \mathbf{x}) \rangle_{\mathcal{N}_{\varphi}(\Omega)} \le \|g\|_{\mathcal{N}_{\varphi}(\Omega)} \|\varphi(\cdot, \mathbf{x})\|_{\mathcal{N}_{\varphi}(\Omega)} = \|g\|_{\mathcal{N}_{\varphi}(\Omega)} \sqrt{\varphi(\mathbf{x}, \mathbf{x})}.$$

Taking the supremum of both sides completes the proof.

Corollary 1 Let  $\nu, \alpha \in \mathbb{R}^d$  such that  $1/2 \le \alpha_j \le \nu_j$  for all  $1 \le j \le d$ . For  $f \in \mathcal{N}_{\Phi_{\nu,2}\mathbf{P}}(\Gamma^d)$ , we have

$$||f - P_{L,\nu,\mathbf{p}}(f)||_{L^{\infty}(\Gamma^d)} \le \sigma ||f - P_{L,\nu,\mathbf{p}}(f)||_{\mathcal{N}_{\Phi_{\alpha,2\mathbf{p}}}(\Gamma^d)}, \tag{21}$$

where  $\sigma = \sigma_1 \sigma_2 \cdots \sigma_d$ , with  $\sigma_j$  the standard deviation of the one-dimensional Matérn kernel  $\phi_{\alpha_j, 2^{p_j}}$ .

*Proof* Directly follows from Proposition 7 by noticing that  $\|\Phi_{\alpha,2P}(\cdot,\cdot)^{1/2}\|_{L^{\infty}(\Gamma^d)} = \sigma$ .

The bound in Theorem 2 is written as the sum of contributions from each k-dimensional subspace  $\mathfrak{u} \in \mathcal{P}_k^d$ , for  $1 \leq k \leq d$ . Each error contribution is scaled by the compounded penalty,  $2^{-c|\mathbf{p}_{\mathbf{u}}|}$ , and hence, in general, higher dimensional subspaces are penalised more. For problems exhibiting anisotropy such that the lengthscale grows with dimension, these constants can quickly become extremely small.

Example 1 Consider an arbitrarily high dimensional target function,  $d \geq 11$ , with a lengthscale-anisotropy such that the penalty grows linearly with dimension,  $p_j = j - 1$ . For c = 1, the largest constant corresponding to an 11-dimensional subspace is given by  $2^{1+2+\cdots+10} = 2^{-55} \approx 3 \times 10^{-17}$ . As such, the relative error contribution from any subspace greater than k = 10 is less than machine precision, in a sense 'capping' the dimensionality of the problem at d = 10. For a slower growth penalty,  $p_j = \lceil \log j \rceil$ , the equivalent effective dimensionality with respect to machine precision is d = 20.

The construction of lengthscale-informed sparse grids exploits this imbalance in error contributions by delaying the onset of additional points in the latter subspaces, instead favouring those with larger compounded penalties and, hence, with more associated error. The result is an approximation scheme with, for a given level  $L \in \mathbb{N}_0$ , improved error over the isotropic case, that also employs many fewer function evaluations. We can explicitly count the number of function evaluations required with the following result.

**Theorem 3** (Counting abscissae in lengthscale-informed sparse grids) For a given function  $f: \Gamma^d \to \mathbb{R}$ , evaluating  $P_{L,\nu,\mathbf{p}}(f)$  employs exactly

$$N_{d,\mathbf{p}}(L) = 1 + \sum_{k=1}^{d} 2^{k} \sum_{\mathbf{u} \in \mathcal{P}_{k}^{d}} N_{k,\mathbf{0}}(L - |\mathbf{p}_{\mathbf{u}}| - k)$$
 (22)

many point evaluations of f, where  $N_{k,\mathbf{0}}(L)$  is the number of points in an isotropic sparse grid of dimension k and level L, given by

$$N_{k,\mathbf{0}}(L) = \begin{cases} \sum_{l=0}^{L} {l+k-1 \choose k-1} 2^l & if \ L \ge 0, \ and, \\ 0 & otherwise. \end{cases}$$
 (23)

Proof See Section 4.2.  $\Box$ 

Theorems 2 and 3 imply the existence of two distinct regimes. Firstly, the pre-asymptotic behaviour of the error driven by the lengthscale anisotropy, and then, once L is large enough such that most k-dimensional subspaces,  $1 \le k \le d$ , contain unique

points, the asymptotic regime begins. Here the rate obeys the same asymptotic rates as in Proposition 1, governed by the smoothness and the dimensionality. Consequently, we view the two main benefits of employing lengthscale-informed sparse grids in kernel interpolation to be:

- 1. For very high dimensional functions,  $d \gg 10$ , where it is practically infeasible to reach L large enough such that the asymptotic rate begins to dominate due to the size of grid required, lengthscale-informed sparse grids offer a tractable approximation scheme for functions exhibiting sufficient lengthscale anisotropy. Furthermore, these benefits are not subject to additional regularity assumptions on f, and as such are applicable to functions with limited or isotropic smoothness.
- 2. Even in lower dimensional settings,  $2 \le d \le 10$ , for any problem exhibiting anisotropy in the lengthscale, lengthscale-informed sparse grids outperform their isotropic counterpart in terms of the required number of evaluations to reach a given error threshold.

#### 3.3 Predictive variance in Gaussian process emulation

In the context of Gaussian process emulation, we can adapt the proof strategy from Section 3, [34], to bound the convergence of the predictive marginal variance by the approximation error bounded in Theorem 2.

**Proposition 8** Let  $\tilde{\Phi}_{L,\nu,\mathbf{p}}: \Gamma^d \times \Gamma^d \to \mathbb{R}_{>0}$  denote the posterior covariance associated with the lengthscale-informed sparse grid design  $\mathcal{X}_{L,\mathbf{p}}^{\otimes}$  and prior covariance  $\Phi_{\nu,2\mathbf{p}}$ . The posterior marginal variance is bounded by

$$\|\tilde{\Phi}_{L,\nu,\mathbf{p}}(\cdot,\cdot)^{1/2}\|_{L^{\infty}(\Gamma^{d})} \leq \sigma \|I - P_{L,\nu,\mathbf{p}}\|_{\mathcal{N}_{\Phi_{\nu,2}\mathbf{p}}(\Gamma^{d}) \to \mathcal{N}_{\Phi_{\alpha,2}\mathbf{p}}(\Gamma^{d})},\tag{24}$$

for all  $\alpha \in \mathbb{R}^d$  such that  $1/2 \le \alpha_j \le \nu_j$ ,  $1 \le j \le d$ . Here,  $\sigma := \sigma_1 \sigma_2 \cdots \sigma_d$ , where  $\sigma_j$  is the standard deviation of the one-dimensional Matérn kernel  $\phi_{\alpha_j,2^{p_j}}$ .

Proof Using Proposition 3.5, [47], we have

$$\tilde{\Phi}_{L,\boldsymbol{\nu},\mathbf{p}}(\mathbf{x},\mathbf{x})^{1/2} = \sup_{\|g\|_{\mathcal{N}_{\Phi_{\boldsymbol{\nu},2}\mathbf{p}}} = 1} |g(x) - P_{L,\boldsymbol{\nu},\mathbf{p}}(g)(x)|, \tag{25}$$

and, as shown in the proof of Theorem 3.8, [34], it follows that

$$\|\tilde{\Phi}_{L,\boldsymbol{\nu},\mathbf{p}}(\cdot,\cdot)^{1/2}\|_{L^{\infty}(\Gamma^{d})} = \sup_{\mathbf{x}\in\Gamma^{d}} \sup_{\|g\|_{\mathcal{N}_{\Phi_{\boldsymbol{\nu},2}\mathbf{p}}} = 1} |g(\mathbf{x}) - P_{L,\boldsymbol{\nu},\mathbf{p}}(g)(\mathbf{x})|, \tag{26}$$

$$= \sup_{\|g\|_{\mathcal{N}_{\Phi_{\boldsymbol{\nu}},2\mathbf{P}}}} \sup_{\mathbf{x} \in \Gamma^d} |g(\mathbf{x}) - P_{L,\boldsymbol{\nu},\mathbf{p}}(g)(\mathbf{x})|, \tag{27}$$

$$= \sup_{\|g\|_{\mathcal{N}_{\Phi_{\nu,2}\mathbf{P}}}} \|g - P_{L,\nu,\mathbf{p}}(g)\|_{L^{\infty}(\Gamma^{d})}.$$
 (28)

Applying Corollary 1 to (28) completes the proof.

# 4 Error analysis

In this section we present the proofs and necessary results for Theorems 2 and 3 in Sections 4.1 and 4.2, respectively.

#### 4.1 Error in L

To derive the error of the lengthscale-informed sparse grid operator in terms of  $L \in \mathbb{N}_0$ , the construction level of the sparse grid, in the Native space norm of the separable Matérn covariance kernel, we first introduce a key property of tensor product operators in tensor product spaces.

**Proposition 9** (Proposition 4.127, [42]) Let  $\alpha \in \mathbb{R}^d_{\geq 0}$  be such that  $\nu_j \geq \alpha_j$  for all  $1 \leq j \leq d$ , and let  $S: \mathcal{N}_{\Phi_{\nu,\lambda}}(\Gamma^d) \to \mathcal{N}_{\Phi_{\alpha,\lambda}}(\Gamma^d)$  be an operator of the form  $S = s_1 \otimes \cdots \otimes s_d$ , where each  $s_j: \mathcal{N}_{\phi_{\nu_j,\lambda_j}}(\Gamma) \to \mathcal{N}_{\phi_{\alpha_j,\lambda_j}}(\Gamma)$  is a one-dimensional linear operator. Then,

$$||S||_{\mathcal{N}_{\Phi_{\nu,\lambda}}(\Gamma^d) \to \mathcal{N}_{\Phi_{\alpha,\lambda}}(\Gamma^d)} = \prod_{j=1}^d ||s_j||_{\mathcal{N}_{\phi_{\nu_j,\lambda_j}}(\Gamma) \to \mathcal{N}_{\phi_{\alpha_j,\lambda_j}}(\Gamma)}.$$
 (29)

This property allows us to rewrite the error of our sparse grid interpolation operator, Definition 8, entirely in terms of one dimensional errors. As such, we need only establish a connection between the interpolation error and the lengthscale parameter in the case of d=1. We start by establishing a key result for kernel interpolant extensions in Native spaces over general intervals  $\tilde{\Gamma} \subseteq \mathbb{R}$ .

**Proposition 10** Let  $\tilde{\Gamma} \subset \mathbb{R}$  be an interval. For  $f \in \mathcal{N}_{\phi_{\nu,\lambda}}(\tilde{\Gamma})$ , we have

$$\|R_{\tilde{\Gamma}}(s_{\mathcal{X},\phi_{\nu,\lambda}}(f))\|_{\mathcal{N}_{\phi_{\nu,\lambda}}(\tilde{\Gamma})} = \|s_{\mathcal{X},\phi_{\nu,\lambda}}(f)\|_{\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})}.$$
(30)

*Proof* Define  $\mathcal{E}_f$  as the set of all possible extensions

$$\mathcal{E}_{f} \coloneqq \left\{ u \in \mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R}) : u|_{\tilde{\Gamma}} = R_{\tilde{\Gamma}}(s_{\mathcal{X},\phi_{\nu,\lambda}}(f)) \right\},\tag{31}$$

then, by definition of extensions in Hilbert spaces, we have

$$||R_{\tilde{\Gamma}}(s_{\mathcal{X},\phi_{\nu,\lambda}}(f))||_{\mathcal{N}_{\phi_{\nu,\lambda}}(\tilde{\Gamma})} := \inf_{u \in \mathcal{E}_f} ||u||_{\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})}.$$
 (32)

In particular, we note that the unrestricted interpolant,  $s_{\mathcal{X},\phi_{\nu,\lambda}}(f)$ , is in  $\mathcal{E}_f$ , and hence

$$||s_{\mathcal{X},\phi_{\nu,\lambda}}||_{\mathcal{N}_{\phi}(\mathbb{R})} \ge \inf_{u \in \mathcal{E}_f} ||u||_{\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})} = ||R_{\tilde{\Gamma}}(s_{\mathcal{X},\phi_{\nu,\lambda}}(f))||_{\mathcal{N}_{\phi_{\nu,\lambda}}(\tilde{\Gamma})}.$$
 (33)

Reintroducing the sampling operators  $\mathcal{T}_{\mathcal{X}}$  used in the definition of  $s_{\mathcal{X},\phi}(f)$  in Definition 2, clearly we have, for all  $u \in \mathcal{E}_f$ ,  $\mathcal{T}_{\mathcal{X}}(u) = \mathcal{T}_{\mathcal{X}}(f)$ . In other words, each  $u \in \mathcal{E}_f$  interpolates f at the points in  $\mathcal{X}$ . Hence,

$$\|R_{\tilde{\Gamma}}(s_{\mathcal{X},\phi_{\nu,\lambda}}(f))\|_{\mathcal{N}_{\phi_{\nu,\lambda}}(\tilde{\Gamma})} = \inf_{u \in \mathcal{E}_f} \|u\|_{\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})}, \tag{34}$$

$$\geq \inf_{\substack{u \in \mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R}) \\ \mathcal{T}_{\mathcal{X}}(u) = \mathcal{T}_{\mathcal{X}}(f)}} \|u\|_{\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})}, \tag{35}$$

$$=: \|s_{\mathcal{X},\phi_{\nu,\lambda}}(f)\|_{\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})},\tag{36}$$

simply by inclusion and then by Definition 2. Combining (33) and (36) gives us our result.  $\Box$ 

We wish to extend these results to restrictions of the difference between successive interpolants, as employed in the construction of sparse grid operators. This is possible since we are able rewrite the differences themselves as kernel interpolants.

**Proposition 11** Let  $\tilde{\mathcal{X}} \subset \mathcal{X}$  and define  $id : \mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R}) \to \mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})$  to be the one-dimensional identity operator. Let  $f \in \mathcal{N}_{\phi_{\nu,\lambda}}(\Gamma)$ , then

1. 
$$(s_{\mathcal{X},\phi_{\nu,\lambda}} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(f) = (\mathrm{id} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(s_{\mathcal{X},\phi_{\nu,\lambda}}(f)), \text{ and}$$

2. 
$$(s_{\mathcal{X},\phi_{\nu,\lambda}} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(f) = s_{\mathcal{X},\phi_{\nu,\lambda}}((\mathrm{id} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(f)).$$

Proof Statement 1. follows simply from noticing that  $s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}} = s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}}(s_{\mathcal{X},\phi_{\nu,\lambda}}(f))$ . For Statement 2., we first note that the difference is a linear combination of N-many kernels,  $N = |\mathcal{X}|$ , and accordingly, there exist unique real-valued  $\{\beta_i\}_{i=1}^N$  such that

$$(s_{\mathcal{X},\phi_{\nu,\lambda}} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(f) = \sum_{i=1}^{N} \beta_i \phi_{\nu,\lambda}(\cdot, x_i), \tag{37}$$

for a given ordering  $\mathcal{X} = \{x_1, \dots, x_N\}$ . By definition of kernel interpolant in Definition 2, there also exist unique real-valued  $\{\gamma_i\}_{i=1}^N$  such that

$$s_{\mathcal{X},\phi_{\nu,\lambda}}((\mathrm{id} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(f)) = \sum_{i=1}^{N} \gamma_i \phi_{\nu,\lambda}(\cdot, x_i).$$
 (38)

Let  $1 \leq i \leq N$ , then,

$$(s_{\mathcal{X},\phi_{\nu,\lambda}} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(f)(x_i) = s_{\mathcal{X},\phi_{\nu,\lambda}}(f)(x_i) - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}}(f)(x_i), \tag{39}$$

$$= f(x_i) - s_{\tilde{\mathcal{X}},\phi_{i+1}}(f)(x_i), \tag{40}$$

and,

$$s_{\mathcal{X},\phi_{\nu,\lambda}}((\mathrm{id} - s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}})(f))(x_i) = s_{\mathcal{X},\phi_{\nu,\lambda}}(x_i) - s_{\mathcal{X},\phi_{\nu,\lambda}}(s_{\tilde{\mathcal{X}},\phi_{\nu,\lambda}}(f))(x_i), \tag{41}$$

$$= f(x_i) - s_{\tilde{\mathcal{X}}_i,\phi_{i+1}}(f)(x_i). \tag{42}$$

Therefore, for all  $1 \le i \le N$ , by (37) and (38), we have

$$\sum_{i=1}^{N} \beta_i \phi_{\nu,\lambda}(x, x_i) = \sum_{i=1}^{N} \gamma_i \phi_{\nu,\lambda}(x, x_i) = f(x_i) - s_{\tilde{\mathcal{X}}, \phi_{\nu,\lambda}}(f)(x_i), \tag{43}$$

a uniquely determined system, and hence  $\gamma_i = \beta_i$  for all  $1 \le i \le N$ .

Our next goal is to outline the relationship between the lengthscale parameter and the Native space norm of interpolants in the one-dimensional setting. To do this, we first define stretching operators, and associate them to changing the lengthscales of Matérn kernels and their interpolants.

**Definition 10** Let  $a \in \mathbb{R}_{>0}$  and let  $\widehat{\mathcal{X}} = \{x_1, \ldots, x_m\} \subset (-a, a)$  be a finite discrete set. For a given  $\lambda \in \mathbb{R}_{>0}$ , we define the *point-stretching operator*  $\mathcal{T}_{\lambda}(\{x_1, \ldots, x_m\}) := \{\lambda x_1, \ldots, \lambda x_m\} \subset (-\lambda a, \lambda a)$ . Similarly, we define the *stretching operator*  $\mathcal{S}_{\lambda}(g) : (-\lambda a, \lambda a) \to \mathbb{R}$  by  $\mathcal{S}_{\lambda}(g)(\lambda x) := g(x)$  for all  $x \in (-a, a)$ .

Remark 5 Note that clearly, for finite  $\lambda, a \in \mathbb{R}_{>0}$  and  $\alpha \in \mathbb{N}$ , if  $g \in H^{\alpha}((-\lambda a, \lambda a))$ , then  $S_{\lambda}(g) \in H^{\alpha}((-a, a))$ .

**Proposition 12** Let  $\nu, \lambda_1, \lambda_2 \in \mathbb{R}_{>0}$ . Then, for all  $x, x' \in \mathbb{R}$ ,

$$\phi_{\nu,\lambda_1}(x,x') = \phi_{\nu,\lambda_2}\left(\frac{\lambda_2}{\lambda_1}x, \frac{\lambda_2}{\lambda_1}x'\right). \tag{44}$$

Proof Since Matérn kernels are stationary, we can write a Matérn kernel as a function of the scaled Euclidean distance between the arguments,

$$\phi_{\nu,\lambda} = \tilde{\phi}_{\nu} \left( \frac{|x - x'|}{\lambda} \right). \tag{45}$$

This is clear from Definition 3. Consequently, it follows

$$\phi_{\nu,\lambda_2}\left(\frac{\lambda_2}{\lambda_1}x, \frac{\lambda_2}{\lambda_1}x'\right) = \tilde{\phi}_{\nu}\left(\frac{\left|\frac{\lambda_2}{\lambda_1}x - \frac{\lambda_2}{\lambda_1}x'\right|}{\lambda_2}\right),\tag{46}$$

$$=\tilde{\phi}_{\nu}\left(\frac{|x-x'|}{\lambda_1}\right),\tag{47}$$

$$=\phi_{\nu,\lambda_1}(x,x'). \tag{48}$$

**Lemma 1** (Stretching kernel interpolants) Let  $a \in \mathbb{R}_{>0}$  and let  $\widehat{\mathcal{X}} = \{x_1, \dots, x_m\} \subset (-a, a)$  be a finite discrete set. For a given bounded function,  $f: (-a, a) \to \mathbb{R}$ , and lengthscales  $\lambda_1, \lambda_2 \in \mathbb{R}_{>0}$ , we have

$$s_{\mathcal{T}_{\lambda_2/\lambda_1}(\widehat{\mathcal{X}}),\phi_{\lambda_2}}(\mathcal{S}_{\lambda_2/\lambda_1}(f))\left(\frac{\lambda_2}{\lambda_1}x\right) = s_{\widehat{\mathcal{X}},\phi_{\lambda_1}}(f)(x),\tag{49}$$

for all  $x \in (-a, a)$ .

Proof By Proposition 1, there exists a unique expansion

$$s_{\widehat{\mathcal{X}},\phi_{\lambda_1}}(f)(x) = \sum_{i=1}^m \beta_i \phi_{\nu,\lambda_1}(x,x_i),\tag{50}$$

for all  $x \in (-a, a)$ , where each  $\beta_i \in \mathbb{R}$  is determined as the solution to the linear system

$$\sum_{i=1}^{m} \beta_i \phi_{\nu, \lambda_1}(x_k, x_i) = f(x_k)$$

$$\tag{51}$$

for all  $1 \leq k \leq m$ . Equally, there exists a unique expansion

$$s_{\mathcal{T}_{\lambda_2/\lambda_1}(\widehat{\mathcal{X}}),\phi_{\nu,\lambda_2}}(\mathcal{S}_{\lambda_2/\lambda_1}(f))\left(\frac{\lambda_2}{\lambda_1}x\right) = \sum_{i=1}^m \gamma_i \phi_{\nu,\lambda_2}\left(\frac{\lambda_2}{\lambda_1}x, \frac{\lambda_2}{\lambda_1}x_i\right),\tag{52}$$

where each  $\gamma_i \in \mathbb{R}$  is again determined by the system

$$\sum_{i=1}^{m} \gamma_{i} \phi_{\nu, \lambda_{2}} \left( \frac{\lambda_{2}}{\lambda_{1}} x_{k}, \frac{\lambda_{2}}{\lambda_{1}} x_{i} \right) = \mathcal{S}_{\lambda_{2} / \lambda_{1}}(f) \left( \frac{\lambda_{2}}{\lambda_{1}} x_{k} \right), \tag{53}$$

for all  $1 \le k \le m$ . By Proposition 12 and the definitions of  $\mathcal{S}_{\lambda}$  and  $\mathcal{T}_{\lambda}$  in Definition 10, we see that this system reduces to the first. Thus we deduce  $\beta_i = \gamma_i$  for all  $1 \le i \le m$ , and hence, for all  $x \in (-a, a)$ 

$$s_{\widehat{\mathcal{X}},\phi_{\nu,\lambda_1}}(f)(x) = \sum_{i=1}^m \beta_i \phi_{\nu,\lambda_1}(x,x_i), \tag{54}$$

$$= \sum_{i=1}^{m} \beta_i \phi_{\nu, \lambda_2} \left( \frac{\lambda_2}{\lambda_1} x, \frac{\lambda_2}{\lambda_1} x_i \right), \tag{55}$$

$$= s_{\mathcal{T}_{\lambda_2/\lambda_1}(\widehat{\mathcal{X}}), \phi_{\nu, \lambda_2}}(\mathcal{S}_{\lambda_2/\lambda_1}(f)) \left(\frac{\lambda_2}{\lambda_1} x\right). \tag{56}$$

**Lemma 2** (Native space norm of stretched kernel interpolants) Let  $\Gamma_p := (-2^{-p-1}, 2^{-p-1})$  for  $p \in \mathbb{N}_0$  and, for  $l \in \mathbb{N}_0$ , let  $\mathcal{X}_l \subset \Gamma_0 = (-1/2, 1/2)$  be the uniformly spaced point set defined as in Definition 5. Then

$$||R_{\Gamma_0}(s_{\mathcal{X}_l,\phi_{\nu,2^p}}(f))||_{\mathcal{N}_{\phi_{\nu,2^p}}(\Gamma_0)} = ||R_{\Gamma_p}(s_{\mathcal{X}_{l+p}\cap\Gamma_p,\phi_{\nu,1}}(\mathcal{S}_{2^{-p}}(f)))||_{\mathcal{N}_{\phi_{\nu,1}}(\Gamma_p)}.$$
 (57)

*Proof* Using Proposition 10 we have that the restricted norm is equal to the unrestricted,

$$||R_{\Gamma_0}(s_{\mathcal{X}_l,\phi_{\nu,2^p},\Gamma_0}(f))||_{\mathcal{N}_{\phi_{\nu,2^p}}}(\Gamma_0) = ||s_{\mathcal{X}_l,\phi_{\nu,2^p}}(f)||_{\mathcal{N}_{\phi_{\nu,2^p}}}(\mathbb{R}).$$
 (58)

Let  $\{\beta_i\}_{i=1}^{|\mathcal{X}_l|}$  be the unique real-valued coefficients such that, for all  $x \in \mathbb{R}$ ,

$$s_{\mathcal{X}_{l},\phi_{\nu,2^{p}}}(f)(x) = \sum_{i=1}^{|\mathcal{X}_{l}|} \beta_{i}\phi_{\nu,2^{p}}(x,x_{i}), \tag{59}$$

whose existence is assured by Proposition 1. By Lemma 1, we have that this is also equal to  $s_{\mathcal{T}_{2^p}(\mathcal{X}_l),\phi_1}(\mathcal{S}_{2^{-p}}(f))$ . The Native space norm of the unrestricted interpolant is then given by

$$||s_{\mathcal{X}_{l},\phi_{\nu,2^{p}}}(f)||_{\mathcal{N}_{\phi_{\nu,2^{p}}}}(\mathbb{R}) := \sum_{i=1}^{|\mathcal{X}_{l}|} \sum_{k=1}^{|\mathcal{X}_{l}|} \beta_{i}\beta_{k}\phi_{\nu,2^{p}}(x_{i},x_{k}), \tag{60}$$

$$= \sum_{i=1}^{|\mathcal{X}_l|} \sum_{k=1}^{|\mathcal{X}_l|} \beta_i \beta_k \phi_{\nu,1} \left( \frac{x_i}{2^p}, \frac{x_k}{2^p} \right), \tag{61}$$

$$=: \|s_{\mathcal{T}_{2^p}(\mathcal{X}_l),\phi_1}(\mathcal{S}_{2^{-p}}(f))\|_{\mathcal{N}_{\phi_{\nu,1}}(\mathbb{R})}, \tag{62}$$

by Proposition 12, where  $\mathcal{T}_{\lambda}$  is defined in Definition 10. By Proposition 10, since  $\mathcal{T}_{2^p}(\mathcal{X}_l) \subset \Gamma_p$ , we have

$$||s_{\mathcal{T}_{2p}(\mathcal{X}_l),\phi_1}(\mathcal{S}_{2^{-p}}(f))||_{\mathcal{N}_{\phi_{i,1}}(\mathbb{R})} = ||R_{\Gamma_p}(s_{\mathcal{T}_{2p}(\mathcal{X}_l),\phi_1}(\mathcal{S}_{2^{-p}}(f)))||_{\mathcal{N}_{\phi_{i,1}}(\Gamma_p)}.$$
 (63)

Finally, we note that

$$\mathcal{T}_{2^p}(\mathcal{X}_l) = \mathcal{T}_{2^p}\left(\left\{\frac{n}{2^{l+1}} \in \left(-\frac{1}{2}, \frac{1}{2}\right) : n \in \mathbb{Z}\right\}\right),\tag{64}$$

$$= \left\{ \frac{n}{2^{l+p+1}} \in \left( -\frac{1}{2^{p+1}}, \frac{1}{2^{p+1}} \right) : n \in \mathbb{Z} \right\}, \tag{65}$$

$$= \mathcal{X}_{l+p} \cap \Gamma_p. \tag{66}$$

**Corollary 2** Let  $l, p \in \mathbb{N}_0$  and let the p-penalised point set  $\mathcal{X}_l^p$  be defined as in Definition 7. Then, for a given  $f \in \mathcal{N}_{\phi_{\nu,2^p}}(\Gamma_0)$ ,

$$\|R_{\Gamma_{0}}((s_{\mathcal{X}_{l}^{p},\phi_{\nu,2^{p}}} - s_{\mathcal{X}_{l-1}^{p},\phi_{\nu,2^{p}}})(f))\|_{\mathcal{N}_{\phi_{\nu,2^{p}}}(\Gamma_{0})}$$

$$= \begin{cases} \|R_{\Gamma_{p}}((s_{\mathcal{X}_{l}\cap\Gamma_{p},\phi_{\nu,1}} - s_{\mathcal{X}_{l-1}\cap\Gamma_{p},\phi_{\nu,1}})(\mathcal{S}_{2^{-p}}(f)))\|_{\mathcal{N}_{\phi_{\nu,1}}(\Gamma_{p})} & \text{if } l \geq p+1, \\ 0 & \text{if } 1 \leq l \leq p, \\ \|R_{\Gamma_{p}}(s_{\{0\},\phi_{\nu,1}}(\mathcal{S}_{2^{-p}}(f)))\|_{\mathcal{N}_{\phi_{\nu,1}}(\Gamma_{p})} & \text{if } l = 0. \end{cases}$$

$$(67)$$

Proof For l=0, we have  $(s_{\mathcal{X}_l^p,\phi_{\nu,2^p}}-s_{\mathcal{X}_{l-1}^p,\phi_{\nu,2^p}})(f)=s_{\mathcal{X}_l^p,\phi_{\nu,2^p}}(f)$ , since interpolants of negative level are set to 0. Then apply Lemma 2, noting that  $\mathcal{X}_p\cap\Gamma_p=\{0\}$ . For  $1\leq l\leq p$ , trivially we have  $\mathcal{X}_l^p=\mathcal{X}_{l-1}^p=\{0\}$ , and so the difference is 0. Finally, for  $l\geq p+1$ , we can rewrite  $(s_{\mathcal{X}_l^p,\phi_{\nu,2^p}}-s_{\mathcal{X}_{l-1}^p,\phi_{\nu,2^p}})(f)$  as  $s_{\mathcal{X}_l^p,\phi_{\nu,2^p}}((\mathrm{id}-s_{\mathcal{X}_{l-1}^p,\phi_{\nu,2^p}})(f))$  by Statement 2, Proposition 11, since  $\mathcal{X}_l^p\subset\mathcal{X}_{l-1}^p$ , and hence we can again apply Lemma 2, giving

$$||R_{\Gamma_{0}}((s_{\mathcal{X}_{l}^{p},\phi_{\nu,2^{p}}} - s_{\mathcal{X}_{l-1}^{p},\phi_{\nu,2^{p}}})(f))||_{\mathcal{N}_{\phi_{\nu,2^{p}}}(\Gamma_{0})}$$

$$= ||R_{\Gamma_{0}}(s_{\mathcal{X}_{l}^{p},\phi_{\nu,2^{p}}}((\mathrm{id} - s_{\mathcal{X}_{l-1}^{p},\phi_{\nu,2^{p}}})(f))||_{\mathcal{N}_{\phi_{\nu,2^{p}}}(\Gamma_{0})},$$
(68)

$$= \|R_{\Gamma_p}(s_{\mathcal{X}_{l+p}\cap\Gamma_p,\phi_{\nu,1}}(\mathcal{S}_{2^{-p}}((\mathrm{id} - s_{\mathcal{X}_{l-1}^p,\phi_{\nu,2^p}})(f))))\|_{\mathcal{N}_{\phi_{\nu,1}}(\Gamma_p)}.$$
(69)

It follows that

$$S_{2^{-p}}((\mathrm{id} - s_{\mathcal{X}_{l-1}^p, \phi_{\nu, 2^p}})(f)) = (\mathrm{id} - s_{\mathcal{X}_{l+p-1} \cap \Gamma_p, \phi_{\nu, 1}})(S_{2^{-p}}(f)),$$

and by Proposition 11 we recover the result.

Through Proposition 9, these one-dimensional results allow us to equate the error of our operator with an anisotropic kernel  $\Phi_{\nu,2P}$  over the isotropic domain  $\Gamma^d$  to the error of a corresponding 'stretched' operator with an isotropic kernel  $\Phi_{\nu,1}$  over an anisotropic domain  $\prod_{j=1}^d \Gamma_{p_j}$ . Smaller intervals clearly require fewer points to maintain the same fill-distance, and it is in this way that we have found a link between increasing the lengthscale and reducing the approximation error. In order to apply the error bounds in Proposition 5, we must move into the appropriate Sobolev norm. For this, we use the following equivalence relationship.

**Proposition 13** Let  $\lambda \in \mathbb{R}_{>0}$ ,  $\nu + 1/2 \in \mathbb{N}$  and, for  $f \in H^{\nu+1/2}(\mathbb{R})$ , define the one-dimensional Sobolev norm by

$$||f||_{H^{\nu+1/2}(\mathbb{R})} := \int_{\mathbb{R}} |\widehat{f}(\omega)|^2 (1 + |w|_2^2)^{\nu+1/2} d\omega.$$
 (70)

The following norm-equivalence relation holds,

$$||f||_{H^{\nu+1/2}(\mathbb{R})}^2 = \sigma^2 \frac{\Gamma(\nu+1/2)\lambda}{\Gamma(\nu)\pi^{1/2}} \frac{\int_{\mathbb{R}} |\widehat{f}(\omega)|^2 (1+|\omega|^2)^{\nu+1/2} d\omega}{\int_{\mathbb{R}} |\widehat{f}(\omega)|^2 (1+\lambda^2 |\omega|^2)^{\nu+1/2} d\omega} ||f||_{\mathcal{N}_{\phi_{\nu,\lambda}}(\mathbb{R})}^2.$$
(71)

This relationship further holds for restrictions to compact sets  $\Omega \subset \mathbb{R}$ 

*Proof* Follows from Theorem 10.12, [1], using the Fourier transform of Matérn kernels given in Example 7.17, [41], as done in the proof of Lemma 3.4, [34].  $\Box$ 

Remark 6 In particular, we note that for  $\lambda = 1$  this relationship simplifies considerably to

$$||f||_{H^{\nu+1/2}(\mathbb{R})}^2 = \sigma^2 \frac{\Gamma(\nu+1/2)}{\Gamma(\nu)\pi^{1/2}} ||f||_{\mathcal{N}_{\phi_{\nu,1}}(\mathbb{R})}^2.$$
 (72)

We give an alternative formulation of the Sobolev approximation error in Proposition 5, specifically for one-dimensional interpolation operators defined on the sets  $\mathcal{X}_{i}^{p}$ .

**Lemma 3** (Section 3, Proposition 4, [19]) Let  $0 \le \alpha \le \nu$ , then

$$||R_{\Gamma_0}(\mathrm{id} - s_{\mathcal{X}_l, \phi_{\nu, \lambda}})||_{H^{\nu+1/2}(\Gamma_0) \to H^{\alpha+1/2}(\Gamma_0)} \le C_3^{(\nu, \alpha)} h_{\mathcal{X}_l, \Gamma_0}^{\nu - \alpha},$$
 (73)

where the fill-distance is now given by  $h_{\mathcal{X}_l,\Gamma_0} = 2^{-(l+1)}$ , and  $C_3^{(\nu,\alpha)}$  is independent of l.

The following Lemmas aim to combine the previous results by first directly deriving the error bound of the corresponding 'stretched' problem, and then by employing Corollary 5 in Appendix A to address the awkward  $\mathbf{Q}_{\nu,\alpha}$  term that arises. Finally, we prove Theorem 2 for the case where  $\nu - \alpha = c\mathbf{1}$  for some  $c \in \mathbb{N}$ . Whilst these methods are also applicable to settings where  $\nu$  and  $\alpha$  do not satisfy this simple relationship, for conciseness we leave that to the reader.

**Lemma 4** Let  $L \in \mathbb{N}$ ,  $\mathbf{p} \in \mathbb{N}_0^d$ ,  $\Gamma := (-1/2, 1/2)$  and let  $\boldsymbol{\nu}, \boldsymbol{\alpha} \in \mathbb{R}_{\geq 0}^d$  be such that  $\alpha_j \leq \nu_j$  for all  $1 \leq j \leq d$ . Define the multi-index set  $\mathcal{K}_k^d := \{\boldsymbol{l} \in \mathbb{N}_0^d : |\{1 \leq j \leq d : l_j \neq 0\}| = k\}$ . Then,

$$||I - P_{L,\mathbf{p},\Phi_{\nu,2\mathbf{p}}}||_{\mathcal{N}_{\Phi_{\nu,2\mathbf{p}}}(\Gamma^d) \to \mathcal{N}_{\Phi_{\alpha,2\mathbf{p}}}(\Gamma^d)} \le C_4^{(\nu,\alpha)} \sum_{k=1}^d \sum_{\boldsymbol{l} \in \mathcal{K}_b^d \setminus \mathcal{I}_I^d} \prod_{j=1}^d \mathbf{Q}_{\nu,\alpha}(\boldsymbol{l},\mathbf{p})_j,$$
(74)

where

$$\mathbf{Q}_{\boldsymbol{\nu},\boldsymbol{\alpha}}(\boldsymbol{l},\mathbf{p})_{j} \coloneqq \begin{cases} C_{3}^{(\nu_{j},\alpha_{j})} 2^{-(\nu_{j}-\alpha_{j})l_{j}} & \text{if } l_{j} \geq p_{j}+1, \\ 0 & \text{if } 1 \leq l_{j} \leq p_{j}, \text{ and} \\ 1 & \text{if } l_{j} = 0, \end{cases}$$
(75)

with constant  $C_4^{(\boldsymbol{\nu},\boldsymbol{\alpha})}$  given by

$$C_4^{(\boldsymbol{\nu},\boldsymbol{\alpha})} = \prod_{j=1}^d \frac{\Gamma(\alpha_j + 1/2)\Gamma(\nu_j)}{\Gamma(\alpha_j)\Gamma(\nu_j + 1/2)}.$$
 (76)

*Proof* As before, by Lemma 2.2, [19], we can write the error operator as the sum over all multi-indices *not* included in Definition 8, that is,

$$I - P_{L,\mathbf{p},\Phi_{\nu,2}\mathbf{p}} = \sum_{\boldsymbol{l} \in \mathbb{N}_0^d \setminus \mathcal{I}_L^d} \bigotimes_{j=1}^d \left( R_{\Gamma} \circ \left( s_{\mathcal{X}_{l_j}^{p_j},\phi_{\nu_j,2^{p_j}}} - s_{\mathcal{X}_{l_j-1}^{p_j},\phi_{\nu_j,2^{p_j}}} \right) \right). \tag{77}$$

Clearly we have  $\mathcal{K}_0^d \cup \mathcal{K}_1^d \cup \cdots \cup \mathcal{K}_d^d = \mathbb{N}_0^d$  and  $\mathcal{K}_j^d \cap \mathcal{K}_{j'}^d = \emptyset$  for all  $j \neq j'$ , and so we can rewrite (77) as

$$I - P_{L,\mathbf{p},\Phi_{\nu,2}\mathbf{p}} = \sum_{k=0}^{d} \sum_{l \in \mathcal{K}_{\nu}^{d} \setminus \mathcal{I}_{r}^{d}} \bigotimes_{j=1}^{d} \left( R_{\Gamma} \circ \left( s_{\mathcal{X}_{l_{j}}^{p_{j}},\phi_{\nu_{j},2}^{p_{j}}} - s_{\mathcal{X}_{l_{j}-1}^{p_{j}},\phi_{\nu_{j},2}^{p_{j}}} \right) \right).$$
 (78)

Since  $\mathcal{K}_k^d = \{\mathbf{0}\} = \mathcal{I}_L^d$ , we may ignore the case k = 0. By the triangle inequality we have

$$||I - P_{L,\mathbf{p},\Phi_{\nu,2\mathbf{p}}}||_{\mathcal{N}_{\Phi_{\nu,2\mathbf{p}}}(\Gamma) \to \mathcal{N}_{\Phi_{\alpha,2\mathbf{p}}}(\Gamma)}$$

$$\leq \sum_{k=1}^{d} \sum_{\boldsymbol{l} \in \mathcal{K}_{k}^{d} \backslash \mathcal{I}_{L}^{d}} \left\| \bigotimes_{j=1}^{d} R_{\Gamma} \circ \left( s_{\mathcal{X}_{l_{j}}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} - s_{\mathcal{X}_{l_{j}-1}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} \right) \right\|_{\mathcal{N}_{\Phi_{\nu, 2^{\mathbf{p}}}}(\Gamma) \to \mathcal{N}_{\Phi_{\alpha, 2^{\mathbf{p}}}}(\Gamma)},$$

$$= \sum_{k=1}^{d} \sum_{\boldsymbol{l} \in \mathcal{K}_{k}^{d} \backslash \mathcal{I}_{L}^{d}} \prod_{j=1}^{d} \left\| R_{\Gamma} \circ \left( s_{\mathcal{X}_{l_{j}}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} - s_{\mathcal{X}_{l_{j}-1}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} \right) \right\|_{\mathcal{N}_{\phi_{\nu_{j}, 2^{p_{j}}}}(\Gamma) \to \mathcal{N}_{\phi_{\alpha_{j}, 2^{p_{j}}}}(\Gamma)},$$

$$=: \sum_{k=1}^{d} \sum_{\boldsymbol{l} \in \mathcal{K}_{k}^{d} \backslash \mathcal{I}_{l}^{d}} \prod_{j=1}^{d} \| \boldsymbol{f} \|_{\mathcal{N}_{\phi_{\nu_{j}, 2^{p_{j}}}}(\Gamma) = 1} \left\| R_{\Gamma} \left( \left( s_{\mathcal{X}_{l_{j}}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} - s_{\mathcal{X}_{l_{j}-1}^{p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} \right) (\boldsymbol{f}) \right) \right\|_{\mathcal{N}_{\phi_{\alpha_{j}, 2^{p_{j}}}}(\Gamma)},$$

by Proposition 9 since  $\mathcal{N}_{\Phi_{\nu,2P}}(\Gamma^d) := \bigotimes_{j=1}^d \mathcal{N}_{\phi_{\nu,2}p_j}(\Gamma)$ , where  $\Gamma := \Gamma_0 = (-1/2,1/2)$ , is indeed a tensor product of Hilbert spaces. We now consider the three cases presented in Corollary 2. Firstly, for l > p+1, we have

$$\left\| R_{\Gamma_0} \left( \left( s_{\mathcal{X}_{l_j}^{p_j}, \phi_{\nu_j, 2^{p_j}}} - s_{\mathcal{X}_{l_{j-1}}^{p_j}, \phi_{\nu_j, 2^{p_j}}} \right) (f) \right) \right\|_{\mathcal{N}_{\phi_{\alpha_i, 2^{p_j}}}(\Gamma_0)}$$
(79)

$$= \left\| R_{\Gamma_{p_j}} \left( \left( s_{\mathcal{X}_{l_j} \cap \Gamma_{p_j}, \phi_{\nu_j, 1}} - s_{\mathcal{X}_{l_j - 1} \cap \Gamma_{p_j}, \phi_{\nu_j, 1}} \right) \left( \mathcal{S}_{2^{-p}}(f) \right) \right) \right\|_{\mathcal{N}_{\phi_{\alpha_j, 1}}(\Gamma_{p_j})}. \tag{80}$$

Using Statement 2 in Proposition 11, since  $\mathcal{X}_{l_j-1} \subset \mathcal{X}_{l_j}$ , we rewrite the difference between successive interpolants in terms of the identity operator, change norm using the equality in Remark 6, and then apply the Sobolev error bound in Lemma 3:

$$\begin{split} & \left\| R_{\Gamma_{p_{j}}} \left( \left( s_{\mathcal{X}_{l_{j}} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} - s_{\mathcal{X}_{l_{j}-1} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} \right) (\mathcal{S}_{2^{-p}}(f)) \right) \right\|_{\mathcal{N}_{\phi_{\alpha_{j}, 1}}(\Gamma_{p_{j}})} \\ &= \left\| R_{\Gamma_{p_{j}}} \left( \left( \operatorname{id} - s_{\mathcal{X}_{l_{j}-1} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} \right) \left( s_{\mathcal{X}_{l_{j}} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} (\mathcal{S}_{2^{-p}}(f)) \right) \right) \right\|_{\mathcal{N}_{\phi_{\alpha_{j}, 1}}(\Gamma_{p_{j}})}, \\ &= \sigma_{j} \sqrt{\frac{\Gamma(\alpha_{j} + 1/2)}{\Gamma(\alpha_{j})^{\pi 1/2}}} \left\| R_{\Gamma_{p_{j}}} \left( \left( \operatorname{id} - s_{\mathcal{X}_{l_{j}-1} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} \right) \left( s_{\mathcal{X}_{l_{j}} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} (\mathcal{S}_{2^{-p}}(f)) \right) \right) \right\|_{H^{\alpha_{j}+1/2}(\Gamma_{p_{j}})}, \\ &\leq \sigma_{j} \sqrt{\frac{\Gamma(\alpha_{j} + 1/2)}{\Gamma(\alpha_{j})^{\pi 1/2}}} C_{3}^{(\nu_{j}, \alpha_{j})} h_{\mathcal{X}_{l_{j}-1} \cap \Gamma_{p_{j}}, \Gamma_{p_{j}}}^{\nu_{j}} \left\| R_{\Gamma_{p_{j}}} \left( s_{\mathcal{X}_{l_{j}} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} (\mathcal{S}_{2^{-p}}(f)) \right) \right\|_{H^{\nu_{j}+1/2}(\Gamma_{p_{j}})}. \end{split}$$

The fill-distance here is given by  $h_{\mathcal{X}_{l_j}\cap\Gamma_{p_j},\Gamma_{p_j}}=h_{\mathcal{X}_{l_j-1},\Gamma_0}=2^{-l_j}$ . We then argue away the supremum of the remaining norm by reversing the previous steps; first moving back to the Native space norm using Remark 6, and then stretching back to the unit domain with Lemma 2.

$$\begin{aligned}
& \left\| R_{\Gamma_{p_{j}}} \left( s_{\mathcal{X}_{l_{j}} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} (\mathcal{S}_{2^{-p}}(f)) \right) \right\|_{H^{\nu_{j}+1/2}(\Gamma_{p_{j}})} \\
&= \left( \sigma_{j} \sqrt{\frac{\Gamma(\nu_{j}+1/2)}{\Gamma(\nu_{j})\pi^{1/2}}} \right)^{-1} \left\| R_{\Gamma_{p_{j}}} \left( s_{\mathcal{X}_{l_{j}} \cap \Gamma_{p_{j}}, \phi_{\nu_{j}, 1}} (\mathcal{S}_{2^{-p}}(f)) \right) \right\|_{\mathcal{N}_{\phi_{\nu_{j}}, 1}(\Gamma_{p_{j}})}, \\
&= \left( \sigma_{j} \sqrt{\frac{\Gamma(\nu_{j}+1/2)}{\Gamma(\nu_{j})\pi^{1/2}}} \right)^{-1} \left\| R_{\Gamma_{0}} \left( s_{\mathcal{X}_{l_{j}-p_{j}}, \phi_{\nu_{j}, 2^{p_{j}}}} (f) \right) \right\|_{\mathcal{N}_{\phi_{\nu_{j}}, 2^{p_{j}}}(\Gamma_{0})}, \end{aligned} (83)$$

Then, by the definition of kernel interpolant in Definition 2 as the interpolant of minimum Native space norm, we have

$$\sup_{\|f\|_{\mathcal{N}_{\phi_{\nu_{j}},2}p_{j}}(\Gamma)=1}\left\|R_{\Gamma_{0}}\left(s_{\mathcal{X}_{l_{j}-p_{j}},\phi_{\nu_{j},2}p_{j}}(f)\right)\right\|_{\mathcal{N}_{\phi_{\nu_{j}},2}p_{j}}(\Gamma_{0})\leq1,\tag{84}$$

since  $\Gamma = \Gamma_0$ . Combining (79), (80), (81) and (84) gives us the first case. By Corollary 2, the case  $0 \le l_j \le p_j$  is trivial and, for the case  $l_j = 0$ , we have

$$\left\| R_{\Gamma_0} \left( \left( s_{\mathcal{X}_{l_j}^{p_j}, \phi_{\nu_j, 2^{p_j}}} - s_{\mathcal{X}_{l_j - 1}^{p_j}, \phi_{\nu_j, 2^{p_j}}} \right) (f) \right) \right\|_{\mathcal{N}_{\phi_{\alpha_j, 2^{p_j}}}(\Gamma_0)} \tag{85}$$

$$= \|R_{\Gamma_{p_j}}(s_{\{0\},\phi_{\nu_j,1}}(\mathcal{S}_{2^{p_j}}(f)))\|_{\mathcal{N}_{\phi_{\alpha_j,1}}(\Gamma_{p_j})},$$

$$= \left(\sigma_{j} \sqrt{\frac{\Gamma(\alpha_{j}+1/2)}{\Gamma(\alpha_{j})\pi^{1/2}}}\right) \|R_{\Gamma_{p_{j}}}(s_{\{0\},\phi_{\nu_{j},1}}(\mathcal{S}_{2^{-p}}(f)))\|_{H^{\alpha_{j}+1/2}(\Gamma_{p_{j}})}, \tag{86}$$

$$\leq \left(\sigma_{j} \sqrt{\frac{\Gamma(\alpha_{j}+1/2)}{\Gamma(\alpha_{j})\pi^{1/2}}}\right) \|R_{\Gamma_{p_{j}}}(s_{\{0\},\phi_{\nu_{j},1}}(\mathcal{S}_{2^{-p}}(f)))\|_{H^{\nu_{j}+1/2}(\Gamma_{p_{j}})}, \tag{87}$$

$$= \left(\sqrt{\frac{\Gamma(\alpha_j + 1/2)\Gamma(\nu_j)}{\Gamma(\alpha_j)\Gamma(\nu_j + 1/2)}}\right) \|R_{\Gamma_{p_j}}(s_{\{0\},\phi_{\nu_j,1}}(\mathcal{S}_{2^{-p}}(f)))\|_{\mathcal{N}_{\phi_{\nu_j,1}}(\Gamma_{p_j})}, \tag{88}$$

$$= \left( \sqrt{\frac{\Gamma(\alpha_j + 1/2)\Gamma(\nu_j)}{\Gamma(\alpha_j)\Gamma(\nu_j + 1/2)}} \right) \|R_{\Gamma_0}(s_{\{0\},\phi_{\nu_j,2^{p_j}}}(f))\|_{\mathcal{N}_{\phi_{\nu_j,2^{p_j}}}(\Gamma_0)}, \tag{89}$$

where we have used both Lemma 2 and the equivalence relation in Remark 6, twice. We then apply (84) again to arrive at the final result.

**Lemma 5** Let  $L \in \mathbb{N}_0$ ,  $\mathbf{p} \in \mathbb{N}_0^d$ , and let  $\boldsymbol{\nu}, \boldsymbol{\alpha} \in \mathbb{R}_{\geq 0}^d$  be such that  $\alpha_j \leq \nu_j$  for all  $1 \leq j \leq d$ . Then,

$$\sum_{\boldsymbol{l} \in \mathcal{K}_{k}^{d} \setminus \mathcal{I}_{L}^{d}} \prod_{j=1}^{d} \mathbf{Q}_{\boldsymbol{\nu}, \boldsymbol{\alpha}}(\boldsymbol{l}, \mathbf{p})_{j} = \sum_{\mathfrak{u} \in \mathcal{P}_{k}^{d}} C_{5}^{(\boldsymbol{\nu}_{\mathfrak{u}}, \boldsymbol{\alpha}_{\mathfrak{u}})} \sum_{\boldsymbol{l} \in \mathbb{N}_{0}^{k} \setminus \mathcal{I}_{\max\{0, L - |\mathbf{p}_{\mathfrak{u}}| - k\}}} 2^{-(\boldsymbol{\nu}_{\mathfrak{u}} - \boldsymbol{\alpha}_{\mathfrak{u}}) \cdot (\boldsymbol{l} + \mathbf{p}_{\mathfrak{u}} + \mathbf{1})}, \quad (90)$$

where  $C_5^{(\boldsymbol{\nu}_{\mathfrak{u}},\boldsymbol{\alpha}_{\mathfrak{u}})} := \prod_{i=1}^k C_3^{(\boldsymbol{\nu}_{\mathfrak{u}_i},\boldsymbol{\alpha}_{\mathfrak{u}_i})}$ .

*Proof* By Corollary 5, we have  $\rho: \mathcal{K}_k^d \setminus \mathcal{I}_L^d \to \mathcal{P}_k^d \times \mathbb{N}^k \setminus \mathcal{I}_L^k$  is bijective, and hence

$$\sum_{\boldsymbol{l} \in \mathcal{K}_{k}^{d} \setminus \mathcal{I}_{L}^{d}} \prod_{j=1}^{d} \mathbf{Q}_{\boldsymbol{\nu}, \boldsymbol{\alpha}}(\boldsymbol{l}, \mathbf{p})_{j} = \sum_{\mathfrak{u} \in \mathcal{P}_{k}^{d}} \sum_{\mathbf{a} \in \mathbb{N}^{k} \setminus \mathcal{I}_{L}^{k}} \prod_{j=1}^{d} \mathbf{Q}_{\boldsymbol{\nu}, \boldsymbol{\alpha}}(\boldsymbol{\rho}^{-1}(\mathfrak{u}, \mathbf{a}), \mathbf{p})_{j}.$$
(91)

We also have, by definition of  $\rho$ , and since  $0 < \mathbf{a} \in \mathbb{N}^k$ , that  $\rho^{-1}(\mathfrak{u}, \mathbf{a})_j = 0$  if and only if  $j \notin \mathfrak{u}$ . Hence we can split the product in (91) as

$$= \sum_{\mathbf{u} \in \mathcal{P}_k^d} \sum_{\mathbf{a} \in \mathbb{N}^k \setminus \mathcal{I}_L^k} \left( \prod_{j \notin \mathbf{u}} \mathbf{Q}_{\nu, \alpha} (\boldsymbol{\rho}^{-1}(\mathbf{u}, \mathbf{a}), \mathbf{p})_j \right) \left( \prod_{j \in \mathbf{u}} \mathbf{Q}_{\nu, \alpha} (\boldsymbol{\rho}^{-1}(\mathbf{u}, \mathbf{a}), \mathbf{p})_j \right), \tag{92}$$

$$= \sum_{\mathfrak{u} \in \mathcal{P}_k^d} \sum_{\mathbf{a} \in \mathbb{N}^k \setminus \mathcal{I}_L^k} \prod_{j \in \mathfrak{u}} \mathbf{Q}_{\boldsymbol{\nu}, \boldsymbol{\alpha}} (\boldsymbol{\rho}^{-1}(\mathfrak{u}, \mathbf{a}), \mathbf{p})_j,$$
since  $\mathbf{Q}_{\boldsymbol{\nu}, \boldsymbol{\alpha}} (\boldsymbol{\rho}^{-1}(\mathfrak{u}, \mathbf{a}), \mathbf{p})_j = 1$  when  $\boldsymbol{\rho}^{-1}(\mathfrak{u}, \mathbf{a})_j = 0$ ,

$$= \sum_{\mathbf{u} \in \mathcal{P}_k^d} \sum_{\mathbf{a} \in \mathbb{N}^k \setminus \mathcal{I}_L^k} \prod_{i=1}^k \mathbf{Q}_{\nu, \alpha}(\rho^{-1}(\mathbf{u}, \mathbf{a}), \mathbf{p})_{\mathbf{u}_i}, \tag{94}$$

$$= \sum_{\mathbf{u} \in \mathcal{P}_k^d} \sum_{\mathbf{a} \in \mathbb{N}^k \setminus \mathcal{I}_L^k} \prod_{i=1}^k \mathbf{1}_{\{>(\mathbf{p}_{\mathbf{u}})_i\}} \mathbf{Q}_{\boldsymbol{\nu}, \boldsymbol{\alpha}} (\boldsymbol{\rho}^{-1}(\mathbf{u}, \mathbf{a}), \mathbf{p})_{\mathbf{u}_i}, \tag{95}$$

since the contributions  $\mathbf{Q}_{\nu,\alpha}(\rho^{-1}(\mathfrak{u},\mathbf{a}),\mathbf{p})_{\mathfrak{u}_i}$  are zero for all  $(\rho^{-1}(\mathfrak{u},\mathbf{a})_{\mathfrak{u}})_i := a_i \leq (\mathbf{p}_{\mathfrak{u}})_i$ ,  $1 \le i \le k$ . By restricting the indices to only those with non-zero contributions by excluding the set  $\{\mathbf{a} \in \mathbb{N}^k : a_i \le (\mathbf{p_u})_i\}$ , we have

$$= \sum_{\mathbf{u} \in \mathcal{P}_k^d} \sum_{\substack{\mathbf{a} \in \mathbb{N}^k \setminus \mathcal{I}_L^k \\ a_i > p_{\mathbf{u}}}} \prod_{i=1}^k \mathbf{Q}_{\nu, \alpha}(\rho^{-1}(\mathbf{u}), \mathbf{p})_{\mathbf{u}_i}, \tag{96}$$

$$= \sum_{\mathbf{u} \in \mathcal{P}_k^d} \sum_{\substack{\mathbf{a} \in \mathbb{N}^k \setminus \mathcal{I}_L^k \\ a_i > p_{\mathbf{u}_i}}} \prod_{i=1}^k C_3^{(\nu_{\mathbf{u}_i}, \alpha_{\mathbf{u}_i})} 2^{-(\nu_{\mathbf{u}_i} - \alpha_{\mathbf{u}_i})a_i}, \tag{97}$$

$$= \sum_{\mathbf{u} \in \mathcal{P}_k^d} C_5^{(\boldsymbol{\nu}_{\mathbf{u}}, \boldsymbol{\alpha}_{\mathbf{u}})} \sum_{\substack{\mathbf{a} \in \mathbb{N}^k \setminus \mathcal{I}_L^k \\ a_i > p_{\mathbf{u}_i}}} 2^{-\sum_{i=1}^k (\boldsymbol{\nu}_{\mathbf{u}_i} - \boldsymbol{\alpha}_{\mathbf{u}_i}) a_i}, \tag{98}$$

and, finally, considering a change of indices, 
$$l_i = a_i - p_{\mathbf{u}_i} - 1$$
, we have
$$= \sum_{\mathbf{u} \in \mathcal{P}_k^d} C_5^{(\boldsymbol{\nu}_{\mathbf{u}}, \boldsymbol{\alpha}_{\mathbf{u}})} \sum_{\boldsymbol{l} \in \mathbb{N}_0^k \setminus \mathcal{I}_{\max\{0, L - |\mathbf{p}_{\mathbf{u}}| - k\}}^k} 2^{-(\boldsymbol{\nu}_{\mathbf{u}} - \boldsymbol{\alpha}_{\mathbf{u}}) \cdot (\boldsymbol{l} + \mathbf{p}_{\mathbf{u}} + \mathbf{1})}. \tag{99}$$

Proof of Theorem 2 First we derive the Sobolev approximation error for interpolating with Matérn kernels on an isotropic sparse grid, as established in [19]. Let L > 0,  $\nu + 1/2$ ,  $\alpha + 1/2 \in$  $\mathbb{N}^d$  and let  $\mathfrak{u} \in \mathcal{P}_k^d$ , then, since  $S_{L,\Phi_{\nu_{\mathfrak{u}}}} = P_{L,\mathbf{0},\Phi_{\nu_{\mathfrak{u}}}}$ , following the proof of Lemma 4, we have

$$||I - S_{L,\Phi_{\nu_{u}}}||_{H_{\min}^{\nu_{u}+1/2}(\Gamma^{k}) \to H_{\min}^{\alpha_{u}+1/2}(\Gamma^{k})}$$

$$\leq \sum_{\boldsymbol{l} \in \mathbb{N}_{0}^{k} \setminus \mathcal{I}_{L}^{k}} \prod_{i=1}^{k} ||R_{\Gamma} \left( s_{\mathcal{X}_{l},\phi_{\nu_{u}_{i},1}} - s_{\mathcal{X}_{l-1},\phi_{\nu_{u}_{i},1}} \right) ||_{H^{\nu_{u}_{i}+1/2}(\Gamma) \to H^{\alpha_{u}_{i}+1/2}(\Gamma)},$$

$$(100)$$

$$\leq \sum_{\boldsymbol{l}\in\mathbb{N}_{0}^{k}\setminus\mathcal{I}_{L}^{k}} \prod_{i=1}^{k} C_{3}^{(\nu_{\mathfrak{u}_{i}},\alpha_{\mathfrak{u}_{i}})} h_{\mathcal{X}_{l-1},\Gamma}^{\nu_{\mathfrak{u}_{i}}-\alpha_{\mathfrak{u}_{i}}}, \tag{101}$$

$$= C_5^{(\boldsymbol{\nu}_{\mathfrak{u}}, \boldsymbol{\alpha}_{\mathfrak{u}})} \sum_{\boldsymbol{l} \in \mathbb{N}_0^k \setminus \mathcal{I}_L^k} 2^{-c|\boldsymbol{l}|_1} =: \epsilon_{\boldsymbol{\nu}_{\mathfrak{u}}, \boldsymbol{\alpha}_{\mathfrak{u}}}^{(k)}(L).$$

$$(102)$$

Here we have used  $\nu_j - \alpha_j = c$  for all  $1 \le j \le d$ , and hence  $\nu_{\mathfrak{u}_i} - \alpha_{\mathfrak{u}_i} = c$  for all  $1 \le i \le k$ . Now, for general  $\mathbf{p} \in \mathbb{N}_0^d$ , applying first Lemma 4 and then Lemma 5, we have

$$||I - P_{L,\mathbf{p},\Phi_{\nu,2\mathbf{p}}}||_{\mathcal{N}_{\Phi_{\nu,2\mathbf{p}}}(\Gamma) \to \mathcal{N}_{\Phi_{\alpha,2\mathbf{p}}}(\Gamma)}$$

$$\leq C_4^{(\nu,\alpha)} \sum_{k=1}^d \sum_{\mathbf{l} \in \mathcal{K}_k^d \setminus \mathcal{I}_L^d} \prod_{j=1}^d \mathbf{Q}_{\nu,\alpha}(\mathbf{l},\mathbf{p})_j$$
(103)

$$\leq C_4^{(\boldsymbol{\nu},\boldsymbol{\alpha})} \sum_{k=1}^d \sum_{\mathbf{u} \in \mathcal{P}_k^d} C_5^{(\boldsymbol{\nu}_{\mathbf{u}},\boldsymbol{\alpha}_{\mathbf{u}})} \sum_{\boldsymbol{l} \in \mathbb{N}_0^k \setminus \mathcal{I}_{\max\{0,L-|\mathbf{p}_{\mathbf{u}}|-k\}}} 2^{-(\boldsymbol{\nu}_{\mathbf{u}}-\boldsymbol{\alpha}_{\mathbf{u}})\cdot(\boldsymbol{l}+\mathbf{p}_{\mathbf{u}}+1)}, \tag{104}$$

$$= C_4^{(\boldsymbol{\nu},\boldsymbol{\alpha})} \sum_{k=1}^d 2^{-ck} \sum_{\mathbf{u} \in \mathcal{P}_k^d} 2^{-c|\mathbf{p}_{\mathbf{u}}|_1} C_5^{(\boldsymbol{\nu}_{\mathbf{u}},\boldsymbol{\alpha}_{\mathbf{u}})} \sum_{\boldsymbol{l} \in \mathbb{N}_0^k \setminus \mathcal{I}_{\max\{0,L-|\mathbf{p}_{\mathbf{u}}|-k\}}} 2^{-c|\boldsymbol{l}|_1}. \tag{105}$$

$$= C_4^{(\nu,\alpha)} \sum_{k=1}^d 2^{-ck} \sum_{\mathbf{u} \in \mathcal{P}_a^d} 2^{-c|\mathbf{p}_{\mathbf{u}}|_1} C_5^{(\nu_{\mathbf{u}},\alpha_{\mathbf{u}})} \sum_{\mathbf{l} \in \mathbb{N}_0^k \setminus \mathcal{I}_{-\infty}^k (o, \mathbf{l}, -c, -b)} 2^{-c|\mathbf{l}|_1}.$$
(105)

Substituting in  $\epsilon_{\boldsymbol{\nu}_{\mathfrak{u}},\boldsymbol{\alpha}_{\mathfrak{u}}}^{(k)}(L-|\mathbf{p}_{\mathfrak{u}}|_{1}-k)$  gives us the statemen

#### 4.2 Counting abscissae

In order to gauge the approximation error in terms of the number required evaluations of f, we must find expressions for the size of a lengthscale-informed sparse grid for any given level  $L \in \mathbb{N}_0$  and penalty  $\mathbf{p} \in \mathbb{N}_0^d$ ,

$$N_{d,\mathbf{p}}(L) \coloneqq |\mathcal{X}_{\mathbf{p},L}^{\otimes}|.$$
 (106)

In general, counting abscissae in sparse grids can be challenging, and often only upper bounds are achievable. Fortunately, for our choice of one-dimensional point sets,  $\mathcal{X}_l \subset (-1/2, 1/2)$ , closed-form expressions for the number of points have been derived for isotropic sparse grids (see Seciton 4, [48]), which we are able to extend to our lengthscale-informed construction. The proof of the following theorem uses similar arguments as in the proof of Lemma 5.

Proof of Theorem 3 The number of point evaluations in a lengthscale-adapted sparse grid is given by

$$N_{d,\mathbf{p}}(L) = \sum_{\mathbf{l} \in \mathcal{I}_L^d} \prod_{j=1}^d \mathbf{B}(\mathbf{l}, \mathbf{p})_j,$$
(107)

where we define  $\mathbf{B}(l,\mathbf{p})_{j} := |\mathcal{X}_{l_{j}}^{p_{j}}| - |\mathcal{X}_{l_{j}-1}^{p_{j}}|$  and  $\mathcal{I}_{L}^{k}$  is as defined in Definition 8, (see [36]). From the definition of  $\mathcal{X}_l^p$  in Definition 7, we have

$$|\mathcal{X}_{l_{j}}^{p_{j}}| = \begin{cases} |\mathcal{X}_{l_{j}-p_{j}}| = 2^{l_{j}-p_{j}+1} - 1 & \text{if } l_{j} \geq p_{j}, \\ 1 & \text{if } 0 \leq l_{j} < p_{j}, \text{ and} \\ 0 & \text{otherwise,} \end{cases}$$
(108)

and hence,

$$\mathbf{B}(\boldsymbol{l}, \mathbf{p})_{j} = \begin{cases} 2^{l_{j} - p_{j}} & \text{if } l_{j} > p_{j}, \\ 0 & \text{if } 0 < l_{j} < p_{j}, \text{ and} \\ 1 & \text{if } l_{j} = 0. \end{cases}$$
 (109)

By Corollary 5,  $\rho: \mathcal{K}_k^d \cap \mathcal{I}_L^d \to \{\mathbf{0}\} \cup \mathcal{P}_k^d \times \mathbb{N}^k \cap \mathcal{I}_L^k$  is bijective, and since, by definition,  $\bigcup_{k=0}^d \mathcal{K}_k^d = \mathbb{N}_0^d$ , and  $\mathcal{K}_{k_1}^d \cap \mathcal{K}_{k_2}^d = \emptyset$  if and only if  $k_1 \neq k_2$ , we have

$$\sum_{\boldsymbol{l} \in \mathcal{I}_{\boldsymbol{l}}^{d}} \prod_{j=1}^{d} \mathbf{B}(\boldsymbol{l}, \mathbf{p})_{j} = \sum_{k=0}^{d} \sum_{\boldsymbol{l} \in \mathcal{K}_{\boldsymbol{l}}^{d} \cap \mathcal{I}_{\boldsymbol{l}}^{d}} \prod_{j=1}^{d} \mathbf{B}(\boldsymbol{l}, \mathbf{p})_{j},$$
(110)

$$=1+\sum_{k=1}^{d}\sum_{\mathfrak{u}\in\mathcal{P}_{k}^{d}}\sum_{\mathbf{a}\in\mathbb{N}^{k}\cap\mathcal{I}_{L}^{k}}\prod_{j=1}^{d}\mathbf{B}(\boldsymbol{\rho}^{-1}(\mathfrak{u},\mathbf{a}),\mathbf{p})_{j},$$
(111)

$$=1+\sum_{k=1}^{d}\sum_{\mathfrak{u}\in\mathcal{P}_{k}^{d}}\sum_{\mathbf{a}\in\mathbb{N}^{k}\cap\mathcal{I}_{L}^{k}}\prod_{i=1}^{k}\mathbf{B}(\mathbf{a},\mathbf{p}_{\mathfrak{u}})_{i},$$
(112)

since  $\rho(\mathfrak{u}, \mathbf{a})_j = 1$  for all  $j \notin \mathfrak{u}$ . We note that  $\mathbf{B}(\mathbf{a}, \mathbf{p}_{\mathfrak{u}})_i = 0$  for all  $0 < a_i < p_{\mathfrak{u}_i}$ , and hence we can further restrict the multi-index set, giving

$$N_{d,\mathbf{p}}(L) = 1 + \sum_{k=1}^{d} \sum_{\mathbf{u} \in \mathcal{P}_k^d} \sum_{\substack{\mathbf{a} \in \mathcal{I}_L^k \\ a_i > 0 \\ a_i > p_{\mathbf{u}}}} 2^{|\mathbf{a}|_1 - |\mathbf{p}_{\mathbf{u}}|_1}.$$
 (113)

Finally, changing the multi-indices by  $l_i = a_i - p_{u_i} - 1$  gives

$$N_{d,\mathbf{p}}(L) = 1 + \sum_{k=1}^{d} \sum_{\mathbf{u} \in \mathcal{P}_k^d} \sum_{l \in \mathcal{I}_{L-|\mathbf{p}_{\mathbf{u}}|-k}} 2^{|l|_1 + k}, \tag{114}$$

$$=1+\sum_{k=1}^{d} 2^{k} \sum_{\mathbf{u}\in\mathcal{P}_{k}^{d}} \sum_{\mathbf{l}\in\mathcal{I}_{L-|\mathbf{p}_{\mathbf{u}}|_{1}-k}} 2^{|\mathbf{l}|_{1}},$$
(115)

where the final sum is exactly the number of points in an isotropic sparse grid,  $N_{k,\mathbf{0}}(L-|\mathbf{p_u}|_1-k)$ , with the closed form expression given in Section 4, [48]. Finally we note that when  $L-|\mathbf{p_u}|_1-k<0$ , the set  $\mathcal{I}_{L-|\mathbf{p_u}|_1-k}^k$  is empty and hence the contribution is zero.

When considering growing penalties as discussed in Section 2.4, the following can be shown.

**Corollary 3** Let  $\{p_j\}_{j\in\mathbb{N}}$  be a non-decreasing sequence of integers,  $p_j\in\mathbb{N}_0$ , such that, for all  $j\in\mathbb{N}$ , there exists an  $m\in\mathbb{N}$  such that  $p_{j+m}>p_j$ . Then, for fixed  $L\in\mathbb{N}_0$ ,  $N_{d,\mathbf{p}}(L)$  is bounded independently of the dimension, d.

Proof Let  $k \in \{1, 2, ..., d\}$  and let  $r(k, L, \mathbf{p}) = \min\{j \in \mathbb{N} : p_j > L - k\}$ . Let  $d > r(k, L, \mathbf{p})$  and  $\mathfrak{u} \in \mathcal{P}_k^d \setminus \mathcal{P}_k^{r(k, L, \mathbf{p})}$ , then  $|\mathbf{p}_{\mathfrak{u}}| \geq p_{r(k, L, \mathbf{p})}$ , since there must exist at least one  $j \in \mathfrak{u}$  such

that  $r(k, L, \mathbf{p}) < j \le d$ . Thus  $L - |\mathbf{p_u}| - k \le L - p_{r(k, L, \mathbf{p})} - k < 0$  and hence  $N_{k, \mathbf{0}}(L - |\mathbf{p_u}| - k) = 0$ . Therefore, for large enough d, we have

$$\sum_{\mathbf{u}\in\mathcal{P}_k^d} N_{k,\mathbf{0}}(L-|\mathbf{p}_{\mathbf{u}}|-k) = \sum_{\mathbf{u}\in\mathcal{P}_k^{r(k,L,\mathbf{p})}} N_{k,\mathbf{0}}(L-|\mathbf{p}_{\mathbf{u}}|-k), \tag{116}$$

for all  $1 \le k \le d$  and hence,

$$N_{d,\mathbf{p}}(L) = 1 + \sum_{k=1}^{d} 2^{k} \sum_{\mathbf{u} \in \mathcal{P}_{k}^{r(k,L,\mathbf{p})}} N_{k,\mathbf{0}}(L - |\mathbf{p}_{\mathbf{u}}| - k).$$
 (117)

by Theorem 3. For a given  $L \in \mathbb{N}_0$ , is clear that there must exist some  $k_{\max} \in \mathbb{N}$  such that  $|\mathbf{p_u}| + k > L$  for all  $k > k_{\max}$  and all  $\mathfrak{u} \in \mathcal{P}_k^{r(k,L,\mathbf{p})}$ . Accordingly, we complete the proof by replacing d with  $k_{\max}$  in (117).

# 5 Fast implementation

In Algorithm 1, Plumlee 2014 [36], a fast inference algorithm was outlined to perform quick inversions of the induced covariance matrix when employing product kernels on sparse grid designs. In this section, we adapt this algorithm to general lengthscale-informed sparse grids, enhancing its efficiency for high dimensional problems, especially when the penalty grows with dimension. We start by introducing a key result.

**Proposition 14** (Theorem 2, [36]) Define the multi-index set  $\mathcal{J}_L^d = \{l \in \mathbb{N}_0^d : \max\{0, L - d + 1\} \leq |l|_1 \leq L\}$ . The lengthscale-informed sparse grid operator in Definition 8 can be rewritten

$$P_{d,\mathbf{p},L} = \sum_{\boldsymbol{l} \in \mathcal{J}_L^d} b_L(\boldsymbol{l}) \bigotimes_{j=1}^d s_{\mathcal{X}_{l_j}^{p_j}},$$
(118)

where

$$b_L(\mathbf{l}) = (-1)^{L-|\mathbf{l}|_1} \binom{d-1}{L-|\mathbf{l}|_1}.$$
 (119)

As an immediate consequence of Proposition 14, the inverse covariance matrix can be written entirely in terms of Kronecker products of much smaller Toeplitz matrices, each corresponding to one-dimensional designs,

$$\Phi_{\boldsymbol{\nu},2^{\mathbf{p}}}(\mathcal{X}_{\mathbf{p},L}^{\otimes},\mathcal{X}_{\mathbf{p},L}^{\otimes})^{-1} = \sum_{\boldsymbol{l}\in\mathcal{J}_{L}^{d}} b_{L}(\boldsymbol{l})A(\boldsymbol{l}) \left[\bigotimes_{j=1}^{d} \phi_{\nu_{j},2^{p_{j}}}(\mathcal{X}_{l_{j}}^{p_{j}},\mathcal{X}_{l_{j}}^{p_{j}})^{-1}\right] A(\boldsymbol{l})^{T}, \qquad (120)$$

where each  $A(\mathbf{l})$  is an  $N_{d,\mathbf{p}}(L) \times (|\mathcal{X}_{l_1}| \times \cdots \times |\mathcal{X}_{l_d}|)$  matrix with exactly one entry equal to 1 in each column and zeros elsewhere, determined by the indexing of the covariance matrix. Accordingly, to evaluate  $P_{d,\mathbf{p},L}$ , we only need compute the inverses of these

component matrices and the coefficients  $b_L(\mathbf{l})$ . We can immediately implement this algorithm for lengthscale-informed sparse grids and, in general, we observe a large computational speed up; the the slowest single procedure now being the inversion of the largest Toeplitz matrix of order  $\mathcal{O}(L2^L)$ . Many of these matrices are also identical, enabling even faster computations when storing individual components. However, this method requires summation over the set  $\mathcal{J}_L^d$ , which grows extremely quickly for  $d \gg$ 10, eventually losing its computational advantage over a simple Cholesky factorisation. Fortunately, with the inclusion of a non-trivial penalty **p**, significant redundancy is introduced into these calculations. To exploit this, we express  $P_{d,\mathbf{p},L}$  instead as a sum over a reduced multi-index set,  $\mathcal{A}_{\mathbf{p},L}^d$ , now depending on the penalty. We define this set via the following map.

**Definition 11** We define the mapping between multi-indices,  $\mathbf{q}_{d,\mathbf{p}}: \mathcal{J}_L^d \to \mathbb{N}_0^d$ , by  $\mathbf{q}_{d,\mathbf{p}}(l) = \mathbf{a}$ , such that  $a_j = \max\{l_j - p_j, 0\}$ , for all  $1 \leq j \leq d$ . We denote the image of  $\mathbf{q}_{d,\mathbf{p}}$  by  $\mathcal{A}_{\mathbf{p},L}^d$ . For a given  $\mathbf{a} \in \mathcal{A}_{\mathbf{p},L}^d$ , we also define the sets  $\mathfrak{u}(\mathbf{a}) \coloneqq \{j \in \{1,\ldots,d\} : a_j = 0\}$  and  $\mathfrak{v}(\mathbf{a}) \coloneqq \{1,\ldots,d\} \setminus \mathfrak{u}(\mathbf{a})$ .

**Lemma 6** For  $\mathbf{a} \neq \mathbf{a}' \in \mathcal{A}_{\mathbf{p},L}^d$ , the pre-images of  $\mathbf{q}_{d,\mathbf{p}}$  are disjoint;  $\mathbf{q}_{d,\mathbf{p}}(\mathbf{a}) \cap \mathbf{q}_{d,\mathbf{p}}(\mathbf{a}') = \emptyset$ .

Proof Consider 
$$d = 1$$
, i.e.  $\mathbf{p} = p \in \mathbb{N}_0$ . Then, for  $a \in \mathcal{A}_p^1$ , we have
$$q_{1,p}^{-1}(a) = \begin{cases} a+p & \text{if } a > 0, and \\ \{0,\dots,p\} & \text{if } a = 0. \end{cases}$$
(121)

For general dimension d > 1, the pre-image is then simply the product

$$\mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a}) = \sum_{j=1}^{d} \mathbf{q}_{1,p_j}^{-1}(a_j). \tag{122}$$

Let  $\mathbf{a} \neq \mathbf{a}' \in \mathcal{A}_{\mathbf{a},L}^d$ , then there exists at least one index  $j, 1 \leq j \leq d$ , such that  $a_j \neq a_j'$ . Firstly, assume  $a_j, a_j' \neq 0$ . Then, in both cases, the pre-image is a single multi-index, and  $\mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a})_j = a_j + p_j \neq a_j' + p_j = \mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a}')_j$ . Next we assume  $a_j = 0$ , and hence  $a_j' > 0$ . Then, for all  $l \in \mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a})$ , we have  $l_j \in \{0,\ldots,p_j\}$ . Therefore,  $l_j \neq a_j' + p_j = \mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a}')_j$ . By symmetry of the last argument, all cases are considered, an hence  $\mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a}) \cap \mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a}') = \emptyset$ , as required.  $\square$ 

Proposition 15 We have that

$$P_{d,\mathbf{p},L} = \sum_{\mathbf{a} \in \mathcal{A}_{\mathbf{p},L}^d} u_{\mathbf{p},L}(\mathbf{a}) \bigotimes_{j=1}^d s_{\mathcal{X}_{l_j}}, \tag{123}$$

where

$$u_{\mathbf{p},L(\mathbf{a})} = \sum_{m=0}^{|\mathbf{p}_{\mathbf{u}(\mathbf{a})}|} \mathscr{S}_{\mathbf{a},\mathbf{p}}(m)(-1)^{L-m-|(\mathbf{a}+\mathbf{p})_{\mathbf{v}(\mathbf{a})}|_1} \begin{pmatrix} d-1\\ L-m-|(\mathbf{a}+\mathbf{p})_{\mathbf{v}(\mathbf{a})}|_1 \end{pmatrix}, \tag{124}$$

and

$$\mathscr{S}_{\mathbf{a},\mathbf{p}}(m) = \sum_{\mathbf{w} \subset \mathbf{u}(\mathbf{a})} (-1)^{|\mathbf{w}|} \binom{m + |\mathbf{u}(\mathbf{a})| - |\mathbf{w}| - |\mathbf{p}_{\mathbf{w}}|_1 - 1}{|\mathbf{u}(\mathbf{a})| - 1}.$$
 (125)

Proof For all  $l \in \mathcal{J}_L^d$ , we have  $s_{\mathcal{X}_{l_1}^{p_1}} \otimes \cdots \otimes s_{\mathcal{X}_{l_d}^{p_d}} = s_{\mathcal{X}_{\mathbf{q}_{d,\mathbf{p}}(l)_1}} \otimes \cdots \otimes s_{\mathcal{X}_{\mathbf{q}_{d,\mathbf{p}}(l)_d}}$ , since,

$$\mathcal{X}_{\mathbf{q}_{d,\mathbf{p}}(l)_{j}} = \begin{cases} \mathcal{X}_{l_{j}-p_{j}} & \text{for } l_{j} \geq p_{j}+1, \text{ and} \\ \mathcal{X}_{0} & \text{for } 0 \leq l_{j} \leq p_{j}, \end{cases}$$

$$(126)$$

for all  $1 \leq j \leq d$ , which is exactly the definition of  $\mathcal{X}_{l_j}^{p_j}$  in Definition 7. By Lemma 6, we can rearrange the expression for  $P_{d,\mathbf{p},L}$  in Proposition 14 into a sum over multi-indices in  $\mathcal{A}_{\mathbf{p},L}^d$  as,

$$P_{d,\mathbf{p},L} = \sum_{\mathbf{a} \in \mathcal{A}_{\mathbf{p},L}^d} \left( \sum_{\mathbf{l} \in \mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a})} b_L(\mathbf{l}) \right) \bigotimes_{j=1}^d s_{\mathcal{X}_{a_j}}.$$
 (127)

We now wish to simplify the sum over the pre-image  $\mathbf{q}_{d,\mathbf{p}}^{-1}(\mathbf{a})$  for a given  $\mathbf{a} \in \mathcal{A}_{\mathbf{p},L}^d$  by considering the zero and non-zero components separately. Assuming  $|\mathfrak{u}(\mathbf{a})| = k$ , we have

$$\sum_{\mathbf{l} \in \mathbf{q}_{d,\mathbf{p}_{l}}^{-1}(\mathbf{a})} b_{L}(\mathbf{l}) = \sum_{l_{1} \in \mathbf{q}_{d,p_{1}}^{-1}(a_{1})} \cdots \sum_{l_{d} \in \mathbf{q}_{d,p_{d}}^{-1}(a_{d})} (-1)^{L-|\mathbf{l}|_{1}} \binom{d-1}{L-|\mathbf{l}|_{1}}, \tag{128}$$

$$= \sum_{l_{\mathbf{u}(\mathbf{a})_{1}} \in \mathbf{q}_{d,p_{\mathbf{u}(\mathbf{a})_{1}}}^{-1}} \dots \sum_{l_{\mathbf{u}(\mathbf{a})_{k}} \in \mathbf{q}_{d,p_{\mathbf{u}(\mathbf{a})_{k}}}^{-1}} (a_{\mathbf{u}(\mathbf{a})_{k}})$$

$$(-1)^{L-|l_{\mathbf{u}(\mathbf{a})}|_{1}-|(\mathbf{a}+\mathbf{p})_{\mathbf{v}(\mathbf{a})}|_{1}} \begin{pmatrix} d-1 \\ L-|l_{\mathbf{u}(\mathbf{a})}|_{1}-|(\mathbf{a}+\mathbf{p})_{\mathbf{v}(\mathbf{a})}|_{1} \end{pmatrix}.$$

$$(129)$$

For all  $1 \le i \le k$ , we have  $\mathbf{q}_{d,p_{\mathfrak{u}(\mathbf{a})_i}}^{-1}(a_{\mathfrak{u}(\mathbf{a})_i}) = \{0,\ldots,p_{\mathfrak{u}(\mathbf{a})_i}\}$ . Therefore, we can rewrite (129) as

$$\sum_{\boldsymbol{l} \in \mathbf{q}_{-}^{-1}(\mathbf{a})} b_{L}(\boldsymbol{l}) = \sum_{m=0}^{|\mathbf{p}_{\mathbf{u}(\mathbf{a})}|} \mathscr{S}_{\mathbf{a},\mathbf{p}}(m) (-1)^{L-m-|(\mathbf{a}+\mathbf{p})_{\boldsymbol{v}(\mathbf{a})}|_{1}} \binom{d-1}{L-m-|(\mathbf{a}+\mathbf{p})_{\boldsymbol{v}(\mathbf{a})}|_{1}},$$

where  $\mathscr{S}_{\mathbf{a},\mathbf{p}}(m) := \#\{l \in \mathbb{N}_0^k : |l|_1 = m, l_i \leq p_{\mathfrak{u}(\mathbf{a})_i}\}$ , with an explicit expression given by inclusion-exclusion (see Chapter 2, [49]).

Given  $L \in \mathbb{N}_0$ ,  $\mathbf{p} \in \mathbb{N}_0^d$  and a target function  $f : \Gamma^d \to \mathbb{R}$ , we outline the procedural construction of the weight vector  $\mathbf{w} = \Phi_{\nu,2P}(\mathcal{X}_{\mathbf{p},L}^{\otimes}, \mathcal{X}_{\mathbf{p},L}^{\otimes})^{-1} f(\mathcal{X}_{\mathbf{p},L}^{\otimes})$  in Algorithm 1, adapted for lengthscale-informed sparse grids from Algorithm 1, [36]. Here, for a given  $\mathbf{a} \in \mathcal{A}_{\mathbf{p},L}^d$ , we define  $u_{\mathbf{p},L}(\mathbf{a})$  as in Proposition 15, and let  $\mathbf{w}_{\mathbf{a}}$  denote the sub-vector of  $\mathbf{w}$  corresponding to the design points in the component grid  $\mathcal{X}_{a_1} \times \cdots \times \mathcal{X}_{a_d} \subset \mathcal{X}_{\mathbf{p},L}^{\otimes}$ .

#### **Algorithm 1** Fast inference algorithm for lengthscale-informed sparse grids.

Initialise 
$$\mathbf{w} = \mathbf{0} \in \mathbb{R}^{N_{d,\mathbf{p}}(L)}$$
 for  $\mathbf{a} \in \mathcal{A}_{\mathbf{p},L}^d$  do 
$$\mathbf{w}_{\mathbf{a}} = \mathbf{w}_{\mathbf{a}} + u_{\mathbf{p},L}(\mathbf{a}) \left[ \bigotimes_{j=1}^d \phi_{\nu_j,2^{p_j}} (\mathcal{X}_{a_j},\mathcal{X}_{a_j})^{-1} \right] f(\mathcal{X}_{a_1} \times \cdots \times \mathcal{X}_{a_d})$$
 end for

The explicit computational cost of constructing  $\mathcal{A}_{\mathbf{p},L}^d$ , and consequently the algorithm, is difficult to assess as it is heavily dependent on the penalty; the greater

the anisotropy, the smaller the set  $\mathcal{A}_{\mathbf{p},L}^d$ . In the worst case, for a trivial penalty  $\mathbf{p} = (0, \dots, 0)$ , we recover isotropic sparse grids, and therefore the set  $|\mathcal{A}_{\mathbf{p},L}^d| = |\mathcal{J}_L^d| \le {L+d-1 \choose d-1}$ . In the case of growing penalties as discussed in Section 2.4, we have the following result.

**Proposition 16** Let  $\{p_j\}_{j\in\mathbb{N}}$  be a non-decreasing sequence of integers,  $p_j\in\mathbb{N}_0$ , such that, for all  $j\in\mathbb{N}$ , there exists an  $m\in\mathbb{N}$  such that  $p_{j+m}>p_j$ . Then, for fixed  $L\in\mathbb{N}_0$ ,  $|\mathcal{A}_{\mathbf{p},L}^d|$  is bounded independently of d.

Proof Let  $L \in \mathbb{N}_0$  be given and let  $\boldsymbol{l} \in \mathcal{J}_L^d$ . Clearly for all  $d \in \mathbb{N}$  we have  $|\mathcal{A}_{\mathbf{p},L}^d| \leq |\mathcal{A}_{\mathbf{p},L}^{d+1}|$ . By definition of  $\{p_j\}_{j \in \mathbb{N}}$ , for d large enough, there must exist a  $k_{\max} < d$  such that  $l_k < p_k$  for all  $k > k_{\max}$ , and therefore  $\mathbf{q}_{k,\mathbf{p}}(\boldsymbol{l})_k = 0$  for all  $k > k_{\max}$ . It suffices to show that, for any  $k_2 \geq k_1 \geq \max\{k_{\max}, L+1\}$ ,  $|\mathcal{A}_{\mathbf{p},L}^{k_1}| = |\mathcal{A}_{\mathbf{p},L}^{k_2}|$ . We achieve this by defining a mapping between these sets,  $t: \mathcal{A}_{\mathbf{p},L}^{k_1} \to \mathcal{A}_{\mathbf{p},L}^{k_2}$ ,  $t(\mathbf{a}^{(1)}) = (a_1^{(1)}, a_2^{(1)}, \dots, a_{k_1}^{(1)}, 0, \dots, 0) \in \mathbb{N}_0^{k_2}$ , and show that it is bijective. First we show that the image is indeed contained in  $\mathcal{A}_{\mathbf{p},L}^{k_2}$ . Let  $\mathbf{a}^{(1)} \in \mathcal{A}_{\mathbf{p},L}^{k_1}$ , then the pre-image  $\mathbf{q}_{k_1,L}^{-1}(\mathbf{a}^{(1)})$  is non-empty in  $\mathcal{J}_L^{k_1}$  by Definition 11. Define an analogous map  $t^*: \mathcal{J}_L^{k_1} \to \mathcal{J}_L^{k_2}$  by  $t^*(\boldsymbol{l}^{(1)}) = (l_1^{(1)}, l_2^{(1)}, \dots, l_{k_1}^{(1)}, 0, \dots, 0) \in \mathbb{N}_0^{k_2}$ . We have both  $|t^*(\boldsymbol{l}^{(1)})|_1 = |\boldsymbol{l}^{(1)}|_1 \leq L$  and  $|t^*(\boldsymbol{l}^{(1)})|_1 \geq \max\{0, L-k_2+1\} = 0$ , and so  $t^*(\boldsymbol{l}^{(1)}) \in \mathcal{J}_L^{k_2}$  for all  $\boldsymbol{l}^{(1)} \in \mathbf{q}_{k_1,L}^{-1}(\mathbf{a}^{(1)})$ . We then have

$$\mathbf{q}_{k_2,\mathbf{p}}(t^*(\boldsymbol{l}^{(1)})) = (\max\{t^*(\boldsymbol{l}^{(1)})_1 - p_1, 0\}, \dots, \max\{t^*(\boldsymbol{l}^{(1)})_{k_2} - p_{k_2}, 0\}), \tag{130}$$

$$= (\max\{t^*(\boldsymbol{l}^{(1)})_1 - p_1, 0\}, \dots, \max\{t^*(\boldsymbol{l}^{(1)})_{k_1} - p_{k_1}, 0\}, 0, \dots, 0), \tag{131}$$

$$= (\max\{\boldsymbol{l}_1^{(1)} - p_1, 0\}, \dots, \max\{\boldsymbol{l}_{k_1}^{(1)} - p_{k_1}, 0\}, 0, \dots, 0), \tag{132}$$

$$= (\mathbf{q}_{k_1, \mathbf{p}}(\mathbf{l}^{(1)}), 0, \dots, 0) = t(\mathbf{a}^{(1)}), \tag{133}$$

and therefore  $t(\mathbf{a}^{(1)})$  is indeed contained in  $\mathcal{A}_{\mathbf{p},L}^{k_2}$ . Clearly t is injective, what remains to show is surjectivity. Let  $\mathbf{a}^{(2)} \in \mathcal{A}_{\mathbf{p},L}^{k_2}$ . Since  $k_1 > k_{\max}$ , we have established that  $\mathbf{a}^{(2)} = (a_1^{(2)}, \cdots, a_{k_1}^{(2)}, 0, \ldots, 0) \in \mathbb{N}_0^{k_2}$ . Furthermore, there must exist an  $t^{(2)} \in \mathcal{J}_L^{k_2}$  such that  $\mathbf{q}_{k_2,\mathbf{p}}(t^{(2)}) = \mathbf{a}^{(2)}$ . Therefore,  $\max\{l_j^{(2)} - p_j^{(2)}, 0\} = a_j^{(2)}$  for all  $1 \leq j \leq k_2$ , and in particular,  $\max\{l_k^{(2)} - p_k^{(2)}, 0\} = 0$  for all  $k_1 \leq k \leq k_2$ . Consider the multi-index  $t'^{(2)} \coloneqq (l_1^{(2)}, \ldots, l_{k_1}^{(2)}, 0, \ldots, 0) \in \mathbb{N}_0^{k_2}$ . Clearly  $|t'^{(2)}|_1 \leq |t^{(2)}|_1 \leq L$ , and since  $k_2 > L + 1$ , we have  $|t'^{(2)}|_1 > \max\{0, L - k_2 - 1\} = 0$ . Therefore  $t'^{(2)} \in \mathcal{J}_L^{k_2}$  and hence  $t'^{(2)} \in \mathbf{q}_{k_2,\mathbf{p}}^{-1}(\mathbf{a}^{(2)})$ . Now define  $t'^{(1)} \coloneqq (l_1'^{(2)}, \ldots, l_{k_1}^{(2)})$ , then  $|t'^{(1)}|_1 = |t'^{(2)}|_1$ , and since  $k_1 > L + 1$ , we have  $t'^{(1)} \in \mathcal{J}_L^{k_1}$ . Then, by definition,

$$\mathcal{A}_{\mathbf{p},L}^{k_1} \ni \mathbf{q}_{k_1,\mathbf{p}}(\mathbf{l}^{\prime(1)}) = (\max\{l_1^{\prime(1)} - p_1, 0\}, \dots, \max\{l_{k_1}^{\prime(1)} - p_{k_1}, 0\}), \tag{134}$$

$$= (\max\{l_1^{(1)} - p_1, 0\}, \dots, \max\{l_{k_1}^{(1)} - p_{k_1}, 0\}), \tag{135}$$

$$= (a_1^{(2)}, \dots, a_1^{(2)}), \tag{136}$$

and 
$$t((a_1^{(2)}, \dots, a_1^{(2)})) = \mathbf{a}^{(2)}$$
, as required.

### 6 Numerical experiments

In this section, we present numerical results for approximating known test functions,  $f:\Gamma^d\to\mathbb{R},\ \Gamma=(-1/2,1/2).$  We compare the performance of separable Matérn kernel interpolants across three different point sets: lengthscale-informed sparse grids (LISG), standard isotropic sparse grids (SG), and Monte Carlo points (MC) (uniformly distributed points  $\mathbf{x}_i\sim U(\Gamma^d)$ ). For our test functions we use random linear combinations of separable Matérn kernels with unit standard deviation,  $\boldsymbol{\sigma}=\mathbf{1}\in\mathbb{R}^d$ ,

$$f(\mathbf{x}) = \sum_{i=1}^{M} \xi_i \Phi_{\nu, \lambda}(\mathbf{y}_i, \mathbf{x})$$
(137)

where the random parameters  $\xi_i$  and  $\mathbf{y}_i$  are i.i.d. according to  $\xi_i \sim \mathcal{N}(0,5)$  and  $\mathbf{y}_i \sim U\left(\Gamma^d\right)$ , respectively. The Native space norms of these functions are known, see Proposition 2, and are independent of the dimension d.

In each experiment, see Figures 4, 5, 6 and 7, we consider two distinct length-scale anisotropy behaviours; exponential and linear growth, corresponding to linearly,  $\mathbf{p}_{\mathrm{lin}}$ , and logarithmically,  $\mathbf{p}_{\mathrm{log}}$ , growing penalties, respectively. Specifically, we take  $p_{\mathrm{lin},j}=j-1$  and  $p_{\mathrm{log},j}=\lceil\log_2(j)\rceil$ , where  $\lceil\cdot\rceil$  corresponds to the standard ceiling function, enforcing integer valued penalties. In Figures 4-6, the relative  $L^2$ -errors presented are averaged over 10 runs on independent realisations of f, and the errors are each approximated with 100 Monte Carlo samples. For large designs in high dimensions, for example  $d \geq 25$  and  $L \geq 8$ , due to the efficiency of Algorithm 1, the major bottleneck becomes sampling the emulator with each sample requiring  $d \times N$ -many kernel evaluations. Hence, to compute the  $L^2$ -error in reasonable time, we have chosen the number of Monte Carlo samples to be as small as possible while ensuring sufficiently small Monte Carlo error. In practice, evaluating emulators is trivially parallelisable, and so we do not view this as a particular drawback of GP emulation. We use Algorithm 1 to evaluate the interpolants for both sparse grid methods, and for Monte Carlo points we use a standard Cholesky decomposition.

In the first experiment, see Figure 4, we compare the error of lengthscale-informed sparse grids with standard isotropic sparse grids and Monte Carlo points in approximating realisations of f. We employ both lengthscale-informed kernels, where we matched the lengthscale hyperparameters in each axial direction with the lengthscale-anisotropy in f, and isotropic kernels, where we set  $\lambda = 1$ . The results shown assume  $\nu_j = 1.5$  in all directions,  $1 \le j \le d$ , for both f and the interpolating kernels; similar relationships were observed for the values  $\nu_j = 0.5$  and  $\nu_j = 2.5$ .

We immediately see a clear separation between the methods employing isotropic kernels and those with lengthscales adapted to the anisotropy in f, with the latter converging much faster. The difference in the errors between the SG and LISG methods is more pronounced in the higher dimensional case, d=8, and for linearly growing penalties,  $\mathbf{p}=\mathbf{p}_{\text{lin}}$ , as supported by our results and discussion in Section 3.2. For both isotropic and lengthscale-informed interpolating kernels, we see that the error consistently converges fastest with Monte Carlo designs. We believe this

discrepancy may be partially explained by the extrapolation behaviour of the onedimensional interpolants  $s_{\mathcal{X}_l,\phi_{\nu,\lambda}}$  near the endpoints of the intervals, and thus inherited by sparse grid designs in higher dimensions. Consequently, we have also presented the corresponding results for lengthscale-informed sparse grids based on point-sets weighted towards the endpoints; namely Clenshaw-Curtis abscissae (excluding endpoints),  $\mathcal{X}_{\text{CC},l} \coloneqq \{\sin(\theta)/2 : -\pi < \theta < \pi, \theta = n\pi/2^l, n \in \mathbb{Z}\}$ , and uniformly-spaced abscissae (including endpoints),

$$\mathcal{X}_{B,l} := \begin{cases}
\mathcal{X}_{l-1} \cup \{-1/2, 1/2\} & \text{if } l \ge 2, \\
\{-1/2, 0, 1/2\} & \text{if } l = 1, \text{ and} \\
\{0\} & \text{if } l = 0.
\end{cases}$$
(138)

In both cases, the error is improved over the uniformly-spaced grids defined in Section 3. Otherwise, to the authors' knowledge, no such approximation bounds have been derived that are able to explain the convergence rate observed in the Monte Carlo case, however we point the reader to [50], which indicates that the choice of point sets may be secondary to the choice of basis functions, which mirrors our observations. We also note that it is difficult to compare these methods for  $d \geq 10$ , due to how quickly isotropic sparse grid designs grow, and for  $N > 10^4$ , due to the inefficiency of evaluating emulators based on unstructured designs, such as with Monte Carlo points.

In Figure 5, we assess the effectiveness of Lengthscale-Informed Sparse Grids in significantly higher dimensions. Although theoretically applicable in arbitrarily high dimensions, for ease of implementation we consider up to a maximum dimension of d = 100, by which point clear trends are established. For the case  $\nu_j = 2.5$ , the number of points for which we can test is limited due to ill conditioning of the covariance matrices.

As discussed in Section 3.2, in all-but-one of the six penalty and smoothness combinations, we observe the presence of two regimes: The pre-asymptotic regime driven by the penalty, p, and hence the lengthscale anisotropy, and the asymptotic regime governed by the smoothness,  $\nu_j$ , and the dimensionality, d. For smaller dimensions, there is a quick onset of the asymptotic behaviour, seen clearly for dimensions d=2,3and, in some instances, d=5. For these dimensions, the asymptotic convergence rate is faster than the presymptomatic rate, and accordingly we see an increased convergence rate once L is large enough. This effect is diminished with increasing d, and eventually we would expect a significant slow down. The exception to this pattern occurs for  $\nu_j = 0.5$  and  $\mathbf{p} = \mathbf{p}_{\log}$ , however we note that this behaviour is present for slightly faster, quadratic growth in the lengthscale,  $p_j = \lceil j^2 \rceil$ . As we increase the smoothness, the pre-asymptotic convergence rate increases, as expected. Notably, this increase is much larger from  $\nu_i = 0.5$  to 1.5, than with  $\nu_i = 1.5$  to 2.5. We also observe an increased convergence rate when employing linearly, instead of logarithmically, growing penalties, however the difference is small relative to the additional anisotropy present. A limitation of the error bound in Theorem 2 is that we require lengthscales of the form  $\lambda_i = 2^p$ ,  $p \in \mathbb{N}_0$ . Furthermore, lengthscales are rarely known a priori in practice, and instead are more likely to be estimated. Hence, to test the robustness of the method, in Figure 6 we explore the effect of misspecifying the penalty. We take

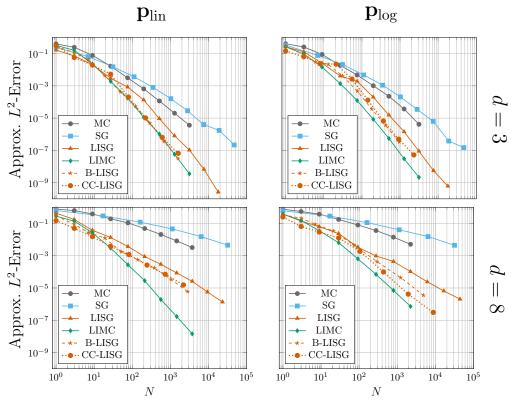


Fig. 4: Relative  $L^2$ -error in approximating realisations of f when (a), interpolating with isotropic kernels ( $\lambda = 1$ ) on Monte Carlo (MC) and standard sparse grid (SG) designs, and (b), interpolating with anisotropic kernels ( $\lambda = 2^{\mathbf{p}}$ ) on Monte Carlo (LIMC) and lengthscale-informed sparse grid designs, based on uniformly spaced-points (LISG), uniformly-spaced including boundary points (B-LISG), and Clenshaw-Curtis points (CC-LISG). We consider input dimensions 3 and 8, both linearly and logarithmically growing penalties, and employ separable Matérn kernels with  $\nu_j = 1.5$  for all  $1 \leq j \leq d$ .

realisations of f with linearly growing penalties,  $\mathbf{p} = \mathbf{p}_{\text{lin}}$ , and approximate using LISG designs, with separable Matérn kernels now stretched according to a perturbed penalty,  $\mathbf{p}_{\text{lin}}^{\eta}$ , defined in terms of a perturbation parameter,  $\eta$ , by  $p_{\text{lin},j}^{\eta} = \lceil (1+\eta)p_j \rceil$ .

Predictably, we observe in all cases that misspecifying the penalty by a small degree only has a marginal effect on the error, whereas a large discrepancy between the anisotropy in f and the kernels results in a significantly worse error. We note that all of these cases perform better than isotropic sparse grids (equivalent to  $\eta=-1$ ), which are infeasible in d=50 due to their size. Interestingly, for  $\nu_j=0.5$ , we see a small improvement when slightly overestimating the lengthscale according to  $\eta=0.2$ . This is not true for  $\nu_j=1.5$ , where instead underestimating the lengthscale according to  $\eta=-0.2$  results in a similar error as when using the exact penalties.

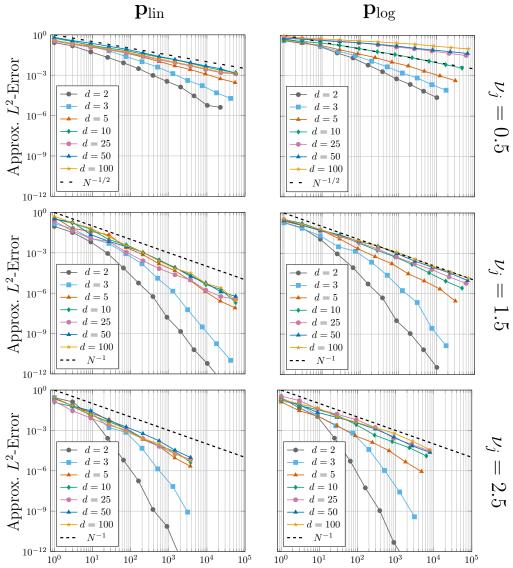
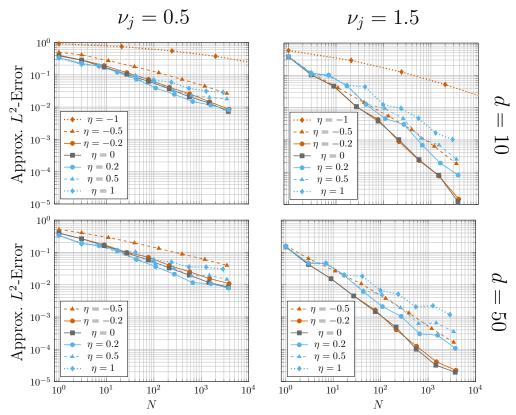


Fig. 5: Relative  $L^2$ -approximation error when interpolating target functions, f, of increasing dimension, d, using lengthscale-informed sparse grids.

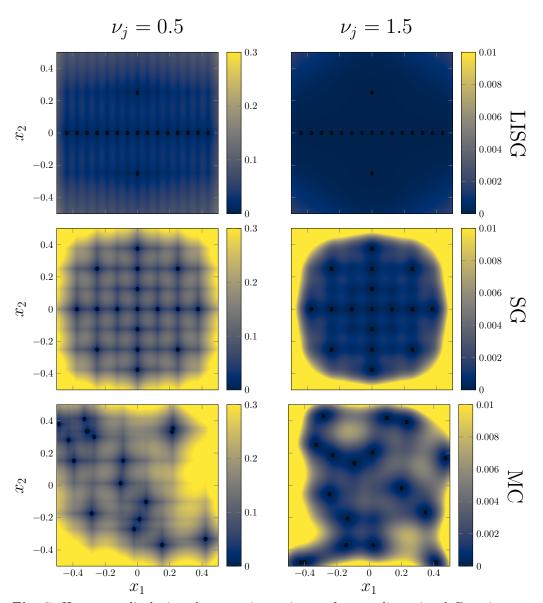
Finally, in Figure 7, we present heatmaps representing the posterior marginal variance of two-dimensional Gaussian processes, whose mean functions correspond to kernel interpolants on LISG, SG and MC designs. We note that only the LISG method employs anisotropic kernels, which accounts for most of the discrepancy to the other two methods.



**Fig. 6**: Effect of misspecifying lengthscale anisotropy on the convergence of the relative  $L^2$ -approximation error in N, the number of function evaluations.

# 7 Conclusion

We have presented lengthscale-informed sparse grids (LISGs); a novel sparse grid construction for interpolation with separable Matérn kernels, designed to exploit lengthscale-anisotropy in the target function f. For sparse grid approximation methods to apply, we assume f lies in a Sobolev space with bounded mixed smoothness, and to be considered anisotropic, f is assumed to be bounded independently of the dimension in the Native space norm of a separable Matérn kernel with the prescribed lengthscales. In Theorem 2, we derived a general error bound indicating the superior performance of LISG approximation over isotropic methods given the presence of anisotropy, especially in a high-dimensional setting. Making the connection to Gaussian process regression, we additionally derive an analogous error bound for the posterior marginal variance in Proposition 8. We included an adaptation to the fast inference algorithm from [36] to LISG, resulting in an algorithm that scales well with both input dimension and the number of function evaluations. We tested the method



**Fig. 7**: Heat map displaying the posterior variance of a two-dimensional Gaussian process trained on approximately 17 function evaluations arranged in different designs. For the LISG method, a penalty of  $\mathbf{p}=(1,3)$  is assumed. Values exceeding the maximum are displayed as the maximum.

on a series of numerical experiments on target functions with known anisotropy in up to 100 dimensions.

To the best of our knowledge, this is the first result proving error bounds in the high-dimensional setting assuming only anisotropy in the lengthscales, not requiring anisotropic (or infinite) regularity. Although we in this work have assumed that the anisotropy structure, i.e. the lengthscales  $\{\lambda_j\}_{j=1}^d$ , is known a-priori, we expect that our method will perform equally well in practice when lengthscales have to be estimated, provided that that target function exhibits the required anisotropy. Our numerical experiments with misspecified lengthscales indicate a level of robustness to errors in the estimation of the lengthscales. Furthermore, since a typical workflow already involves the estimation of lengthscales, the application of our method is not much more cumbersome than that of isotropic sparse grids.

# Acknowledgements

The authors would like to thank the Isaac Newton Institute for Mathematical Sciences, Cambridge, for support and hospitality during the programme *Mathematical and statistical foundation of future data-driven engineering*, where work on this paper was undertaken, supported by EPSRC (EP/R014604/1). The authors further thank Abdul-Lateef Haji-Ali and Ken Newman for helpful discussions and support. EA was supported by Biomathematics and Statistics Scotland (BioSS) and the EPSRC Centre for Doctoral Training in Mathematical Modelling, Analysis and Computation (MAC-MIGS) funded by the EPSRC (EP/S023291/1), Heriot-Watt University, and The University of Edinburgh.ALT was partially supported by EPSRC grants EP/X01259X/1 and EP/Y028783/1.

# Appendix A

This section contains results related to the isomorphism of multi-index sets used in the proofs in Section 3.

**Lemma 7** Let  $d \in \mathbb{N}$  and  $k \in \mathbb{N}_0$ . Define subsets of  $\mathbb{N}_0^d$  by  $\mathcal{K}_k^d := \{ \mathbf{l} \in \mathbb{N}_0^d : | \{1 \leq j \leq d : l_j \neq 0\} | = k \}$  and  $\mathcal{P}_k^d := \{ \mathbf{u} \subset \{1, \dots, d\} : |\mathbf{u}| = k, \mathbf{u}_i < \mathbf{u}_{i+1} \}$ . We have that  $\mathcal{K}_k^d \cong \{ \mathbf{0} \} \cup \mathcal{P}_k^d \times \mathbb{N}^k$  with bijection, for a given  $\mathbf{l} \in \mathbb{N}_0^d$ ,

$$\rho(\mathbf{l}) = \begin{cases} \mathbf{0} \in \mathbb{N}_0^k & \text{if } \mathbf{l} = \mathbf{0}, \text{ and} \\ \left(\mathfrak{u}(\mathbf{l}), l_{\mathfrak{u}(\mathbf{l})}\right) & \text{otherwise,} \end{cases}$$
(A1)

where  $\mathfrak{u}(\boldsymbol{l}) \coloneqq \{j \in \{1, \dots, d\} : l_j = 0\} \subset \mathcal{P}_k^d \text{ and, if } |\mathfrak{u}(\boldsymbol{l})| = k, \text{ we define, for a given } \mathbf{b} \in \mathbb{N}_0^d, \mathbf{b}_{\mathfrak{u}(\boldsymbol{l})} \coloneqq (b_{\mathfrak{u}(\boldsymbol{l})_1}, \dots, b_{\mathfrak{u}(\boldsymbol{l})_k}).$ 

Proof Define the candidate inverse of 
$$\rho$$
 by  $\rho^{-1}(\mathbf{0}) = \mathbf{0} \in \mathbb{N}_0^d$ , and for  $(\mathfrak{u}, \mathbf{a}) \in \mathcal{P}_k^d \times \mathbb{N}^k$ ,  $\rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}_i} = a_i$  for  $1 \le i \le k$  and  $\rho^{-1}(\mathfrak{u}, \mathbf{a})_j = 0$  for  $j \notin \mathfrak{u}$ . (A2)

Let  $l \in \mathcal{K}_k^d$ . If l = 0, then trivially  $\rho^{-1}(\rho(0)) = 0$ . Otherwise, for  $1 \le i \le k$ , we have

$$\rho^{-1}(\rho(l))_{\mathfrak{u}(l)_i} = \rho^{-1}(\mathfrak{u}(l), l_{\mathfrak{u}(l)})_{\mathfrak{u}(l)_i} = l_{\mathfrak{u}(l)_i}, \tag{A3}$$

and for all  $j \notin \mathfrak{u}(\boldsymbol{l})$ , by definition  $\boldsymbol{l}_j = 0$ , and

$$\rho^{-1}(\rho(l))_j = \rho^{-1}(\mathfrak{u}(l), l_{\mathfrak{u}(l)})_j = 0.$$
(A4)

Therefore, for all  $1 \leq j \leq d$ ,  $\rho^{-1}(\rho(l))_j = l_j$ , and so  $\rho^{-1}(\rho(l)) = l$ . In the opposite direction, trivially we have  $\rho(\rho^{-1}(\mathbf{0})) = \mathbf{0}$ . Otherwise, let  $(\mathfrak{u}, \mathbf{a}) \in \mathcal{P}_k^d \times \mathbb{N}^k$ . For  $1 \leq i \leq k$ , we have  $\rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}_i} = a_i \in \mathbb{N}$ . Specifically,  $\rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}_i} \neq 0$ , and so by definition,  $\mathfrak{u}_i \in \mathfrak{u}(\rho^{-1}(\mathfrak{u}, \mathbf{a}))$ . Furthermore, if  $j \notin \mathfrak{u}$ , we have  $\rho^{-1}(\mathfrak{u}, \mathbf{a})_j = 0$ , and so  $j \notin (-1, 1)$ .  $\mathfrak{u}(\boldsymbol{\rho}^{-1}(\mathfrak{u},\mathbf{a}))$ . Hence

$$\mathfrak{u}(\rho^{-1}(\mathfrak{u}, \mathbf{a})) = \{\mathfrak{u}_i\}_{1 \le i \le k} = \mathfrak{u} \tag{A5}$$

Finally, we then have

$$\rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}(\rho^{-1}(\mathfrak{u}, \mathbf{a}))} = \rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}},$$

$$:= \left(\rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}_{1}}, \dots, \rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}_{k}}\right),$$

$$= (a_{1}, \dots, a_{k}),$$

$$= \mathbf{a}$$
(A6)

Therefore,

$$\rho(\rho^{-1}(\mathfrak{u}, \mathbf{a})) := \left(\mathfrak{u}(\rho^{-1}(\mathfrak{u}, \mathbf{a})), \rho^{-1}(\mathfrak{u}, \mathbf{a})_{\mathfrak{u}(\rho^{-1}(\mathfrak{u}, \mathbf{a}))}\right),$$

$$= (\mathfrak{u}, \mathbf{a}),$$
(A7)

as required.

Corollary 4 Let  $d, k \in \mathbb{N}$ . Let  $\rho : \mathcal{K}_k^d \leftrightarrow \{\mathbf{0}\} \cup \mathcal{P}_k^d \times \mathbb{N}^k$  be defined as in Lemma 7 and let  $\mathbf{0} \neq \mathbf{l} \in \mathcal{K}_k^d$ ,  $\rho(\mathbf{l}) = (\mathfrak{u}, \mathbf{a})$ . For  $L \in \mathbb{N}_0$ , define the multi-index set  $\mathcal{I}_L^d := \{\mathbf{l} \in \mathbb{N}_0^d : |\mathbf{l}| \leq L\}$ . Then  $\mathbf{l} \in \mathcal{I}_L^d$  if and only if  $\mathbf{a} \in \mathcal{I}_L^k$ .

Proof Let  $\mathbf{l} \in \mathcal{I}_L^d$ , then  $\sum_{j=1}^d l_j \leq L$ . By definition,  $\mathbf{a} = \mathbf{l}_{\mathfrak{u}(\mathbf{l})}$ , and hence  $\sum_{i=1}^k a_i = \sum_{i=1}^k l_{\mathfrak{u}(\mathbf{l})_i} \leq \sum_{j=1}^d l_j \leq L$ , since  $l_j \geq 0$ . Thus  $\mathbf{a} \in \mathcal{I}_L^k$ .

Let  $\mathbf{a} \in \mathcal{I}_L^k$ . By definition,  $l_j = 0$  if  $j \notin \mathfrak{u}(\mathbf{l})$ . Since  $\mathbf{l} \in \mathcal{K}_k^d$ , we have  $|\mathfrak{u}(\mathbf{l})| = k$ , and hence  $\sum_{j=1}^d l_j = \sum_{i=1}^k l_{\mathfrak{u}(\mathbf{l})_i} = \sum_{i=1}^k a_i \leq L$ . Thus  $\mathbf{l} \in \mathcal{I}_L^d$  also.

**Corollary 5** Let  $d, k \in \mathbb{N}$ . Let  $\mathcal{K}_k^d$ ,  $\mathcal{P}_k^d$  and  $\mathcal{I}_L^d$  be defined as in 7 and 4. Then  $\mathcal{K}_k^d \cap \mathcal{I}_L^d \cong \{\mathbf{0}\} \cup \mathcal{P}_k^d \times \mathbb{N}^k \cap \mathcal{I}_L^k$  and  $\mathcal{K}_k^d \setminus \mathcal{I}_L^d \cong \mathcal{P}_k^d \times \mathbb{N}^k \setminus \mathcal{I}_L^k$ .

*Proof* This follows directly from the two previous results as  $\rho$  acts as a bijection in both cases, noting that  $\mathbf{0} \in \mathcal{I}_L^d$  for all  $L \geq 0$ .

# References

- [1] Wendland, H.: Scattered Data Approximation. Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, Cambridge (2004)
- [2] Buhmann, M.D.: Radial basis functions. Acta numerica 9, 1–38 (2000)
- [3] Narcowich, F., Ward, J., Wendland, H.: Sobolev bounds on functions with scattered zeros, with applications to radial basis function surface fitting. Mathematics of Computation **74**(250), 743–763 (2005)
- [4] Narcowich, F.J., Ward, J.D., Wendland, H.: Sobolev error estimates and a Bernstein inequality for scattered data interpolation via radial basis functions. Constructive Approximation 24(2), 175–186 (2006)
- [5] Arcangéli, R., Silanes, M.C.L., Torrens, J.J.: Extension of sampling inequalities to sobolev semi-norms of fractional order and derivative data. Numerische Mathematik 121(3), 587–608 (2012)
- [6] Rasmussen, C.E., Williams, C.K.I.: Gaussian Processes for Machine Learning. The MIT Press, Cambridge, MA (2005)
- [7] Gramacy, R.B.: Surrogates: Gaussian Process Modeling, Design, and Optimization for the Applied Sciences. Chapman & Hall/CRC Texts in Statistical Science. CRC Press, Boca Raton, FL (2020)
- [8] Stein, M.L.: Interpolation of Spatial Data: Some Theory for Kriging. Springer, New York, NY (1999)
- [9] Kennedy, M.C., O'Hagan, A.: Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology) **63**(3), 425–464 (2001)
- [10] Higdon, D., Kennedy, M., Cavendish, J.C., Cafeo, J.A., Ryne, R.D.: Combining field data and computer simulations for calibration and prediction. SIAM Journal on Scientific Computing 26(2), 448–466 (2004)
- [11] Scheuerer, M., Schaback, R., Schlather, M.: Interpolation of spatial data—A stochastic or a deterministic problem? European Journal of Applied Mathematics **24**(04), 601–629 (2013)
- [12] Matérn, B.: Spatial Variation vol. 36. Springer, New York, NY (2013)
- [13] Porcu, E., Bevilacqua, M., Schaback, R., Oates, C.J.: The matérn model: A journey through statistics, numerical analysis and machine learning. Statistical Science **39**(3), 469–492 (2024)

- [14] Adams, R.A., Fournier, J.J.: Sobolev Spaces. Elsevier, Amsterdam (2003)
- [15] Vaart, A., Zanten, H.: Information rates of nonparametric gaussian process methods. Journal of Machine Learning Research 12(6) (2011)
- [16] Santner, T.J., Williams, B.J., Notz, W.I.: The Design and Analysis of Computer Experiments. Springer Series in Statistics. Springer, New York, NY (2003)
- [17] Vernon, I., Goldstein, M., Bower, R.G.: Galaxy formation: a bayesian uncertainty analysis. Bayesian Analysis **05**, 619–670 (2010)
- [18] Nobile, F., Tempone, R., Webster, C.G.: An anisotropic sparse grid stochastic collocation method for partial differential equations with random input data. SIAM Journal on Numerical Analysis 46(5), 2411–2442 (2008)
- [19] Nobile, F., Tempone, R., Wolfers, S.: Sparse approximation of multilinear problems with applications to kernel-based methods in uq. Numerische Mathematik 139 (2018)
- [20] Rieger, C., Wendland, H.: Sampling inequalities for anisotropic tensor product grids. IMA Journal of Numerical Analysis **40**(1), 285–321 (2019)
- [21] Sloan, I.H., Woźniakowski, H.: When are quasi-monte carlo algorithms efficient for high dimensional integrals? Journal of Complexity 14(1), 1–33 (1998)
- [22] Dick, J., Kuo, F.Y., Sloan, I.H.: High-dimensional integration: the quasi-monte carlo way. Acta Numerica 22, 133–288 (2013)
- [23] Rieger, C., Wendland, H.: On the approximability and curse of dimensionality of certain classes of high-dimensional functions. SIAM Journal on Numerical Analysis **62**(2), 842–871 (2024)
- [24] Rieger, C., Wendland, H.: Constructive approximation of high-dimensional functions with small efficient dimension with applications in uncertainty quantification. arXiv preprint arXiv:2411.18128 (2024)
- [25] Yang, Y., Tokdar, S.T.: Minimax-optimal nonparametric regression in high dimensions. The Annals of Statistics, 652–674 (2015)
- [26] Liu, X., Guillas, S.: Dimension reduction for gaussian process emulation: An application to the influence of bathymetry on tsunami heights. SIAM/ASA Journal on Uncertainty Quantification 5(1), 787–812 (2017)
- [27] Rasmussen, C.E.: Gaussian processes in machine learning. In: Summer School on Machine Learning, pp. 63–71. Springer, Berlin, Heidelberg (2004)
- [28] Vaart, A.W., Zanten, J.H.: Adaptive Bayesian estimation using a Gaussian random field with inverse Gamma bandwidth. The Annals of Statistics **37**(5B),

- 2655-2675 (2009)
- [29] Bhattacharya, A., Pati, D., Dunson, D.: Anisotropic function estimation using multi-bandwidth gaussian processes. The Annals of Statistics 42(1), 352–381 (2014)
- [30] MacKay, D.J.: Bayesian interpolation. Neural computation 4(3), 415–447 (1992)
- [31] Neal, R.M.: Bayesian Learning for Neural Networks. Springer, New York, NY (2012)
- [32] Wipf, D., Nagarajan, S.: A new view of automatic relevance determination. Advances in neural information processing systems **20** (2007)
- [33] Fasshauer, G.E., Hickernell, F.J., Woźniakowski, H.: On dimension-independent rates of convergence for function approximation with gaussian kernels. SIAM Journal on Numerical Analysis 50(1), 247–271 (2012)
- [34] Teckentrup, A.L.: Convergence of gaussian process regression with estimated hyper-parameters and applications in bayesian inverse problems. SIAM/ASA Journal on Uncertainty Quantification 8(4), 1310–1337 (2020)
- [35] Jagadeeswaran, R., Hickernell, F.J.: Fast automatic bayesian cubature using lattice sampling. Statistics and Computing **29**(6), 1215–1229 (2019)
- [36] Plumlee, M.: Fast prediction of deterministic functions using sparse grid experimental designs. Journal of the American Statistical Association 109(508), 1581–1591 (2014)
- [37] Conrad, P.R., Girolami, M., Särkkä, S., Stuart, A., Zygalakis, K.: Statistical analysis of differential equations: introducing probability measures on numerical solutions. Statistics and Computing 27, 1065–1082 (2017)
- [38] Bai, T., Teckentrup, A.L., Zygalakis, K.C.: Gaussian processes for bayesian inverse problems associated with linear partial differential equations. Statistics and Computing **34**(4), 139 (2024)
- [39] Schölkopf, B., Herbrich, R., Smola, A.J.: A generalized representer theorem. In: Proceedings of the 14th Annual Conference on Computational Learning Theory and the 5th European Conference on Computational Learning Theory, pp. 416–426. Springer, Berlin, Heidelberg (2001)
- [40] Novak, E., Ullrich, M., Woźniakowski, H., Zhang, S.: Reproducing kernels of sobolev spaces on  $\mathbb{R}^d$  and applications to embedding constants and tractability. Analysis and Applications **16**(05), 693–715 (2018)
- [41] Lord, G.J., Powell, C.E., Shardlow, T.: An Introduction to Computational

- Stochastic PDEs. Cambridge Texts in Applied Mathematics. Cambridge University Press, Cambridge (2014)
- [42] Hackbusch, W.: Tensor Spaces and Numerical Tensor Calculus. Springer, Cham (2012)
- [43] Bungartz, H.-J., Griebel, M.: Sparse grids. Acta numerica 13, 147–269 (2004)
- [44] Wasilkowski, G.W., Wozniakowski, H.: Explicit cost bounds of algorithms for multivariate tensor product problems. Journal of Complexity 11(1), 1–56 (1995)
- [45] Rieger, C., Wendland, H.: Sampling inequalities for sparse grids. Numerische Mathematik **136**(2), 439–466 (2017)
- [46] Aronszajn, N.: Theory of reproducing kernels. Transactions of the American Mathematical Society **63**(3), 337–404 (1950)
- [47] Stuart, A.M., Teckentrup, A.L.: Posterior consistency for gaussian process approximations of bayesian posterior distributions. Mathematics of Computation 87(310), 721–753 (2018)
- [48] Burkhardt, J.: Counting Abscissas in Sparse Grids (2014). https://people.math.sc.edu/Burkardt/presentations/sgmga counting.pdf Accessed 2025-06-02
- [49] Stanley, R.P.: Enumerative Combinatorics. Volume 1. Cambridge University Press, New York, NY (2012)
- [50] Adcock, B., Brugiapaglia, S.: Monte carlo is a good sampling strategy for polynomial approximation in high dimensions. arXiv preprint arXiv:2208.09045 (2023)