

Gaussian process regression: Optimality, robustness, and relationship with kernel ridge regression

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Abstract

Gaussian process regression is widely used in many fields, for example, machine learning, reinforcement learning and uncertainty quantification. One key component of Gaussian process regression is the unknown correlation function, which needs to be specified. In this paper, we investigate what would happen if the correlation function is misspecified. We derive upper and lower error bounds for Gaussian process regression with possibly misspecified correlation functions. We find that when the sampling scheme is quasi-uniform, the optimal convergence rate can be attained even if the smoothness of the imposed correlation function exceeds that of the true correlation function. We also obtain convergence rates of kernel ridge regression with misspecified kernel function, where the underlying truth is a deterministic function. Our study reveals a close connection between the convergence rates of Gaussian process regression and kernel ridge regression, which is aligned with the relationship between sample paths of Gaussian process and the corresponding reproducing kernel Hilbert space. This work establishes a bridge between Bayesian learning based on Gaussian process and frequentist kernel methods with reproducing kernel Hilbert space.

Keywords: Gaussian process regression; Bayesian machine learning; Kernel ridge regression; Reproducing kernel Hilbert space; Space-filling designs

1. Introduction

Gaussian process regression is widely applied in machine learning (Rasmussen and Williams, 2006), including reinforcement learning (Rasmussen et al., 2003) and Bayesian optimization (Shahriari et al., 2016; Frazier, 2018; Bull, 2011; Klein et al., 2017); spatial statistics

(Cressie, 2015; Stein, 1999; Matheron, 1963); computer experiments (Santner et al., 2003; Sacks et al., 1989), and many others, to capture the intrinsic randomness of the underlying function. The goal of Gaussian process regression is to recover an underlying function based on noisy observations. As a Bayesian machine learning method, the key idea of Gaussian process regression is to impose a probabilistic structure, which is a Gaussian process, on the underlying truth. Based on this assumption, the conditional distribution at each unobserved point in the interested domain is normal with explicit mean and variance. The conditional mean provides a natural predictor of the function value, and the pointwise confidence interval constructed based on the conditional variance can be used for statistical uncertainty quantification.

In this work, we establish error bounds on Gaussian process regression, where the smoothness of the correlation function can be misspecified, and the observations have noise. We consider that the underlying truth is a Gaussian process, which is a standard setting in Gaussian process modeling (Stein, 1999; Santner et al., 2003; Gramacy, 2020). Although the noisy observations have been extensively considered in the setting that the underlying truth is a deterministic function (Wynne et al., 2021; Steinwart et al., 2009; Fischer and Steinwart, 2020; van der Vaart and van Zanten, 2011, and references therein), (see Section 2 for more discussions), it is somewhat surprising that there has been little study on this in the literature when the underlying truth is a Gaussian process. The difference is that, the convergence results for a deterministic function usually depend on some quantities related to the underlying function (e.g., the norm of the underlying function in some function space), while for a Gaussian process, these quantities themselves may be random. Thus, the convergence for a Gaussian process regression needs to be analyzed with a different approach. We derive prediction lower and upper error bounds under L_2 metric and with fixed design. Specifically, we show that if the smoothness of the true correlation function is m_0 and the smoothness of the imposed correlation function lies in $[m_0, \infty)$, with an appropriate regularization parameter and quasi-uniform design points, the convergence rate under L_2 metric is $n^{-(m_0-d/2)/(2m_0)}$, where d is the dimension and n is the sample size. Furthermore, we prove that this convergence rate is optimal under certain assumptions. Our theory can be applied to justifying the use of space-filling designs, where the design points spread approximately evenly in the region of interest, since quasi-uniform designs are space-filling designs. If the smoothness of the imposed correlation function, denoted by m , is less than m_0 , we show that the convergence rate of upper error bound is $n^{-(m-d/2)/(2m)}$.

Here, we should keep in mind not to confuse the setting of Gaussian process regression with the settings of other fields, including nonparametric regression (Gu, 2013; van de Geer, 2000) and posterior contraction of Gaussian process priors (van der Vaart and van Zanten, 2008a, 2011). The hypothesis spaces are different in the later two fields. In particular, the underlying function is assumed to be *deterministic*, which leads to different notions of *smoothness* and convergence rates (Kanagawa et al., 2018; Tuo and Wang, 2020).

We also consider one popular kernel method: kernel ridge regression, where the reproducing kernel Hilbert space can be misspecified. This is a frequentist approach, where the underlying truth is assumed to be a deterministic function. The reason for considering kernel ridge regression is two-fold.

First, the study paves the way to establish the intriguing relationship between Gaussian process regression and kernel ridge regression with more details given later. At first sight, the two areas are very different, for example, completely different approaches have been employed to investigate their convergence rates respectively. On the other hand, the two areas share some striking similarities in certain aspects, for example, their predictors take rather similar forms, and also their model assumptions bear strong resemblance. A thorough review on the differences and connection of Gaussian process and reproducing kernel Hilbert space can be found in Kanagawa et al. (2018). Therefore, it is natural to ask whether there are some deep relationships between Gaussian process regression and kernel ridge regression. Kanagawa et al. (2018) provides a positive answer. Remark 5.5 of Kanagawa et al. (2018) states a theoretical equivalence between Gaussian process regression and kernel ridge regression, where the Gaussian process regression model and the convergence rate (Kanagawa et al., 2018, Theorem 5.1) is based on the posterior contraction of Gaussian process priors in van der Vaart and van Zanten (2011). Although the underlying truth in van der Vaart and van Zanten (2011) is still a deterministic function, Remark 5.5 of Kanagawa et al. (2018) reveals a relationship between Gaussian process regression and kernel ridge regression. Based on the constructed convergence rate in Gaussian process regression, we conduct a further investigation and establish a relationship based on the situations where “the underlying truth in Gaussian process regression is a Gaussian process” and “the underlying truth in kernel ridge regression is a deterministic function”.

We now describe briefly their relationship, which is summarized in Figure 1. If the true correlation function has smoothness m_0 , then the sample paths of the Gaussian process have a smoothness $m_0 - d/2$, but do not lie in the Sobolev space $H^{m_0-d/2}$ with a strictly positive probability (Steinwart, 2019; Kanagawa et al., 2018). For a deterministic function f with smoothness $m_0(f) = m_0 - d/2$, the optimal convergence rate is $n^{-m_0(f)/(2m_0(f)+d)} = n^{-(m_0-d/2)/(2m_0)}$, which coincides with the optimal convergence rate of Gaussian process regression. Furthermore, the optimal value of the regularization parameter in kernel ridge regression coincides with that of the regularization parameter in Gaussian process regression. In other words, we can regard Gaussian process regression as kernel ridge regression with an oversmoothed kernel function shifted by a smoothness $d/2$, from prediction perspective. This coincidence reveals an interesting relationship between kernel ridge regression and Gaussian process regression, and provides more insights on the connection between these two methods.

Second, we will derive some new and interesting results on convergence rates, which complements the existing literature on this topic. Specifically, suppose f has smoothness $m_0(f)$, and the corresponding Sobolev space with smoothness $m_0(f)$ is denoted by $H^{m_0(f)}$. We show that the kernel ridge regression can still achieve the optimal convergence rate, if the corresponding reproducing kernel Hilbert space is associated with a smoothness lying in $[m_0(f)/2, \infty)$. If $f \in H^{m_0(f)}$, this recovers the convergence results in the misspecified kernel ridge regression literature (e.g., Blanchard and Mücke (2018); Dicker et al. (2017); Guo et al. (2017); Lin et al. (2017); Steinwart et al. (2009); Fischer and Steinwart (2020)), while the settings are different. See Section 2.2 for detailed discussion. Nevertheless, we note that if a function has smoothness $m_0(f)$, it may not lie in the corresponding Sobolev space with smoothness $m_0(f)$; examples include triangle function and Matérn kernel functions;

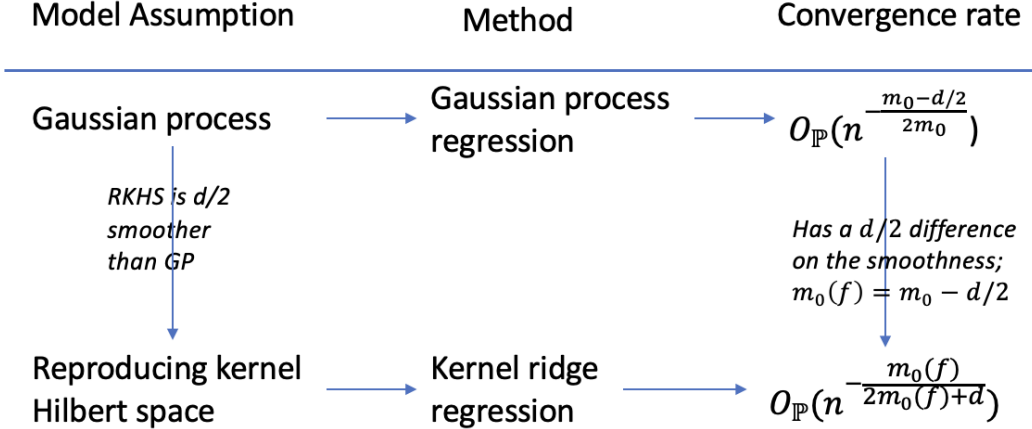


Figure 1: Relationship between the convergence rates of oversmoothed Gaussian process regression ($m_0 \leq m < \infty$) and kernel ridge regression. We use the following abbreviation. RKHS: Reproducing kernel Hilbert space; GP: Gaussian process.

Method	Model Assumption	Convergence rate	
Gaussian process regression	f is a realization of a Gaussian process Z .	$O_{\mathbb{P}}(n^{-\frac{2m_0-d}{2m_0}})$ (optimal rate), for $m_0 \leq m < \infty$.	$O_{\mathbb{P}}(n^{-\frac{2m-d}{2m}})$, for $m \leq m_0$.
Kernel ridge regression	f is a deterministic function.	$f \in H^{m_0(f)}$: $O_{\mathbb{P}}(n^{-\frac{m_0(f)}{2m_0(f)+d}})$, $f \notin H^{m_0(f)}$: $O_{\mathbb{P}}(n^{-\frac{m_0(f)}{2m_0(f)+d}}Q(n))$, for $m_0(f)/2 \leq m < \infty$.	$O_{\mathbb{P}}(n^{-\frac{2m}{4m+d}})$, for $m < m_0(f)/2$.

Table 1: Summary of the L_2 convergence rates of misspecified Gaussian process regression and kernel ridge regression. The function Q satisfies $\lim_{s \rightarrow +\infty} (\log Q(s))/(\log s) = 0$. The two rates on the shaded row were presented in previous literature, while our settings and mathematical development are different.

see Section 5.1.1. We are not aware of any work related to the convergence rate under the scenario $f \notin H^{m_0(f)}$ but has smoothness $m_0(f)$ ¹. Table 1 summarizes the results obtained in this work. For the brevity, we assume the design is quasi-uniform in Table 1, and present general results in the main text.

The rest of this paper is arranged as follows. We first make comparison to related works in Section 2. In Section 3, we introduce some preliminaries. In Section 4, we provide convergence rates of misspecified Gaussian process regression. In Section 5, we discuss the relationship between the convergence rates of misspecified Gaussian process regression and kernel ridge regression, where we also present convergence rates of misspecified kernel ridge regression. Numerical experiments are conducted in Section 6. Conclusions and discussion are made in Section 7. Technical proofs are provided in Appendix.

1. This implies $f \in H^m$ for all $m < m_0(f)$ but $f \notin H^{m_0(f)}$. Note that this is *not* misspecification. The condition $f \notin H^{m_0(f)}$ is only related to f itself, not the prediction method we use. In previous works, it is often assumed that $f \in H^m$ for all $m \leq m_0(f)$.

2. Related literature

In this subsection, we first remark some differences between our results and previous works. The previous works can be roughly divided into two fields: Gaussian process modeling, where the underlying truth is assumed to be a Gaussian process, and deterministic function reconstruction, where the underlying truth is modeled as a deterministic function. The difference between the convergence rate analysis in these two settings is that, in deterministic function reconstruction, the convergence rate usually involves some kind of function norm of the underlying true function, while for Gaussian process modeling, this norm itself is also random, which needs to be further considered. Although our work focuses on the Gaussian process modeling, we also consider the kernel ridge regression and obtain some interesting results. We utilize mathematical tools from both fields in the present work. For example, Lemma 21 comes from Gaussian process modeling, and the rate of convergence of kernel ridge regression is established based on the previous works Tuo et al. (2020); van de Geer (2000). Moreover, mathematical tools in scattered data approximation (Wendland, 2004) play an important role in our analysis.

2.1 Gaussian process modeling

The rate of convergence of Gaussian process regression without noise has been studied in much literature, see Buslaev and Seleznev (1999); Yakowitz and Szidarovszky (1985); Stein (1990b) for example, where the convergence rate is pointwise or the input points are not general scattered data points. Recent works Wang et al. (2020); Tuo and Wang (2020) study the rate of convergence of Gaussian process regression in the $L_p(\Omega)$ norm, with $1 \leq p \leq \infty$ under different designs and misspecified correlation functions in the noiseless case. To the best of our knowledge, the only work that studies Gaussian process regression with noisy observations is Lederer et al. (2019). In Lederer et al. (2019), a uniform error bound of Gaussian process regression has been provided, where the unknown realization f and the correlation function are assumed to have a Lipschitz continuity, and the noise is normal. Furthermore, the correlation function in Lederer et al. (2019) is well-specified.

In this work, we study the rate of convergence of Gaussian process regression in the $L_2(\Omega)$ norm, under different designs and misspecified correlation functions, but we take the noise into consideration. These settings differentiate our work with the previous works in Gaussian process modeling.

2.2 Deterministic function reconstruction

Comparing with Gaussian process modeling, there are much more literature studying the deterministic function reconstruction. The most related fields to the present work are kernel ridge regression, posterior contraction of Gaussian process priors, and scattered data approximation.

Kernel ridge regression Although we focus on the Gaussian process regression, we also consider the kernel ridge regression and obtain some interesting results. We consider that f has smoothness $m_0(f)$, in the sense that is to be introduced later in Section 5.1.1. If the underlying true function $f \in H^{m_0(f)}$, we recover the convergence rates obtained by Blanchard and Mücke (2018); Dicker et al. (2017); Guo et al. (2017); Lin et al. (2017); Steinwart et al. (2009), while the model settings are different. Specifically, the design points in the above works are random. Moreover, the assumptions are different. The aforementioned works impose conditions on the eigenvalues and eigenfunctions (Blanchard and Mücke, 2018; Dicker et al., 2017; Guo et al., 2017; Lin et al., 2017; Steinwart et al., 2009; Fischer and Steinwart, 2020).

The aforementioned works have different model settings from our work, which provides some additional insights on the study of kernel ridge regression. Specifically, we adopt model settings similar to Tuo et al. (2020), where the widely used Matérn kernel functions can be used and the design points are fixed. These model settings allow us to consider the case that the underlying function $f \notin H^{m_0(f)}$ but has smoothness $m_0(f)$. We employ the empirical process technique together with Fourier transform to derive the convergence rates. Following this approach, we do not need to make assumptions on the eigenvalues and eigenfunctions, but we need additional conditions on the interested region. Moreover, our results show the advantage of space-filling designs.

Posterior contraction of Gaussian process priors In this field, despite the use of Gaussian process priors, the underlying function is still assumed to be deterministic. An incomplete list of papers in this area includes Castillo (2008, 2014); Giordano and Nickl (2019); Nickl and Söhl (2017); Pati et al. (2015); van der Vaart and van Zanten (2011, 2008a); van Waaij and van Zanten (2016). We are not aware of any error bounds in this area in terms of our settings, i.e., fixed designs, fill and separation distances.

Scattered data approximation In the field of scattered data approximation, the goal is to approximate or interpolate an underlying deterministic function. Examples include Wendland (2004); Wendland and Rieger (2005); Rieger and Zwicknagl (2009); Narcowich et al. (2006), which cover the noiseless case, and Wynne et al. (2021); Rieger and Zwicknagl (2009), which cover the case that the observations have noise. The misspecification case is considered in Narcowich et al. (2006); Wynne et al. (2021). Although the observations are corrupted by noise in Wynne et al. (2021); Rieger and Zwicknagl (2009) as we considered in the present work, the convergence rates are different. If one plugs in our settings into their bounds, it can be seen that the prediction error bound does not converge to zero. This is the price for the more general noise assumption in Wynne et al. (2021); Rieger and Zwicknagl (2009). We impose the sub-Gaussian assumption (see Condition (C5) in Section 3.2) and obtain a sharper error bound.

3. Preliminaries

In this section, we introduce problem settings and conditions.

3.1 Problem settings

Suppose that our observations (x_k, y_k) satisfy the following model

$$y_k = f(x_k) + \epsilon_k, k = 1, \dots, n, \quad (1)$$

where $x_k \in \Omega \subset \mathbb{R}^d$ and $\epsilon_k \stackrel{\text{i.i.d.}}{\sim} (0, \sigma_\epsilon^2)$, i.e., independent and identically distributed random noise with mean zero and variance σ_ϵ^2 . In Gaussian process regression, the underlying function f is assumed to be a realization of a Gaussian process Z . From this point of view, we shall not differentiate f and Z in Gaussian process regression. We assume Z is a zero-mean stationary Gaussian process, denoted by $Z \sim GP(0, \sigma^2\Psi)$, with $\text{Cov}(Z(x), Z(x')) = \sigma^2\Psi(x - x')$ for $x, x' \in \mathbb{R}^d$. Here σ^2 is the variance, and Ψ is the true but typically unknown correlation function which is stationary, positive definite and integrable on \mathbb{R}^d .

For a moment, assume ϵ_k 's are normal. Given the correlation function Ψ and conditional on $Y = (y_1, \dots, y_n)^T$, $Z(x)$ is normally distributed at an unobserved point x . The conditional expectation and variance of $Z(x)$ are given by

$$\mathbb{E}[Z(x)|Y] = r(x)^T(R + \mu I_n)^{-1}Y, \quad (2)$$

$$\text{Var}[Z(x)|Y] = \sigma^2(\Psi(x - x) - r(x)^T(R + \mu I_n)^{-1}r(x)), \quad (3)$$

where $r(x) = (\Psi(x - x_1), \dots, \Psi(x - x_n))^T$, $R = (\Psi(x_j - x_k))_{jk}$, I_n is an identity matrix, and $\mu = \sigma_\epsilon^2/\sigma^2$. The conditional expectation (2) is a natural predictor of $Z(x)$, and it can be shown that the conditional expectation is indeed the best linear predictor (Ankenman et al., 2010), in the sense that it has the minimal mean squared prediction error (MSPE), which equals $\text{Var}[Z(x)|Y]$.

In this work, we investigate what happens if another correlation function Φ , referred to as the *imposed correlation function*, is used in Gaussian process regression in place of the *true correlation function* Ψ . The resulting Gaussian process regression predictor after using Φ is

$$\hat{f}_G(x) = r_m(x)^T(R_m + \mu_m I_n)^{-1}Y, \quad x \in \Omega, \quad (4)$$

where $r_m(x) = (\Phi(x - x_1), \dots, \Phi(x - x_n))^T$ and $R_m = (\Phi(x_j - x_k))_{jk}$. We suppose μ_m is chosen according to our will and call it the *regularization parameter*. Clearly, \hat{f}_G in (4) is no longer the best linear unbiased predictor. In this work, we are interested in the L_2 prediction error using the imposed correlation function Φ , i.e.,

$$\|Z - \hat{f}_G\|_{L_2(\Omega)}. \quad (5)$$

Similar problem without the influence of noise has been considered in Tuo and Wang (2020). Other convergence results of Gaussian process regression with misspecified correlation functions can be found in Stein (1988, 1990a,b); Tuo and Wang (2020); Wang et al. (2020); Yakowitz and Szidarovszky (1985), where the observations are noiseless. However, the appearance of noise can significantly change the analysis of convergence when the underlying truth is a Gaussian process², as we will see later.

2. This is different with the settings in Wynne et al. (2021), who also consider the noisy observations case with fixed designs. In Wynne et al. (2021), the underlying truth is a deterministic function.

3.2 Notation and conditions

In the rest of this work, the following definitions are used. For two positive sequences a_n and b_n , we write $a_n \asymp b_n$ if, for some $C, C' > 0$, $C \leq a_n/b_n \leq C'$. Similarly, we write $a_n \gtrsim b_n$ if $a_n \geq Cb_n$ for some constant $C > 0$, and $a_n \lesssim b_n$ if $a_n \leq C'b_n$ for some constant $C' > 0$. Also, $C, C', c_j, C_j, j \geq 0$ are generic positive constants, of which value can change from line to line. We use $Q(s)$ to denote an increasing positive function satisfying

$$\lim_{s \rightarrow +\infty} \frac{\log Q(s)}{\log s} = 0 \quad (6)$$

and not depending on n , which may vary at each occurrence. The Euclidean metric is denoted by $\|\cdot\|_2$. The Fourier transform of $f \in L_1(\mathbb{R}^d)$ is given by

$$\mathcal{F}(f)(\omega) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} f(x) e^{-ix^T \omega} dx.$$

The following conditions will be assumed throughout the paper, unless otherwise specified.

(C1) The region of interest $\Omega \subset \mathbb{R}^d$ is a compact set with positive Lebesgue measure and Lipschitz boundary, and satisfies an interior cone condition, i.e., there exist $\alpha \in (0, \pi/2)$ and $\mathcal{R} > 0$ such that for every $x \in \Omega$, a unit vector $\xi(x)$ exists such that the cone $\mathcal{C}(x, \xi(x), \alpha, \mathcal{R}) := \{x + \lambda y : y \in \mathbb{R}^d, \|y\| = 1, y^T \xi(x) \geq \cos \alpha, \lambda \in [0, \mathcal{R}]\}$ is contained in Ω .

(C2) There exists $m_0 > d/2$ such that,

$$c_1(1 + \|\omega\|_2^2)^{-m_0} \leq \mathcal{F}(\Psi)(\omega) \leq c_2(1 + \|\omega\|_2^2)^{-m_0}, \forall \omega \in \mathbb{R}^d.$$

(C3) There exists $m > d/2$ such that,

$$c_3(1 + \|\omega\|_2^2)^{-m} \leq \mathcal{F}(\Phi)(\omega) \leq c_4(1 + \|\omega\|_2^2)^{-m}, \forall \omega \in \mathbb{R}^d.$$

(C4) Let $\mathcal{X} = \{X_1, X_2, \dots\}$ be a sequence of designs. Without loss of generality, assume that $\text{card}(X_n) = n$, where n takes its value in an infinite subset of \mathbb{N} , and $\text{card}(X)$ denote the cardinality of set X . We call \mathcal{X} a *sampling scheme*. The fill distance of X_n , defined by

$$h_{X_n, \Omega} = \sup_{x \in \Omega} \inf_{x_j \in X_n} \|x - x_j\|_2, \quad (7)$$

satisfies

$$h_{X_n, \Omega} \leq Cn^{-1/d}, \forall n \geq 1.$$

(C5) (Sub-Gaussian) Suppose ϵ_k 's in (1) are independent and identically distributed random variables satisfying

$$C^2(\mathbb{E}e^{|\epsilon_k|^2/C^2} - 1) \leq C', \quad k = 1, \dots, n.$$

Such random variables are called sub-Gaussian (van de Geer, 2000).

Condition (C1) is a geometric condition on the region Ω . We believe it holds in most practical situations, because the compactness and convexity imply the interior cone condition; see Hofmann et al. (2007); Niculescu and Persson (2006).

Conditions (C2) and (C3) imply that the Fourier transforms of the true correlation function and imposed correlation function have an algebraical decay. A prominent class of correlation functions that have an algebraical decay of their Fourier transforms is the (isotropic) Matérn correlation functions. The isotropic Matérn correlation functions (Stein, 1999) is defined by

$$\Psi_M(x; \phi, \nu) = \frac{1}{\Gamma(\nu)2^{\nu-1}}(2\sqrt{\nu}\phi\|x\|_2)^\nu K_\nu(2\sqrt{\nu}\phi\|x\|_2), \quad (8)$$

with the Fourier transform (Tuo and Wu, 2016)

$$\mathcal{F}(\Psi_M)(\omega; \nu, \phi) = 4^{\nu+\frac{d}{2}}\pi^{\frac{d}{2}}\frac{\Gamma(\nu+\frac{d}{2})}{\Gamma(\nu)}(\nu\phi^2)^\nu(4\nu\phi^2+\|\omega\|_2^2)^{-(\nu+\frac{d}{2})}, \quad (9)$$

where $\phi > 0$ is the scale parameter, and K_ν is the modified Bessel function of the second kind. The parameter ν is the smoothness parameter, which is associated with the smoothness of the kernel function Ψ_M .

Another example of correlation functions with algebraically decayed Fourier transforms is the generalized Wendland correlation function (Wendland, 2004; Gneiting, 2002; Chernih and Hubbert, 2014; Bevilacqua et al., 2019; Fasshauer and McCourt, 2015), defined as

$$\Psi_{GW}(x) = \begin{cases} \frac{1}{B(2\kappa, \eta+1)} \int_{\|\phi x\|}^1 u(u^2 - \|\phi x\|^2)^{\kappa-1} (1-u)^\eta du, & 0 \leq \|x\| < \frac{1}{\phi}, \\ 0, & \|x\| \geq \frac{1}{\phi}, \end{cases}$$

where $\phi, \kappa > 0$ and $\eta \geq (d+1)/2 + \kappa$, and B denotes the beta function. See Theorem 1 of Bevilacqua et al. (2019).

In this work, we consider fixed designs, where the design points x_1, \dots, x_n are fixed and can be chosen according to our will. Fixed designs are widely used in the field of computer experiments (Santner et al., 2003). Such designs include quasi-uniform designs (Borodachov et al., 2007; Utreras, 1988), maximin Latin hypercube designs (Van Dam et al., 2007), optimal Latin hypercube designs (Park, 1994), and grid points. Condition (C4) states that the fill distance of designs can be controlled at a certain rate. It can be seen that any quasi-uniform sampling scheme satisfies Condition (C4), as stated in the following example.

Definition 1 (Separation radius) For $X = \{x_1, \dots, x_n\}$, define the separation radius as

$$q_X = \min_{1 \leq j \neq k \leq n} \|x_j - x_k\|_2 / 2. \quad (10)$$

Example 1 (Quasi-uniform designs) It is easy to check that $h_{X, \Omega} \geq q_X$ (Wendland, 2004) for any set of points X . A sampling scheme $\mathcal{X} = \{X_1, X_2, \dots\}$ is called quasi-uniform if $h_{X_n, \Omega} / q_{X_n} \leq C$ for all n . For a quasi-uniform sampling scheme, $h_{X_n, \Omega} \asymp q_{X_n} \asymp n^{-1/d}$ (Müller, 2009).

Obviously, a sampling scheme satisfying Condition (C4) may not be quasi-uniform. For example, we can add a point which is very close to one design point of a quasi-uniform design such that the separation radius is close to zero, and $h_{X_n, \Omega}/q_{X_n} \leq C$ does not hold.

Remark 1 *Random samplings do not satisfy Condition (C4); see Example 1 of Tuo and Wang (2020).*

4. Rates of convergence for misspecified Gaussian process regression

In this section, we present our results on the convergence rate of the prediction error of misspecified Gaussian process regression (5).

We start with the easiest case. If the imposed correlation function is the same as the true correlation function, i.e., $\Phi = \Psi$ and $\mu_m = \sigma_\epsilon^2/\sigma^2$, then \hat{f}_G is the best linear predictor and achieves the minimal MSPE, which is $\text{Var}[Z(x)|Y]$; see Section 3.1. Obviously, the best linear predictor achieves the optimal convergence rate for a sampling scheme $\mathcal{X} = \{X_1, X_2, \dots\}$. It can be shown that if μ_m is any fixed positive constant and $\Phi = \Psi$, the optimal convergence rate can still be achieved.

Proposition 2 *Let $\hat{f}_G(x)$ be as in (4) with $\Phi = \Psi$ and $\mu_m = C$, where $C > 0$ is any fixed constant. For any fixed design $X = \{x_1, \dots, x_n\} \subset \Omega$,*

$$\mathbb{E}(\hat{f}_G(x) - Z(x))^2 \leq C_1 \sigma^2 (\Psi(x-x) - r(x)^T (R + \mu I_n)^{-1} r(x)) = C_1 \text{Var}[Z(x)|Y]$$

holds for all $x \in \Omega$, where R , $r(x)$ and μ are as in (2), and the constant C_1 only depends on C , σ_ϵ^2 and σ^2 .

The proof of Proposition 2 can be found in Appendix C. Because $\text{Var}[Z(x)|Y]$ is the minimal MSPE, $\mathbb{E}(\hat{f}_G(x) - Z(x))^2 \geq \text{Var}[Z(x)|Y]$. Proposition 2 shows that if the true correlation function is used, the regularization parameter can be changed to any fixed constant and would not influence the optimal convergence rate. However, Proposition 2 does not provide any assertion on the convergence rate.

In the following, we provide several error bounds of misspecified Gaussian process regression under noisy observations. Suppose that Ψ and Φ satisfy Condition (C2) and Condition (C3), respectively. If $m_0 < m < \infty$, we call this case *oversmoothed* case and call the corresponding imposed correlation function Φ *oversmoothed correlation function*. On the other hand, if $d/2 < m < m_0$, we call this case *undersmoothed* case and call the corresponding imposed correlation function Φ *undersmoothed correlation function*. If $m = m_0$, we call this case *well-specified* case.

We first provide an upper bound on the term $\Psi(x-x) - r(x)^T (R + \mu_1 I_n)^{-1} r(x)$ in the following proposition, which is closely related to the conditional variance in (3). The proof of Proposition 3 is provided in Appendix D. Proposition 3 plays a key role in the proofs of Theorems 6 and 8.

Proposition 3 *Suppose Conditions (C1)-(C4) hold. Then we have for any positive constant $\mu_1 \gtrsim n^{1-2m_0/d}$,*

$$\Psi(x-x) - r(x)^T (R + \mu_1 I_n)^{-1} r(x) \lesssim (\mu_1/n)^{1-\frac{d}{2m_0}}, \quad (11)$$

where $r(x)$ and R are as in (2).

Remark 4 *Proposition 3 is a deterministic version of Lemma F.8 in Wang (2020). In Proposition 3, the design points are fixed, while in Lemma F.8 of Wang (2020), the design points are uniformly distributed on Ω .*

Remark 5 *Note that when the observations are noisy, the convergence rate of the conditional variance (3) can be directly obtained by setting $\mu_1 = \mu$, where μ is as in (2). This result is different with the existing results in scattered data approximation (Wendland, 2004; Wu and Schaback, 1993), where the observations have no noise.*

We start with the oversmoothed case. In the following theorem, we assume that both the true correlation function Ψ and the imposed correlation function Φ are Matérn correlation functions as in (8). Recall that $h_{X,\Omega}$ and q_X are the fill distance and separation radius for a design X as defined in (7) and (10), respectively. The proof of Theorem 6 is in Appendix E.

Theorem 6 (Oversmoothed Matérn correlation function) *Let Ψ and Φ be two Matérn correlation functions as in (8). Suppose Conditions (C1)-(C5) hold. Suppose $m_0 \leq m < \infty$ and $\mu_m \gtrsim n^{1-\frac{2m}{d}}$. Then, for any $t_1, t_2 \geq C_0$ and all n , with probability at least $1 - \exp(-t_1^2) - \exp(-t_2^2)$, we have*

$$\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \leq C \left((1+t_1)^2 T + t_2^2 \mu_m^{-\frac{d}{2m}} n^{-(1-\frac{d}{2m})} \right),$$

where $T = \mu_m^{-\frac{m-m_0}{m}} q_{X_n}^{-\frac{(m-m_0)d}{m}} (\mu_m/n)^{1-\frac{d}{2m}} + \mu_m^{\frac{2m_0-d}{2m}} q_{X_n}^{\frac{(2m_0-d)d}{2m}}$, and the constants C, C_0 do not depend on n, t_1 and t_2 .

The following corollary states that, if a sampling scheme is quasi-uniform, then Gaussian process regression with an oversmoothed Matérn correlation function can still lead to the error bound $O_{\mathbb{P}}(n^{-\frac{2m_0-d}{2m_0}})$. Recall that a sampling scheme $\mathcal{X} = \{X_1, X_2, \dots\}$ is said to be quasi-uniform if $h_{X_n, \Omega}/q_{X_n} \leq C$ for all n (see Example 1). Corollary 7 is a direct result of Theorem 6 and the proof is omitted.

Corollary 7 (Oversmoothed Matérn correlation function and quasi-uniform design) *Let Ψ and Φ be two Matérn correlation functions as in (8). Suppose Conditions (C1)-(C3)*

and (C5) hold. Suppose $m_0 \leq m < \infty$ and the sampling scheme \mathcal{X} is quasi-uniform. Let $\mu_m \asymp n^{-m/m_0+1}$. Then, for all $t \geq C_0$ and n , with probability at least $1 - \exp(-t)$, we have

$$\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \leq C(1+t)n^{-\frac{2m_0-d}{2m_0}},$$

where C_0 and C are constants not depending on n and t . In particular, we have

$$\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 = O_{\mathbb{P}}\left(n^{-\frac{2m_0-d}{2m_0}}\right).$$

Now we consider Gaussian process regression with undersmoothed correlation functions. The following theorem indicates that the convergence rate is slower than that of Gaussian process regression with oversmoothed correlation functions, whose proof is provided in Appendix F. Note that in Theorem 8, the true and imposed correlation functions are not necessarily Matérn correlation functions.

Theorem 8 (Undersmoothed correlation function) *Suppose Conditions (C1)-(C5) hold. Suppose $d/2 < m \leq m_0$ and $\mu_m \gtrsim n^{1-\frac{2m}{d}}$. Then, for any $t_1, t_2 \geq C_0$ and n , with probability at least $1 - \exp(-t_1^2) - \exp(-t_2^2)$, we have*

$$\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \lesssim t_1^2 \mu_m^{-\frac{d}{2m}} n^{-(1-\frac{d}{2m})} + (1+t_2)^2 (\mu_m/n)^{1-\frac{d}{2m}}.$$

In particular, if μ_m is a fixed constant, $\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 = O_{\mathbb{P}}\left(n^{-\frac{2m-d}{2m}}\right)$.

The following corollary provides error bounds in the well-specified case. Corollary 9 is a direct result of Theorem 8, and the proof is omitted.

Corollary 9 (Well-specified correlation function) *Suppose Conditions (C1)-(C5) hold. Furthermore, suppose $m = m_0$ and $\mu_m \asymp 1$. Then, for all $t \geq C_0$ and n , with probability at least $1 - \exp(-t)$, we have*

$$\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \leq C(1+t)n^{-\frac{2m_0-d}{2m_0}},$$

where C_0 and C are constants not depending on n and t . In particular, $\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 = O_{\mathbb{P}}\left(n^{-\frac{2m_0-d}{2m_0}}\right)$.

Theorem 10 provides a lower error bound of Gaussian process regression, whose proof is presented in Appendix G.

Theorem 10 (Lower error bounds of Gaussian process regression) *Suppose Conditions (C1)-(C5) hold. Assume $m_0 > d$ and Assumption G.0.1 holds. Then we have*

$$\mathbb{E}\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \gtrsim n^{-\frac{2m_0-d}{2m_0}}.$$

Remark 11 *Theorem 10 requires a technical assumption Assumption G.0.1 in Appendix G, which essentially requires that there exists a correlation function K with uniformly bounded eigenfunctions such that $\mathcal{F}(K)/\mathcal{F}(\Psi)$ is uniformly bounded. This assumption is slightly weaker than the assumption that Ψ has uniformly bounded eigenfunctions. The later assumption is typical in nonparametric regression literature. See Mendelson et al. (2010); Steinwart et al. (2009) for example. Unfortunately, to the best of our knowledge, whether Assumption G.0.1 holds for Matérn correlation functions is not present in literature.*

Remark 12 *Note that the convergence rate in Theorem 10 is different with the minimax convergence rate in nonparameteric regression, where the underlying truth is a deterministic function. Besides the different settings, another difference is that the minimax convergence rate is considered in the worst case for a given function class, while Theorem 10 can be treated as in an average case. We also note that Tuo and Wang (2020) provide lower error bounds of Gaussian process regression in the noiseless case.*

Combining Theorem 10 and Corollary 7, it can be seen that Gaussian process regression with an oversmoothed Matérn correlation function achieves the optimal convergence rate, if the sampling scheme is quasi-uniform, and the optimal convergence rate for Gaussian process regression is $O_{\mathbb{P}}(n^{-\frac{2m_0-d}{2m_0}})$. Corollary 9 states that the optimal convergence rate can also be achieved if the Gaussian process regression with the true correlation function is used, which is intuitively true.

Theorem 8 provides an upper bound on the L_2 prediction error of Gaussian process regression with an undersmoothed correlation function. The upper bound is larger than that of the Gaussian process regression with the true correlation function. Note that in Tuo and Wang (2020) and Wang et al. (2020), if the observations have no noise, it has been shown that using an oversmoothed Matérn correlation function and a quasi-uniform sampling scheme can achieve the optimal convergence rate, while using an undersmoothed correlation function leads to an upper bound that has a slower convergence rate. Combining their results and ours, we can conclude that if the sampling scheme is quasi-uniform, using oversmoothed correlation functions is not detrimental to the convergence rate, no matter the observations are corrupted by noise or not. Nevertheless, we still recommend practitioners to try to find the correlation function with smoothness closed to the true smoothness. This is because the constant in the convergence rate can be large if the imposed smoothness is too far away from the true smoothness. Moreover, our results suggest that it is important to choose good designs in practice.

5. Relationship of the convergence rates between Gaussian process regression and kernel ridge regression

In this section, we discuss the relationship between the convergence rates of Gaussian process regression and kernel ridge regression. For the conciseness of this paper, we move the introduction to reproducing kernel Hilbert spaces, Sobolev spaces, and kernel ridge regression to Appendix A.

5.1 Rates of convergence for misspecified kernel ridge regression

5.1.1 SMOOTHNESS OF A DETERMINISTIC FUNCTION

We say that a deterministic function $g \in L_2(\mathbb{R}^d)$ has a finite degree of smoothness if the quantity

$$m_0(g) := \sup\{k \geq 0 : g \in H^k(\mathbb{R}^d)\} \quad (12)$$

is finite, where $H^k(\mathbb{R}^d)$ is the Sobolev space with smoothness k . Here k can be a non-integer, and the corresponding Sobolev space is called the *fractional Sobolev space*. We call the quantity (12) the smoothness of g . The functions considered in this work are assumed to have smoothness greater than $d/2$, which implies such function are continuous. Since Ω is compact and has a Lipschitz boundary, there exists an extension operator from $L_2(\Omega)$ to $L_2(\mathbb{R}^d)$, such that the smoothness of each function is maintained (DeVore and Sharpley, 1993; Rychkov, 1999). We define the smoothness of a function $g \in L_2(\Omega)$ by the smoothness of the extended function $g_e \in L_2(\mathbb{R}^d)$ using (12).

From (12), it can be seen that a function g with smoothness $m_0(g)$ can be divided into two scenarios: 1) $g \in H^{m_0(g)}(\Omega)$ but $g \notin H^m(\Omega)$ for any $m > m_0(g)$; 2) $g \in H^m(\Omega)$ for any $m < m_0(g)$ but $g \notin H^{m_0(g)}(\Omega)$. As a simple example, by (9), it can be checked that Matérn correlation functions fall into the second scenario. To the best of our knowledge, the existing results on the kernel ridge regression only investigate the functions in the first scenario.

The following lemma provides a characterization of function g that has smoothness $m_0(g)$ but is not in the Sobolev space $H^{m_0(g)}(\mathbb{R}^d)$.

Lemma 13 *Let $m_0(g) \in (d/2, +\infty)$ be the smoothness of g . If $g \notin H^{m_0(g)}(\mathbb{R}^d)$, there exists an increasing positive function $Q : \mathbb{R}_+ \mapsto \mathbb{R}_+$ satisfying (6) such that*

$$\begin{aligned} \int_{\mathbb{R}^d} \frac{|\mathcal{F}(g)(\omega)|^2}{Q(\|\omega\|)} (1 + \|\omega\|^2)^{m_0(g)} d\omega &\leq 1, \\ \int_{\mathbb{R}^d} \frac{|\mathcal{F}(g)(\omega)|^2}{Q(\|\omega\|)} (1 + \|\omega\|^2)^{m_0(g)+\delta} d\omega &= \infty, \forall \delta > 0. \end{aligned}$$

Note that (6) implies $Q(s)$ increases slower than any s^δ with any $\delta > 0$. The proof of Lemma 13 can be found in Appendix H. We use the following example to illustrate the intuition behind Lemma 13.

Example 2 *Consider the triangle function*

$$f(x) = \begin{cases} 1 - |x|, & |x| \leq 1, \\ 0, & |x| > 1. \end{cases}$$

It can be checked that f has smoothness $3/2$ but $f \notin H^{3/2}(\mathbb{R})$. One can choose $Q(t) := C \log^2(1+t)$ defined on \mathbb{R}_+ with C an appropriate constant such that

$$\int_{\mathbb{R}} \frac{|\mathcal{F}(f)(\omega)|^2}{Q(|\omega|)} (1+|\omega|^2)^{3/2} d\omega \leq 1,$$

$$\int_{\mathbb{R}} \frac{|\mathcal{F}(f)(\omega)|^2}{Q(|\omega|)} (1+|\omega|^2)^{3/2+\delta} d\omega = \infty, \forall \delta > 0.$$

For the proof of the above statements, see Appendix M.

5.1.2 MAIN RESULTS FOR MISSPECIFIED KERNEL RIDGE REGRESSION

Let f be a deterministic function with smoothness $m_0(f)$. The corresponding function space of interest is the Sobolev space $H^{m_0(f)}(\Omega)$, because by the definition of smoothness, $m_0(f) = \sup\{k > d/2 : f \in H^k(\Omega)\}$. Theorem 10.45 of Wendland (2004) suggests that if the kernel function Ψ satisfies Condition (C2) with $m_0 = m_0(f)$, $\mathcal{N}_\Psi(\Omega)$ coincides with the Sobolev space $H^{m_0(f)}(\Omega)$, where $\mathcal{N}_\Psi(\Omega)$ is the reproducing kernel Hilbert space generated by Ψ . Suppose a kernel ridge regression with reproducing kernel Hilbert space $\mathcal{N}_\Phi(\Omega)$ is used to recover the function f . Furthermore, assume Φ satisfies Condition (C3), which implies that the corresponding reproducing kernel Hilbert space $\mathcal{N}_\Phi(\Omega)$ coincides with the Sobolev space $H^m(\Omega)$. We call Φ the *imposed kernel function*, and Ψ the *true kernel function*.

Remark 14 For any constant $c > 0$, it can be seen that $\mathcal{N}_\Psi(\Omega)$ coincides with $\mathcal{N}_{c\Psi}(\Omega)$, and two norms are equivalent. Therefore, we pick any fixed kernel function Ψ satisfying Condition (C2) with $m_0 = m_0(f)$ and call it the *true kernel function*. Any other kernel function is called *imposed kernel function* if it is used in the kernel ridge regression.

With a slight abuse of terminology, we refer to the kernel ridge regression with reproducing kernel Hilbert space $\mathcal{N}_\Phi(\Omega)$ as the misspecified kernel ridge regression. The misspecified kernel ridge regression can be written as

$$\hat{f}_m = \operatorname{argmin}_{\hat{f} \in \mathcal{N}_\Phi(\Omega)} \left(\frac{1}{n} \sum_{k=1}^n (y_k - \hat{f}(x_k))^2 + \lambda_m \|\hat{f}\|_{\mathcal{N}_\Phi(\Omega)}^2 \right), \quad (13)$$

where $\lambda_m > 0$ is a regularization parameter. Note that if $\lambda_m = \mu_m/n$, where μ_m is as in (4), the representer theorem implies that \hat{f}_m has the same form as \hat{f}_G in (4).

There are two cases, according to the smoothness m of the reproducing kernel Hilbert space $\mathcal{N}_\Phi(\Omega)$, or equivalently, the smoothness of the Sobolev space $H^m(\Omega)$. If $m_0(f) \leq m < \infty$, the corresponding Sobolev space $H^m(\Omega) \subset H^{m_0(f)}(\Omega)$. With a slight abuse of terminology, we call this case *oversmoothed* case and call the corresponding kernel function Φ *oversmoothed kernel function*, even if m may equal to $m_0(f)$. On the other hand, if $d/2 < m < m_0(f)$, we call this case *undersmoothed* case and call Φ *undersmoothed kernel function*.

In this work, we are interested in the convergence rate of the L_2 prediction error $\|f - \hat{f}_m\|_{L_2(\Omega)}$. The following theorem states that, using an oversmoothed kernel function can still lead to the optimal convergence rate, if the regularization parameter is appropriately chosen. The proof of Theorem 15 is presented in Appendix I.

Theorem 15 (Kernel ridge regression with oversmoothed kernel function) *Suppose f has smoothness $m_0(f)$. Suppose Conditions (C1)-(C5) hold and $m_0(f) \leq m < \infty$. If $\lambda_m \asymp n^{-\frac{2m}{2m_0(f)+d}}$, the following statements are true for all n .*

1. *If $f \in H^{m_0(f)}(\Omega)$, then*

$$\|f - \hat{f}_m\|_{L_2(\Omega)} = O_{\mathbb{P}}(n^{-\frac{m_0(f)}{2m_0(f)+d}}), \|\hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)} = O_{\mathbb{P}}(n^{\frac{m-m_0(f)}{2m_0(f)+d}}).$$

2. *If $f \notin H^{m_0(f)}(\Omega)$, then*

$$\|f - \hat{f}_m\|_{L_2(\Omega)} = O_{\mathbb{P}}(n^{-\frac{m_0(f)}{2m_0(f)+d}}Q(n)), \|\hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)} = O_{\mathbb{P}}(n^{\frac{m-m_0(f)}{2m_0(f)+d}}Q(n)).$$

The next theorem states the convergence rate of upper error bounds in the undersmoothed case, whose proof is provided in Appendix J.

Theorem 16 (Kernel ridge regression with undersmoothed kernel function) *Suppose f has smoothness $m_0(f)$. Suppose Conditions (C1)-(C5) hold and $d/2 < m < m_0(f)$. If $\lambda_m \asymp n^{-\frac{2m}{2m_0(f)+d}}$, the following statements are true for all n .*

1. *If $m_0(f)/2 \leq m < m_0(f)$, then we have:*

$$\|f - \hat{f}_m\|_{L_2(\Omega)} = \begin{cases} O_{\mathbb{P}}(n^{-\frac{m_0(f)}{2m_0(f)+d}}), & \text{if } f \in H^{m_0(f)}(\Omega), \\ O_{\mathbb{P}}(n^{-\frac{m_0(f)}{2m_0(f)+d}}Q(n)), & \text{if } f \notin H^{m_0(f)}(\Omega). \end{cases}$$

2. *If $d/2 < m < m_0(f)/2$, then we have:*

$$\|f - \hat{f}_m\|_{L_2(\Omega)} = O_{\mathbb{P}}(n^{-\frac{2m}{4m+d}}).$$

From Theorems 15 and 16, we can see that the misspecified kernel ridge regression can still achieve the optimal convergence rate, as long as the imposed kernel function satisfies Condition (C3) with $m \geq m_0(f)/2$. These results generalize the results in Tuo et al. (2020), where the imposed kernel function satisfies $m = m_0(f)/2$. Furthermore, this work establishes the convergence results under the case that $f \notin H^{m_0(f)}(\Omega)$ but has smoothness $m_0(f)$.

5.2 Relationship of the convergence rates of kernel ridge regression and Gaussian process regression

Although kernel ridge regression and Gaussian process regression have different model assumptions, and we have applied completely different approaches to obtain the convergence rates of error bounds, there is an intimate relationship between the constructed convergence rates. This relationship, notably, is aligned with the relationship between the reproducing kernel Hilbert space and Gaussian process, as we will explain in this section. For the ease of mathematical treatment, we assume that the sampling scheme is quasi-uniform. We use Ψ_K , Φ_K , Ψ_G , and Φ_G to denote the true kernel function, the imposed kernel function, the true correlation function, and the imposed correlation function, respectively.

We first link the prediction error of kernel ridge regression and that of Gaussian process regression, as shown in the following proposition. The proof is presented in Appendix K.

Proposition 17 *Suppose $f \in \mathcal{N}_{\Psi_K}(\Omega)$ is a deterministic function, and $Z \sim GP(0, \Psi_G)$ is a Gaussian process. Suppose Ψ_K and Φ_K are stationary, positive definite and integrable on \mathbb{R}^d , $\Psi_G = \Psi_K$, $\Phi_G = \Phi_K$ and $\lambda_m = \mu_m/n$. Then*

$$\mathbb{E}(f(x) - \hat{f}_m(x))^2 \leq C\mathbb{E}(Z(x) - \hat{f}_G(x))^2, \forall x \in \Omega,$$

where \hat{f}_m and \hat{f}_G are as in (13) and (4), respectively, and $C = \max(1, \|f\|_{\mathcal{N}_{\Psi}}^2)$.

Proposition 17 states that the MSPE of kernel ridge regression $\mathbb{E}(f(x) - \hat{f}_m(x))^2$ on any point x can be bounded by the MSPE of Gaussian process regression $\mathbb{E}(Z(x) - \hat{f}_G(x))^2$, when the correlation functions are the same as the kernel functions, and $\lambda_m = \mu_m/n$. However, Proposition 17 does not provide the optimal convergence rate of the MSPE $\mathbb{E}(f(x) - \hat{f}_m(x))^2$. To see this, let $\Psi_K = \Psi_G = \Phi_K = \Phi_G$. Furthermore, assume Ψ_K satisfies Condition (C2). The optimal convergence rate in kernel ridge regression is achieved if $\lambda_m \asymp n^{-\frac{2m_0}{2m_0+d}}$. However, Proposition 2 suggests that the optimal convergence rate of $\|Z - \hat{f}_G\|_{L_2(\Omega)}$ is achieved if μ_m is a fixed constant, and μ_m does not have the same order of magnitude as $n\lambda_m$. On the other hand, if we set $\lambda_m \asymp 1/n$, Theorem 4.1 of Wang (2020) implies that the optimal convergence rate in kernel ridge regression cannot be achieved. In other words, if we use Gaussian process regression with correlation function $\Psi_G = \Psi_K$ and a constant regularization parameter to make prediction on a deterministic function in $\mathcal{N}_{\Psi_K}(\Omega)$, the optimal convergence rate cannot be achieved. The difference between the convergence rates of $\mathbb{E}(f(x) - \hat{f}_m(x))^2$ and $\mathbb{E}(Z(x) - \hat{f}_G(x))^2$ can be interpreted by the difference of the support of a Gaussian process and the corresponding reproducing kernel Hilbert space, where the former is typically larger than the later (van der Vaart and van Zanten, 2008b).

In our results of Gaussian process regression, the smoothness m_0 showing in Condition (C2) for a stationary Gaussian process Z should be interpreted as the mean squared differentiability (Stein, 1999) of the Gaussian process, which is determined by the smoothness of the correlation function Ψ_G . This is different with the smoothness of deterministic functions. Nonetheless, we can consider the smoothness of sample paths of Z , under the usual definition of smoothness for deterministic functions, which reveals an interesting connection between convergence rates of kernel ridge regression and Gaussian process regression.

If $Z \sim GP(0, \Psi_G)$ is a stationary Gaussian process with correlation function Ψ_G satisfying Condition (C2), it can be shown that the sample path smoothness is lower than m_0 with probability one (Driscoll, 1973; Kanagawa et al., 2018; Steinwart, 2019). The difference between the support of a Gaussian process and the corresponding reproducing kernel Hilbert space has been sharply characterized by Steinwart (2019). Specifically, Steinwart (2019) shows that the sample paths of Gaussian process Z lie in Sobolev space $H^\alpha(\Omega)$ with $\alpha \in (d/2, m_0 - d/2)$ with probability one, and do not lie in the Sobolev space $H^{m_0 - d/2}(\Omega)$ with a strictly positive probability. This implies that the sample paths of Gaussian process Z have smoothness $m_0 - d/2$ with a strictly positive probability. Consider a deterministic function f with smoothness $m_0(f) = m_0 - d/2$ but not lying in $H^{m_0 - d/2}(\Omega)$. Theorem 15 suggests that if an oversmoothed kernel function with smoothness m is used and $\lambda_m \asymp n^{-\frac{2m}{2m_0(f)+d}} = n^{-\frac{m}{m_0}}$, then the convergence rate is $n^{-\frac{m_0(f)}{2m_0(f)+d}} = n^{-\frac{m_0 - d/2}{2m_0}}$, up to a difference of $Q(n)$ with $Q(n) = o(n^\delta)$ for any $\delta > 0$. This convergence rate coincides with the optimal convergence rate of Gaussian process regression, and the choice of the regularization parameter has the same order of magnitude as $n\lambda_m$, i.e., $\mu_m \asymp n^{1 - \frac{m}{m_0}} \asymp n\lambda_m$. If we choose the optimal order of magnitude of $\lambda_m = Cn^{-\frac{m}{m_0}}$ for any fixed positive constant C and $\mu_m = n\lambda_m$, the predictors of Gaussian process regression and kernel ridge regression are identical (Kimeldorf and Wahba, 1970), and both achieve the optimal convergence rate. In other words, we can regard Gaussian process regression as kernel ridge regression with an oversmoothed kernel function, from the prediction perspective, and the optimal convergence rates are almost the same, up to a small order of n^δ with any $\delta > 0$.

Remark 18 *Kanagawa et al. (2018, Section 5.1) also discuss relationship between Gaussian process regression and kernel ridge regression. The relationship of the convergence rate of kernel ridge regression and the rate of posterior contraction of Gaussian process priors is established. Note that the Gaussian process regression model and the convergence rate (Kanagawa et al., 2018, Theorem 5.1) is based on the posterior contraction of Gaussian process priors in van der Vaart and van Zanten (2011), where the underlying truth is still a deterministic function. We consider “the underlying truth in Gaussian process regression is a Gaussian process” and “the underlying truth in kernel ridge regression is a deterministic function”. This differentiates our discussion with that in Kanagawa et al. (2018).*

6. Numerical experiments

In this section, we conduct numerical experiments to study whether the convergence rates given by Theorems 6 and 8 are accurate. We consider the region of interest $\Omega = [0, 1]$. It has been shown in Theorems 6 and 8 that, if $m_0 \leq m$, taking $\mu \asymp n^{-m/m_0+1}$ leads to the error bound $O_{\mathbb{P}}(n^{-\frac{2m_0-d}{2m_0}})$; on the other hand, if $m_0 > m$, taking $\mu \asymp 1$ yields the error bound $O_{\mathbb{P}}(n^{-\frac{2m-d}{2m}})$.

Let $\mathcal{E} = \mathbb{E}\|Z - \hat{f}_G\|_{L_2(\Omega)}^2$. We consider grid designs, such that the fill distance has the same order of magnitude of the separation distance. If the convergence rates of \mathcal{E} are sharp, then

we have the approximation

$$\begin{aligned} \log \mathcal{E} &\approx \frac{2m_0 - d}{2m_0} \log(1/n) + \log c_1, \text{ if } m_0 \leq m, \\ \log \mathcal{E} &\approx \frac{2m - d}{2m} \log(1/n) + \log c_2, \text{ if } m_0 > m, \end{aligned} \tag{14}$$

where c_1 and c_2 are constants. Therefore, in the numerical experiments, we regress $\log \mathcal{E}$ on $\log(1/n)$ and check whether the estimated slope is close to the theoretical assertion $\frac{2m_0-d}{2m_0}$ and $\frac{2m-d}{2m}$, when $m_0 \leq m$ and $m_0 > m$, respectively.

We consider the sample sizes $n = 10k$, for $k = 2, 3, \dots, 15$. For each k , we simulate 100 realizations of a Gaussian process, where the correlation function is a Matérn correlation function given by (8). We take $\mu = 0.1 \times n^{-m/m_0+1}$ when $m_0 \leq m$, and take $\mu = 0.1$ when $m_0 > m$. The noise is set to be normal with mean zero and variance 0.25. For i -th realization of a Gaussian process, we generate $10k$ grid points as X , and use $\mathcal{E}_i = \frac{1}{200} \sum_{j=1}^{200} (Z(x_j) - \hat{f}_G(x_j))^2$ to approximate $\|Z - \hat{f}_G\|_{L_2(\Omega)}^2$, where x_j 's are the first 200 points of the Halton sequence (Niederreiter, 1992). This should provide a good approximation since the points are dense enough. The expectation \mathcal{E} is approximated by $\frac{1}{100} \sum_{i=1}^{100} \mathcal{E}_i$.

The results are presented in Table 2. The first two columns of Table 2 show the true and imposed smoothness. We consider three scenarios: oversmoothed case (row 1 and row 2), well-specified case (row 3), and undersmoothed case (row 4). The third and the fourth columns show the convergence rates obtained from the numerical experiments and the theoretical analysis, respectively. The fifth column shows the difference between the fourth and the fifth columns, and the last column gives the R -squared values of the linear regression of the simulated data.

m_0	m	Estimated slope	Theoretical slope	Difference	R^2
1.6	3.3	0.7138	0.6875	0.0263	0.9846
2.0	3.0	0.7664	0.7500	0.0164	0.9810
2.0	2.0	0.7691	0.7500	0.0191	0.9817
3.0	2.0	0.7856	0.7500	0.0356	0.9787

Table 2: Numerical studies on the convergence rates of $\mathbb{E}\|Z - \hat{f}_G\|_{L_2(\Omega)}^2$.

From Table 2, it can be seen that the estimated slopes are close to our theoretical assertions for these cases. Figure 2 shows the scattered points and the regression lines under the four combinations of (m_0, m) in Table 2. From the R -squared values and Figure 2, we can see that the regression lines fit the scattered points well.

7. Conclusions and discussion

In this work, we provide some upper and lower error bounds for Gaussian process regression under misspecified correlation functions, when the observations are corrupted by noise. We show that the optimal convergence rate of Gaussian process regression can be achieved by us-

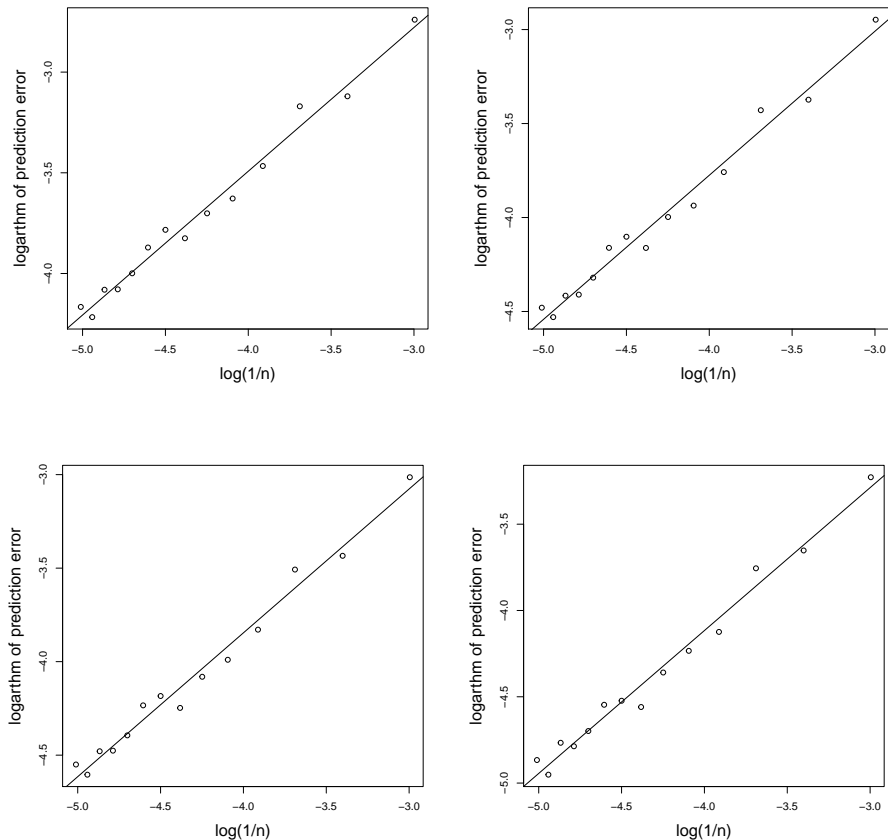


Figure 2: The regression line of $\log \mathcal{E}$ on $\log(1/n)$, under the four combinations of (m_0, m) in Table 2. Each point denotes one average prediction error for each n .

ing an oversmoothed Matérn correlation function and a quasi-uniform sampling scheme. We also show that if the underlying truth is a deterministic function, the optimal convergence rate can still be achieved by kernel ridge regression if the kernel function is oversmoothed or not “too undersmoothed”. Despite the difference of model assumptions and approaches in the proofs, we find an interesting connection between the constructed convergence rates of Gaussian process regression and kernel ridge regression. This connection is aligned with the connection between Gaussian process and reproducing kernel Hilbert space. The finding of the connection could serve as a bridge between Bayesian learning and frequentist learning, and may inspire new advances in these two seemingly separate fields.

There are several remaining problems. First, when the underlying truth is a Gaussian process, we consider fixed designs, which are also considered in Tuo and Wang (2020); Wang et al. (2020); Tuo et al. (2020). Whether the results hold for random sampling needs further study. Second, in addition to prediction, uncertainty quantification plays an important role in statistics. Since Gaussian process regression imposes a probabilistic structure on the underlying truth, it naturally induces an uncertainty quantification methodology via

confidence interval. Uncertainty quantification under misspecification will be pursued in the future.

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Appendix A. Reproducing kernel Hilbert space, Sobolev space and kernel ridge regression

Reproducing kernel Hilbert space plays an important role in the study of kernel ridge regression and Gaussian process regression. Suppose $\Omega \subset \mathbb{R}^d$ satisfies Condition (C1). Assume that $K : \Omega \times \Omega \rightarrow \mathbb{R}$ is a symmetric positive definite kernel function. Define the linear space

$$F_K(\Omega) = \left\{ \sum_{k=1}^n \beta_k K(\cdot, x_k) : \beta_k \in \mathbb{R}, x_k \in \Omega, n \in \mathbb{N} \right\}, \quad (15)$$

and equip this space with the bilinear form

$$\left\langle \sum_{k=1}^n \beta_k K(\cdot, x_k), \sum_{j=1}^m \gamma_j K(\cdot, x'_j) \right\rangle_K := \sum_{k=1}^n \sum_{j=1}^m \beta_k \gamma_j K(x_k, x'_j).$$

Then the *reproducing kernel Hilbert space* $\mathcal{N}_K(\Omega)$ generated by the kernel function K is defined as the closure of $F_K(\Omega)$ under the inner product $\langle \cdot, \cdot \rangle_K$, and the norm of $\mathcal{N}_K(\Omega)$ is $\|f\|_{\mathcal{N}_K(\Omega)} = \sqrt{\langle f, f \rangle_{\mathcal{N}_K(\Omega)}}$, where $\langle \cdot, \cdot \rangle_{\mathcal{N}_K(\Omega)}$ is induced by $\langle \cdot, \cdot \rangle_K$. The following theorem gives another characterization of the reproducing kernel Hilbert space when K is defined by a stationary kernel function Ψ , via the Fourier transform. Note that a kernel function Ψ is said to be stationary if the value $\Psi(x, x')$ only depends on the difference $x - x'$. Thus, we can write $\Psi(x - x') := \Psi(x, x')$.

Theorem 19 (Theorem 10.12 of Wendland (2004)) *Let Ψ be a positive definite kernel function which is stationary, continuous and integrable in \mathbb{R}^d . Define*

$$\mathcal{G} := \{f \in L_2(\mathbb{R}^d) \cap C(\mathbb{R}^d) : \mathcal{F}(f)/\sqrt{\mathcal{F}(\Psi)} \in L_2(\mathbb{R}^d)\},$$

with the inner product

$$\langle f, g \rangle_{\mathcal{N}_\Psi(\mathbb{R}^d)} = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \frac{\mathcal{F}(f)(\omega) \overline{\mathcal{F}(g)(\omega)}}{\mathcal{F}(\Psi)(\omega)} d\omega.$$

Then $\mathcal{G} = \mathcal{N}_\Psi(\mathbb{R}^d)$, and both inner products coincide.

For an integer k , the Sobolev norm for function g on \mathbb{R}^d is defined by

$$\|g\|_{H^k(\mathbb{R}^d)}^2 = \int_{\mathbb{R}^d} |\mathcal{F}(g)(\omega)|^2 (1 + \|\omega\|_2^2)^k d\omega,$$

and the inner product of a Sobolev space $H^k(\mathbb{R}^d)$ is defined by

$$\langle f, g \rangle_{H^k(\mathbb{R}^d)} = \int_{\mathbb{R}^d} \mathcal{F}(f)(\omega) \overline{\mathcal{F}(g)(\omega)} (1 + \|\omega\|_2^2)^k d\omega.$$

This definition can be naturally extended to Sobolev spaces with non-integer orders, which are commonly known as the *fractional Sobolev spaces*, denoted by $H^m(\mathbb{R}^d)$ with a non-integer m .

Remark 20 *In this work, we are only interested in Sobolev spaces with $m > d/2$ because these spaces contain only continuous function according to the Sobolev embedding theorem.*

A Sobolev space can also be defined on $\Omega \subset \mathbb{R}^d$, denoted by $H^m(\Omega)$, with norm

$$\|f\|_{H^m(\Omega)} = \inf\{\|f_e\|_{H^m(\mathbb{R}^d)} : f_e \in H^m(\mathbb{R}^d), f_e|_{\Omega} = f\},$$

where $f_e|_{\Omega}$ denotes the restriction of f_e to Ω . It can be shown that $H^{m_0}(\mathbb{R}^d)$ coincides with the reproducing kernel Hilbert space $\mathcal{N}_{\Psi}(\mathbb{R}^d)$ with equivalent norms, if Ψ satisfies Condition (C2) (Wendland (2004), Corollary 10.13). By the extension theorem (DeVore and Sharpley, 1993), $\mathcal{N}_{\Psi}(\Omega)$ also coincides with $H^{m_0}(\Omega)$, and two norms are equivalent.

Given the observations (x_k, y_k) with relationship (1), the kernel ridge regression reconstructs a function $f \in \mathcal{N}_{\Psi}(\Omega)$ by using

$$\hat{f} = \operatorname{argmin}_{g \in \mathcal{N}_{\Psi}(\Omega)} \left(\frac{1}{n} \sum_{k=1}^n (y_k - g(x_k))^2 + \lambda \|g\|_{\mathcal{N}_{\Psi}(\Omega)}^2 \right), \quad (16)$$

where λ is a prespecified regularization parameter. Under certain conditions and if Ψ satisfies Condition (C2), the optimal order of magnitude of λ is known in the literature (van de Geer, 2000), given by $\lambda = C n^{-\frac{2m_0}{2m_0+d}}$, where C can be any fixed positive constant. The optimal choice of λ leads to the optimal convergence rate under L_2 metric, which is $n^{-\frac{m_0}{2m_0+d}}$ (Stone, 1982).

Appendix B. Notation

We use $\langle \cdot, \cdot \rangle_n$ to denote the empirical inner product, which is defined by

$$\langle f, g \rangle_n = \frac{1}{n} \sum_{k=1}^n f(x_k)g(x_k)$$

for two functions f and g , and let $\|g\|_n^2 = \langle g, g \rangle_n$ be the empirical norm of function g . In particular, let

$$\langle \epsilon, f \rangle_n = \frac{1}{n} \sum_{k=1}^n \epsilon_k f(x_k),$$

where $\epsilon = (\epsilon_1, \dots, \epsilon_n)^T$. For two vectors v and w , we use $\langle v, w \rangle = v^T w$ to denote the inner product.

For notational simplification, let $h_n = h_{X_n, \Omega}$ and $q_n = q_{X_n}$ be the fill distance and separation radius of design X_n , respectively. For the ease of treatment, in the rest of Appendix, we assume the regularization parameter $\lambda_m \asymp n^\alpha$ for some $\alpha \in \mathbb{R}$. We use $\operatorname{tr}(A)$ to denote the trace of a matrix A .

Appendix C. Proof of Proposition 2

Without loss of generality, assume $\sigma = 1$. Notice that for any $u = (u_1, \dots, u_n)^T \in \mathbb{R}^n$ and any constant C_1 ,

$$\Psi(x-x) - 2 \sum_{j=1}^n u_j \Psi(x-x_j) + \sum_{k=1}^n \sum_{j=1}^n u_k u_j \Psi(x_k - x_j) + C_1 \|u\|_2^2 \geq C_1 \|u\|_2^2,$$

because Ψ is positive definite. Plugging $u = (R + C_1 I_n)^{-1} r(x)$, we have

$$C_1 r(x)^T (R + C_1 I_n)^{-2} r(x) \leq \Psi(x-x) - r(x)^T (R + C_1 I_n)^{-1} r(x). \quad (17)$$

If $C \leq \mu = \sigma_\epsilon^2 / \sigma^2$, then direct computation shows that

$$\begin{aligned} & \mathbb{E}(\hat{f}_G(x) - Z(x))^2 \\ &= \Psi(x-x) - 2r(x)^T (R + CI_n)^{-1} r(x) + r(x)^T (R + CI_n)^{-1} (R + \mu I_n) (R + CI_n)^{-1} r(x) \\ &= \Psi(x-x) - 2r(x)^T (R + CI_n)^{-1} r(x) + r(x)^T (R + CI_n)^{-1} (R + CI_n) (R + CI_n)^{-1} r(x) \\ & \quad + (\mu - C) r(x)^T (R + CI_n)^{-2} r(x) \\ &= \Psi(x-x) - r(x)^T (R + CI_n)^{-1} r(x) + (\mu - C) r(x)^T (R + CI_n)^{-2} r(x) \\ &\leq \left(1 + \frac{\mu - C}{C}\right) (\Psi(x-x) - r(x)^T (R + CI_n)^{-1} r(x)) \\ &\leq \frac{\mu}{C} (\Psi(x-x) - r(x)^T (R + \mu I_n)^{-1} r(x)), \end{aligned} \quad (18)$$

where the first inequality is because of (17), and the second inequality is because of $(R + \mu I_n)^{-1} \preceq (R + CI_n)^{-1}$.

If $C > \mu$, then we have

$$\begin{aligned} & \mathbb{E}(\hat{f}_G(x) - Z(x))^2 \\ &= \Psi(x-x) - 2r(x)^T (R + CI_n)^{-1} r(x) + r(x)^T (R + CI_n)^{-1} (R + \mu I_n) (R + CI_n)^{-1} r(x) \\ &\leq \Psi(x-x) - r(x)^T (R + CI_n)^{-1} r(x), \end{aligned} \quad (19)$$

where the first inequality is because of $R + \mu I_n \preceq R + CI_n$.

For any $u = (u_1, \dots, u_n)^T$, the Fourier inversion theorem yields

$$\begin{aligned} & \Psi(x-x) - 2 \sum_{j=1}^n u_j \Psi(x-x_j) + \sum_{k=1}^n \sum_{j=1}^n u_k u_j \Psi(x_k - x_j) + C \|u\|_2^2 \\ &= \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{i\langle x_j, \omega \rangle} - e^{i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + C \|u\|_2^2 \\ &\leq \frac{C}{\mu} \left(\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{i\langle x_j, \omega \rangle} - e^{i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + \mu \|u\|_2^2 \right). \end{aligned} \quad (20)$$

Let $u^{(1)} = (u_1^{(1)}, \dots, u_n^{(1)})^T = (R + \mu I_n)^{-1} r(x)$. Because $u^{(2)} = (u_1^{(2)}, \dots, u_n^{(2)})^T = (R + CI_n)^{-1} r(x)$ is the solution to the optimization problem

$$\min_{u \in \mathbb{R}^n} \Psi(x - x) - 2 \sum_{j=1}^n u_j \Psi(x - x_j) + \sum_{k=1}^n \sum_{j=1}^n u_k u_j \Psi(x_k - x_j) + C \|u\|_2^2,$$

we have

$$\begin{aligned} & \Psi(x - x) - r(x)^T (R + CI_n)^{-1} r(x) \\ &= \Psi(x - x) - 2 \sum_{j=1}^n u_j^{(2)} \Psi(x - x_j) + \sum_{k=1}^n \sum_{j=1}^n u_k^{(2)} u_j^{(2)} \Psi(x_k - x_j) + C \|u^{(2)}\|_2^2 \\ &\leq \Psi(x - x) - 2 \sum_{j=1}^n u_j^{(1)} \Psi(x - x_j) + \sum_{k=1}^n \sum_{j=1}^n u_k^{(1)} u_j^{(1)} \Psi(x_k - x_j) + C \|u^{(1)}\|_2^2 \\ &\leq \frac{C}{\mu} \left(\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j^{(1)} e^{i\langle x_j, \omega \rangle} - e^{i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + \mu \|u^{(1)}\|_2^2 \right) \\ &= \frac{C}{\mu} (\Psi(x - x) - r(x)^T (R + \mu I_n)^{-1} r(x)), \end{aligned} \tag{21}$$

where the second inequality is by (20). Combining (18) and (21), we finish the proof.

Appendix D. Proof of Proposition 3

Let $I(x) = \Psi(x - x) - r(x)^T (R + \mu_1 I_n)^{-1} r(x)$. Consider function $g(t) = \Psi(x - t) - r(x)^T (R + \mu_1 I_n)^{-1} r(t)$. It can be seen that

$$I(x) = g(x) \leq \|g\|_{L_\infty(\Omega)}. \tag{22}$$

Direct computation shows that

$$\begin{aligned} \|g\|_{\mathcal{N}_\Psi(\Omega)}^2 &= \Psi(x - x) - 2r(x)^T (R + \mu_1 I_n)^{-1} r(x) + r(x)^T (R + \mu_1 I_n)^{-1} R (R + \mu_1 I_n)^{-1} r(x) \\ &\leq \Psi(x - x) - r(x)^T (R + \mu_1 I_n)^{-1} r(x) = I(x). \end{aligned} \tag{23}$$

By the Gagliardo–Nirenberg interpolation inequality for functions in Sobolev spaces (Leoni, 2017; Brezis and Mironescu, 2019), it can be seen that

$$\|g\|_{L_\infty(\Omega)} \lesssim \|g\|_{L_2(\Omega)}^{1 - \frac{d}{2m}} \|g\|_{H^m(\Omega)}^{\frac{d}{2m}} \lesssim \|g\|_{L_2(\Omega)}^{1 - \frac{d}{2m}} \|g\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{d}{2m}} \lesssim \|g\|_{L_2(\Omega)}^{1 - \frac{d}{2m}} I(x)^{\frac{d}{4m}}. \tag{24}$$

It remains to bound $\|g\|_{L_2(\Omega)}$. Let $f_1(t) = r(x)^T (R + \mu_1 I_n)^{-1} r(t)$. It can be seen from the representer theorem that

$$f_1 = \operatorname{argmin}_{h \in \mathcal{N}_\Psi(\Omega)} \|\Psi(x - \cdot) - h\|_n^2 + \frac{\mu_1}{n} \|h\|_{\mathcal{N}_\Psi(\Omega)}^2. \tag{25}$$

By Lemma 26,

$$\|g\|_{L_2(\Omega)} \lesssim h_n^{m_0} \|g\|_{H^{m_0}(\Omega)} + \|g\|_n \lesssim h_n^{m_0} \|g\|_{\mathcal{N}_\Psi(\Omega)} + \|g\|_n \lesssim h_n^m I(x)^{1/2} + \|g\|_n, \quad (26)$$

where the second inequality is by the equivalence of $\|\cdot\|_{H^{m_0}(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_\Psi(\Omega)}$, and the last inequality is by (23).

The empirical norm $\|g\|_n$ can be bounded by

$$\begin{aligned} \|g\|_n^2 &= \|\Psi(x - \cdot) - f_1\|_n^2 \\ &= \|\Psi(x - \cdot) - f_1\|_n^2 + \frac{\mu_1}{n} \|f_1\|_{\mathcal{N}_\Psi(\Omega)}^2 - \frac{\mu_1}{n} \|f_1\|_{\mathcal{N}_\Psi(\Omega)}^2 \\ &\leq \|\Psi(x - \cdot) - \Psi(x - \cdot)\|_n^2 + \frac{\mu_1}{n} \|\Psi(x - \cdot)\|_{\mathcal{N}_\Psi(\Omega)}^2 - \frac{\mu_1}{n} r(x)^T (R + \mu_1 I_n)^{-1} R (R + \mu_1 I_n)^{-1} r(x) \\ &= \frac{\mu_1}{n} \Psi(x - x) - \frac{\mu_1}{n} r(x)^T (R + \mu_1 I_n)^{-1} (R + \mu_1 I_n) (R + \mu_1 I_n)^{-1} r(x) \\ &\quad + \frac{\mu_1^2}{n} r(x)^T (R + \mu_1 I_n)^{-2} r(x) \\ &= \frac{\mu_1}{n} \left(\Psi(x - x) - r(x)^T (R + \mu_1 I_n)^{-1} r(x) + \mu_1 r(x)^T (R + \mu_1 I_n)^{-2} r(x) \right), \end{aligned} \quad (27)$$

where the first inequality is because f_1 is the solution to (25).

Notice that for any $u = (u_1, \dots, u_n)^T \in \mathbb{R}^n$,

$$\Psi(x - x) - 2 \sum_{j=1}^n u_j \Psi(x - x_j) + \sum_{k=1}^n \sum_{j=1}^n u_k u_j \Psi(x_k - x_j) + \mu_1 \|u\|_2^2 \geq \mu_1 \|u\|_2^2,$$

because Ψ is positive definite. Plugging $u = (R + \mu_1 I_n)^{-1} r(x)$, we have

$$\mu_1 r(x)^T (R + \mu_1 I_n)^{-2} r(x) \leq \Psi(x - x) - r(x)^T (R + \mu_1 I_n)^{-1} r(x). \quad (28)$$

Therefore, (28) and (27) imply that

$$\|g\|_n^2 \leq \frac{2\mu_1}{n} \left(\Psi(x - x) - r(x)^T (R + \mu_1 I_n)^{-1} r(x) \right) = \frac{2\mu_1}{n} I(x). \quad (29)$$

By (22), (24), (26), and (29), we have

$$\begin{aligned} I(x) &\lesssim (h_n^{m_0} I(x)^{1/2} + \|g\|_n)^{1 - \frac{d}{2m_0}} I(x)^{\frac{d}{4m_0}} \\ &\lesssim \left(h_n^{m_0} I(x)^{1/2} + \frac{\mu_1^{1/2}}{n^{1/2}} I(x)^{1/2} \right)^{1 - \frac{d}{2m_0}} I(x)^{\frac{d}{4m_0}} \\ &\lesssim \left(h_n^{m_0} + \frac{\mu_1^{1/2}}{n^{1/2}} \right)^{1 - \frac{d}{2m_0}} I(x)^{1/2} \lesssim \left(\frac{\mu_1}{n} \right)^{1/2 - \frac{d}{4m_0}} I(x)^{1/2}, \end{aligned} \quad (30)$$

where the last inequality is because $\mu_1 \gtrsim n^{1-2m_0/d}$. It can be seen that (30) implies

$$I(x) \leq \left(\frac{\mu_1}{n} \right)^{1 - \frac{d}{2m_0}}.$$

This finishes the proof.

Appendix E. Proof of Theorem 6

We first present several lemmas used in this proof. Lemma 21 is Lemma 24 in Tuo and Wang (2020). The proof of Lemma 22 is provided in Appendix L.1.

Lemma 21 *Suppose Ω satisfies Condition (C1). Let G be a zero-mean Gaussian process on Ω with continuous sample paths almost surely and with a finite maximum pointwise variance $\sigma_G^2 = \sup_{x \in \Omega} \mathbb{E}G(x)^2 < \infty$. Then for all $u > 0$ and $1 \leq p < \infty$, we have*

$$\begin{aligned} \mathbb{P}(\|G\|_{L_p(\Omega)} - \mathbb{E}\|G\|_{L_p(\Omega)} > u) &\leq e^{-u^2/(2C_p\sigma_G^2)}, \\ \mathbb{P}(\|G\|_{L_p(\Omega)} - \mathbb{E}\|G\|_{L_p(\Omega)} < -u) &\leq e^{-u^2/(2C_p\sigma_G^2)}, \end{aligned}$$

with $C_p = \text{Vol}(\Omega)^{2/p}$. Here $\text{Vol}(\Omega)$ denotes the volume of Ω .

Lemma 22 *Suppose the design points $X = \{x_1, \dots, x_n\}$ and the separation radius of X $q_X \lesssim 1$. Let Ψ be a Matérn correlation function satisfying Condition (C2) and Λ_X be the maximum eigenvalue of matrix $(\Psi(x_j - x_k))_{jk}$. Then*

$$\Lambda_X \leq Cq_X^{-d},$$

where C is a constant depending on Ψ and Ω .

Now we begin to prove Theorem 6. Recall that $y_j = Z(x_j) + \epsilon_j$. Let $\epsilon = (\epsilon_1, \dots, \epsilon_n)^T$ and $F = (Z(x_1), \dots, Z(x_n))^T$. Therefore,

$$\hat{f}_G(x) = r_m(x)^T(R_m + \mu_m I_n)^{-1}F + r_m(x)^T(R_m + \mu_m I_n)^{-1}\epsilon.$$

Direct computation shows that

$$\begin{aligned} (Z(x) - \hat{f}_G(x))^2 &= (Z(x) - r_m(x)^T(R_m + \mu_m I_n)^{-1}F - r_m(x)^T(R_m + \mu_m I_n)^{-1}\epsilon)^2 \\ &\leq 2(Z(x) - r_m(x)^T(R_m + \mu_m I_n)^{-1}F)^2 + 2(r_m(x)^T(R_m + \mu_m I_n)^{-1}\epsilon)^2 \\ &= 2I_1(x) + 2I_2(x), \end{aligned} \tag{31}$$

where the inequality is by the Cauchy-Schwarz inequality. Let $G(x) = Z(x) - r_m(x)^T(R_m + \mu_m I_n)^{-1}F$. It can be seen that G is also a mean zero Gaussian process.

By Jensen's inequality and Fubini's theorem,

$$\begin{aligned} (\mathbb{E}\|G\|_{L_2(\Omega)})^2 &\leq \mathbb{E}\|G\|_{L_2(\Omega)}^2 = \int_{\Omega} \mathbb{E}(Z(x) - r_m(x)^T(R_m + \mu_m I_n)^{-1}F)^2 dx \\ &= \int_{\Omega} \mathbb{E}I_1(x) dx \leq \text{Vol}(\Omega) \sup_{x \in \Omega} \mathbb{E}I_1(x), \end{aligned} \tag{32}$$

where $\text{Vol}(\Omega)$ is the volume of Ω .

Next, we provide a uniform upper bound on $\mathbb{E}I_1(x)$. Direct computation gives us

$$\mathbb{E}I_1 = \Psi(x - x) - 2r_m(x)^T(R_m + \mu_m I_n)^{-1}r(x) + r_m(x)^T(R_m + \mu_m I_n)^{-1}R(R_m + \mu_m I_n)^{-1}r_m(x),$$

where $r(x)$ and R are as in (2).

By the Fourier inversion theorem, for $u = (u_1, \dots, u_n)^T = (R_m + \mu_m I_n)^{-1} r_m(x)$, we have

$$\begin{aligned}
 \mathbb{E}I_1(x) &= \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega \\
 &= \int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + \int_{\|\omega\|_2 > \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega \\
 &= I_{11} + I_{12}, \tag{33}
 \end{aligned}$$

where $\gamma > 1$ will be determined later.

The first term I_{11} can be bounded by

$$\begin{aligned}
 I_{11} &\lesssim \int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m_0} d\omega \\
 &\lesssim \gamma^{2m-2m_0} \int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m} d\omega \\
 &\lesssim \gamma^{2m-2m_0} \int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Phi)(\omega) d\omega, \tag{34}
 \end{aligned}$$

where the first and third inequalities are because of Conditions (C2) and (C3), respectively.

By the Cauchy-Schwarz inequality, the second term I_{12} can be further split to

$$\begin{aligned}
 I_{12} &\leq 2 \int_{\|\omega\|_2 > \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + 2 \int_{\|\omega\|_2 > \gamma} \left| e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega \\
 &= I_3 + I_4. \tag{35}
 \end{aligned}$$

Since Ψ satisfies Condition (C2), the term I_4 can be bounded by

$$I_4 \lesssim \int_{\|\omega\|_2 > \gamma} (1 + \|\omega\|_2^2)^{-m_0} d\omega \lesssim \gamma^{-2m_0+d}, \tag{36}$$

and the term I_3 can be bounded by

$$\begin{aligned}
 I_3 &\lesssim \int_{\|\omega\|_2 > \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m_0} d\omega \\
 &\lesssim \gamma^d \int_{\|\omega\|_2 > 1} \left| \sum_{j=1}^n u_j e^{-i\gamma \langle x_j, \omega \rangle} \right|^2 (1 + \gamma^2 \|\omega\|_2^2)^{-m_0} d\omega \\
 &\lesssim \gamma^{d-2m_0} \int_{\|\omega\|_2 > 1} \left| \sum_{j=1}^n u_j e^{-i\gamma \langle x_j, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m_0} d\omega \\
 &\lesssim \gamma^{d-2m_0} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\gamma \langle x_j, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m_0} d\omega, \tag{37}
 \end{aligned}$$

where the second inequality is by the change of variables, and the third inequality is by the fact that $(1 + \gamma^2 \|\omega\|_2^2)^{-m_0} \leq (\gamma^2(1 + \|\omega\|_2^2)/2)^{-m_0}$ for $\|\omega\|_2 \geq 1$.

Putting (36) and (37) into (35), we obtain

$$\begin{aligned}
 I_{12} &\lesssim \gamma^{d-2m_0} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\gamma \langle x_j, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m_0} d\omega + \gamma^{-2m_0+d} \\
 &\lesssim \gamma^{d-2m_0} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\gamma \langle x_j, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + \gamma^{-2m_0+d} \\
 &= \gamma^{d-2m_0} \sum_{j,k=1}^n u_j u_k \Psi(\gamma x_j - \gamma x_k) + \gamma^{-2m_0+d} \\
 &\leq \gamma^{d-2m_0} \Lambda_{\gamma X} \|u\|_2^2 + \gamma^{-2m_0+d}, \tag{38}
 \end{aligned}$$

where the second inequality is because Ψ satisfies Condition (C2), and $\gamma X = \{\gamma x_1, \dots, \gamma x_n\}$. The separation distance of γX is γq_X , which, together with Lemma 22, implies $\Lambda_{\gamma X} \leq C(\gamma q_X)^{-d}$ (it can be seen by the choice of γ later, $\gamma q_X \lesssim 1$). Plugging (34) and (38) into

(33), we have

$$\begin{aligned}
 & \mathbb{E}I_1(x) \\
 & \lesssim \gamma^{2m-2m_0} \int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Phi)(\omega) d\omega + \gamma^{d-2m_0} \Lambda_{\gamma X} \|u\|_2^2 + \gamma^{-2m_0+d} \\
 & \lesssim \gamma^{2m-2m_0} \int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Phi)(\omega) d\omega + \gamma^{d-2m_0} (\gamma q_X)^{-d} \|u\|_2^2 + \gamma^{-2m_0+d} \\
 & \lesssim \gamma^{2m-2m_0} \left(\int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Phi)(\omega) d\omega + \gamma^{-2m} (q_X)^{-d} \|u\|_2^2 \right) + \gamma^{-2m_0+d}.
 \end{aligned} \tag{39}$$

Take $\gamma = \mu_m^{-\frac{1}{2m}} (q_X)^{-d/2m}$ such that $\gamma^{-2m} (q_X)^{-d} = \mu_m$. Clearly, $\gamma q_X \lesssim 1$. By (39), $\mathbb{E}I_1(x)$ can be further bounded by

$$\begin{aligned}
 \mathbb{E}I_1(x) & \lesssim \mu_m^{-\frac{m-m_0}{m}} q_X^{-\frac{(m-m_0)d}{m}} \left(\int_{\|\omega\|_2 \leq \gamma} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Phi)(\omega) d\omega + \mu_m \|u\|_2^2 \right) \\
 & \quad + \mu_m^{\frac{2m_0-d}{2m}} (q_X)^{\frac{(2m_0-d)d}{2m}} \\
 & \lesssim \mu_m^{-\frac{m-m_0}{m}} q_X^{-\frac{(m-m_0)d}{m}} \left(\int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Phi)(\omega) d\omega + \mu_m \|u\|_2^2 \right) \\
 & \quad + \mu_m^{\frac{2m_0-d}{2m}} (q_X)^{\frac{(2m_0-d)d}{2m}} \\
 & = \mu_m^{-\frac{m-m_0}{m}} q_X^{-\frac{(m-m_0)d}{m}} \left(\Phi(x-x) - 2 \sum_{j=1}^n u_j \Phi(x-x_j) + \sum_{j,k=1}^n u_j u_k \Phi(x_j-x_k) + \mu_m \|u\|_2^2 \right) \\
 & \quad + \mu_m^{\frac{2m_0-d}{2m}} (q_X)^{\frac{(2m_0-d)d}{2m}} \\
 & = \mu_m^{-\frac{m-m_0}{m}} q_X^{-\frac{(m-m_0)d}{m}} (\Phi(x-x) - r_m(x)^T (R_m + \mu_m I_n)^{-1} r_m(x)) + \mu_m^{\frac{2m_0-d}{2m}} (q_X)^{\frac{(2m_0-d)d}{2m}} \\
 & \lesssim \mu_m^{-\frac{m-m_0}{m}} q_X^{-\frac{(m-m_0)d}{m}} (\mu_m/n)^{1-\frac{d}{2m}} + \mu_m^{\frac{2m_0-d}{2m}} (q_X)^{\frac{(2m_0-d)d}{2m}},
 \end{aligned} \tag{40}$$

where the last inequality is by applying Proposition 3 to the correlation function Φ .

Let $T = \mu_m^{-\frac{m-m_0}{m}} q_X^{-\frac{(m-m_0)d}{m}} (\mu_m/n)^{1-\frac{d}{2m}} + \mu_m^{\frac{2m_0-d}{2m}} (q_X)^{\frac{(2m_0-d)d}{2m}}$. Lemma 21, (32), and (40) imply that for all $t_1 > 0$, with probability at least $1 - \exp(-Ct_1^2)$,

$$\|G\|_{L_2(\Omega)} \lesssim (1+t_1)T^{1/2}.$$

which implies

$$\|G\|_{L_2(\Omega)}^2 \lesssim (1+t_1)^2 T. \tag{41}$$

Next, we consider $I_2(x)$. This can be done by applying Theorem 29. Recall that $I_2(x) = (r_m(x)^T(R_m + \mu_m I_n)^{-1}\epsilon)^2$. Define $f_2(x) = 0$ for all $x \in \Omega$, i.e., f_2 is a zero function. Clearly, $f_2 \in \mathcal{N}_\Phi(\Omega)$ with $\|f_2\|_{\mathcal{N}_\Phi(\Omega)} = 0$. Let $\hat{f}_2(x) = r_m(x)^T(R_m + \mu_m I_n)^{-1}\epsilon$, then $\|\hat{f}_2\|_{L_2(\Omega)}^2 = \int_{x \in \Omega} I_2(x) dx$. By the representer theorem, \hat{f}_2 is the solution to

$$\min_{\hat{g} \in \mathcal{N}_\Phi(\Omega)} \frac{1}{n} \sum_{j=1}^n (\hat{g}(x_j) - \epsilon_j)^2 + \frac{\mu_m}{n} \|\hat{g}\|_{\mathcal{N}_\Phi(\Omega)}.$$

Theorem 29 tells us that for all $t > C_0$ (with appropriate changes of notation), with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\|f_2 - \hat{f}_2\|_{L_2(\Omega)}^2 \leq C_3 t^2 n^{-1} (\mu_m/n)^{-\frac{d}{2m}},$$

which implies

$$\int_{x \in \Omega} I_2(x) dx = \|\hat{f}_2\|_{L_2(\Omega)}^2 \leq C_3 t^2 n^{-1} (\mu_m/n)^{-\frac{d}{2m}} \quad (42)$$

since $f_2 = 0$. Note that (31) implies $\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \lesssim \|G\|_{L_2(\Omega)}^2 + \|\hat{f}_2\|_{L_2(\Omega)}^2$. Thus, by (41) and (42), we finish the proof of Theorem 6.

Appendix F. Proof of Theorem 8

Note that $y_j = Z(x_j) + \epsilon_j$. Let $\epsilon = (\epsilon_1, \dots, \epsilon_n)^T$ and $F = (Z(x_1), \dots, Z(x_n))^T$. Therefore,

$$\hat{f}_G(x) = r_m(x)^T (R_m + \mu_m I_n)^{-1} F + r_m(x)^T (R_m + \mu_m I_n)^{-1} \epsilon.$$

Similar to (31), we have

$$\begin{aligned} (Z(x) - \hat{f}_G(x))^2 &\leq 2(Z(x) - r_m(x)^T (R_m + \mu_m I_n)^{-1} F)^2 + 2(r_m(x)^T (R_m + \mu_m I_n)^{-1} \epsilon)^2 \\ &= 2I_1(x) + 2I_2(x). \end{aligned}$$

Let $G(x) = Z(x) - r_m(x)^T (R_m + \mu_m I_n)^{-1} F$, which is also a mean zero Gaussian process.

Similar to (32), we can obtain that

$$(\mathbb{E}\|G\|_{L_2(\Omega)})^2 \leq \text{Vol}(\Omega) \sup_{x \in \Omega} \mathbb{E}I_1(x). \quad (43)$$

Direct computation gives us

$$\mathbb{E}I_1(x) = \Psi(x-x) - 2r_m(x)^T (R_m + \mu_m I_n)^{-1} r(x) + r_m(x)^T (R_m + \mu_m I_n)^{-1} R (R_m + \mu_m I_n)^{-1} r_m(x).$$

By the Fourier inversion theorem and Conditions (C2) and (C3), for $u = (u_1, \dots, u_n)^T = (R_m + \mu_m I_n)^{-1} r_m(x)$, we have

$$\begin{aligned}
 \mathbb{E}I_1(x) &= \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega \\
 &\leq C_1 \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m_0} d\omega \\
 &\leq C_1 \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 (1 + \|\omega\|_2^2)^{-m} d\omega \\
 &\leq C_2 \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Phi)(\omega) d\omega \\
 &= C_2 (\Phi(x - x) - r_m(x)^T (R_m + \mu_m I_n)^{-1} r_m(x)) =: I_3(x), \tag{44}
 \end{aligned}$$

where the second inequality is because $m \leq m_0$.

Applying Proposition 3 to the correlation function Φ implies that

$$I_3(x) \leq C_3 (\mu_m/n)^{1 - \frac{d}{2m}}. \tag{45}$$

Lemma 21, (43), (44), and (45) imply that for all $t_1 > 0$, with probability at least $1 - \exp(-Ct_1^2)$,

$$\|G\|_{L_2(\Omega)}^2 \leq C_4 (1 + t_1)^2 (\mu_m/n)^{1 - \frac{d}{2m}}. \tag{46}$$

Similar to the proof of (42), for all $t_2 \geq C_0$, with probability at least $1 - \exp(-t_2^2)$,

$$\int_{x \in \Omega} I_2(x) dx \leq C_5 t_2^2 \mu_m^{-\frac{d}{2m}} n^{-(1 - \frac{d}{2m})}. \tag{47}$$

By the fact $\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \lesssim \|G\|_{L_2(\Omega)}^2 + \|\hat{r}_m(x)^T (R_m + \mu_m I_n)^{-1} \epsilon\|_{L_2(\Omega)}^2$, (46), and (47), we finish the proof of Theorem 8.

Appendix G. Proof of Theorem 10

We first present several lemmas. Lemma 23 is Lemma F.7 of Wang (2020).

Lemma 23 *Suppose A, B and $C \in \mathbb{R}^{n \times n}$ are positive definite matrices. We have*

$$\begin{aligned}
 &\text{tr}((A + B)(A + B + C)^{-1}) \geq \text{tr}(A(A + C)^{-1}), \\
 &\text{and } \text{tr}((A + B)^2(A + B + C)^{-2}) \geq \text{tr}(A^2(A + C)^{-2}).
 \end{aligned}$$

Let K be a stationary correlation function. Since a correlation function is positive definite, by Mercer's theorem, there exists a countable set of positive eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots > 0$ and an orthonormal basis for $L_2(\Omega)$ $\{\varphi_k\}_{k \in \mathbb{N}}$ such that

$$K(x - y) = \sum_{k=1}^{\infty} \lambda_k \varphi_k(x) \varphi_k(y), \quad x, y \in \Omega, \quad (48)$$

where the summation is uniformly and absolutely convergent.

Lemma 24 states the asymptotic rate of the eigenvalues of K , which is implied by the proof of Lemma 18 of Tuo and Wang (2020).

Lemma 24 *Suppose Condition (C1) holds. Suppose K is a stationary correlation function satisfying Condition (C2) and has an expansion as in (48). Then, $\lambda_k \asymp k^{-2m_0/d}$.*

We need the following technical assumption.

Assumption G.0.1 *Suppose there exists a stationary correlation function K satisfying Condition (C2) and a constant $A_0 > 0$ such that*

$$\left\| \frac{\mathcal{F}(K)}{\mathcal{F}(\Psi)} \right\|_{L_\infty(\mathbb{R}^d)} \leq A_0, \quad (49)$$

and K has an expansion as in (48) with eigenfunctions $\|\varphi_k\|_{L_\infty(\Omega)} \leq C$ for all $k = 1, 2, \dots$, where $C > 0$ not depending on k .

Lemma 25 states that the MSPE $\mathbb{E}(Z(x) - \hat{f}_G(x))^2$ can be further bounded by the term related to K , and the proof is in Appendix L.2.

Lemma 25 *Let Ψ be a correlation function satisfying Condition (C2), and $Z \sim GP(0, \sigma^2 \Psi)$. Assume Assumption G.0.1 holds. Let $\{x_1, \dots, x_n\}$ be a set of design points. Then for all $x \in \Omega$,*

$$\text{Var}[Z(x)|Y] \gtrsim K(x - x) - r_K(x)^T (R_K + \mu I_n)^{-1} r_K(x),$$

where $R_K = (K(x_j - x_k))_{jk}$, $r_K(x) = (K(x - x_1), \dots, K(x - x_n))^T$, and Y and μ are as in (2).

Lemma 26 and Lemma 28 state that under fixed designs, the empirical norm is close to the L_2 norm. Lemma 26 can be found in Madych and Potter (1985); Rieger (2008). The proof of Lemma 28 is merely repeating the process of proving Lemma 26 as in Madych and Potter (1985), thus is omitted.

Lemma 26 *Suppose $g \in H^m(\Omega)$ for some $m > d/2$. Suppose Condition (C4) holds. Then we have*

$$\|g\|_{L_2(\Omega)} \leq C(h_n^m \|g\|_{H^m(\Omega)} + \|g\|_n)$$

holds for all n , where C is a positive constant not depending on g and n .

Remark 27 *Lemma 26 is a stronger version of Lemma 3.4 in Utreras (1988). In Lemma 3.4 of Utreras (1988), the fixed designs are assumed to be quasi-uniform. Lemma 3.4 of Utreras (1988) is used in Tuo et al. (2020).*

Lemma 28 *Suppose $g \in H^m(\Omega)$ for some $m > d/2$. Suppose Condition (C4) holds. Then we have*

$$\|g\|_n \leq C(h_n^m \|g\|_{H^m(\Omega)} + \|g\|_{L_2(\Omega)})$$

holds for all n , where C is a positive constant not depending on g and n .

By Lemma 25, it suffices to show

$$\int_{x \in \Omega} K(x-x) - r_K(x)^T (R_K + \mu I_n)^{-1} r_K(x) dx \gtrsim n^{-\frac{2m_0-d}{2m_0}},$$

where K, r_K, R_K, μ are as in Lemma 25. This is because for any linear predictor \hat{f}_G ,

$$\mathbb{E}(Z(x) - \hat{f}_G(x))^2 \geq \text{Var}[Z(x)|Y], \forall x \in \Omega.$$

Notice that for any $u = (u_1, \dots, u_n)^T \in \mathbb{R}^n$,

$$K(x-x) - 2 \sum_{j=1}^n u_j K(x-x_j) + \sum_{k=1}^n \sum_{j=1}^n u_k u_j K(x_k-x_j) + \mu \|u\|_2^2 \geq \mu \|u\|_2^2, \quad (50)$$

since K is positive definite. Let $u(x) = (u_1(x), \dots, u_n(x))^T = (R_K + \mu I_n)^{-1} r_K(x)$, (50) implies

$$\mu r_K(x)^T (R_K + \mu I_n)^{-2} r_K(x) \leq K(x-x) - r_K(x)^T (R_K + \mu I_n)^{-1} r_K(x). \quad (51)$$

From (51), it can be seen that it is sufficient to provide a lower bound on $I(x) := r_K(x)^T (R_K + \mu I_n)^{-2} r_K(x)$, because μ is a constant.

Let $p = \lfloor n^{d/(2m_0)} \rfloor$, where $\lfloor \cdot \rfloor$ is the floor function. Let $K_1 = \frac{1}{\sqrt{n}}(\varphi_1(X), \dots, \varphi_p(X))$, and $K_2 = \frac{1}{\sqrt{n}}(\varphi_{p+1}(X), \varphi_{p+2}(X), \dots)$, where $\varphi_k(X) = (\varphi_k(x_1), \dots, \varphi_k(x_n))^T$ for $k = 1, 2, \dots$, and φ_k 's are as in (48). Let $\Lambda_1 = \text{diag}(n\lambda_1, \dots, n\lambda_p)$ and $\Lambda_2 = \text{diag}(n\lambda_{p+1}, \dots)$, where λ_k 's are as in (48). Therefore, $R_K = \sum_{k=1}^{\infty} \lambda_k \varphi_k(X) \varphi_k(X)^T = K_1 \Lambda_1 K_1^T + K_2 \Lambda_2 K_2^T$. Note that for any

functions $v_1, v_2 \in H^{m_0}(\Omega)$, $\|v_1 v_2\|_{H^{m_0}(\Omega)} \leq C \|v_1\|_{H^{m_0}(\Omega)} \|v_2\|_{H^{m_0}(\Omega)}$ (Adams and Fournier, 2003). Because $I(x) = u(x)^T u(x)$, we have

$$\begin{aligned} \|I\|_{H^{m_0}(\Omega)} &= \left\| \sum_{k=1}^n u_k^2 \right\|_{H^{m_0}(\Omega)} \leq C \sum_{k=1}^n \|u_k\|_{H^{m_0}(\Omega)}^2 \leq C_1 \sum_{k=1}^n \|u_k\|_{\mathcal{N}_K(\Omega)}^2 \\ &= C_1 \sum_{k=1}^n ((R_K + \mu I_n)^{-1})_k^T R_K ((R_K + \mu I_n)^{-1})_k = C_1 \text{tr}((R_K + \mu I_n)^{-2} R_K), \end{aligned} \quad (52)$$

where the first inequality is by the triangle inequality, and $((R_K + \mu I_n)^{-1})_k$ denotes the k -th row of $(R_K + \mu I_n)^{-1}$.

Next we provide a lower bound on $\lambda_{\min}(K_1^T K_1)$ and an upper bound on $\text{tr}(K_2^T \Lambda_2 K_2)$. For any $a = (a_1, \dots, a_p)^T \in \mathbb{R}^p$ such that $\|a\|_2 = 1$, consider function $g_1 = \sum_{k=1}^p a_k \varphi_k$. Since φ_i 's are orthonormal, $\|g\|_{L_2(\Omega)} = 1$. By Lemma 24, $\|g_1\|_{H^{m_0}(\Omega)}^2 \leq C_1 \|g_1\|_{\mathcal{N}_K(\Omega)}^2 \leq C_1 \|\varphi_p\|_{\mathcal{N}_K(\Omega)}^2 \leq C_2 / \lambda_p \leq C_3 p^{2m_0/d} \leq C_3 n$. Therefore, by Lemma 26 and Condition (C4),

$$\begin{aligned} \|g\|_{L_2(\Omega)} &\leq C_4 (h_n^{m_0} \|g_1\|_{H^{m_0}(\Omega)} + \|g\|_n) \\ &\leq C_5 (n^{-m_0/d} n^{1/2} + \|g\|_n) \end{aligned}$$

which implies

$$\|g\|_n \geq \frac{1}{C_5} \|g\|_{L_2(\Omega)} - n^{(d-2m_0)/2d} \geq \frac{1}{2C_5},$$

for some $n > N_0$, since $m_0 > d/2$ and $n^{(d-2m_0)/2d}$ converges to zero. Then we have

$$\lambda_{\min}(K_1^T K_1) = \inf_{a \in \mathbb{R}^p} \|g\|_n^2 \geq C_6, \quad (53)$$

for some constant $C_6 > 0$.

Considering $\text{tr}(K_2^T \Lambda_2 K_2)$, we have

$$\text{tr}(K_2^T \Lambda_2 K_2) = \sum_{k=p+1}^{\infty} \lambda_k \left(\sum_{j=1}^n \varphi_k(x_j)^2 \right) \leq n C_7^2 \sum_{k=p+1}^{\infty} \lambda_k \leq C_8 n p^{-\frac{2m_0}{d}+1} \leq C_8 n^{\frac{d}{2m_0}}, \quad (54)$$

where the first inequality is by Assumption G.0.1, and the second inequality is by Lemma 24 and the basic inequality $\sum_{k=m}^{\infty} k^{-2m_0/d} \lesssim m^{-2m_0/d+1}$.

By (52), $\|I\|_{H^{m_0}(\Omega)}$ can be further bounded by

$$\begin{aligned} \|I\|_{H^{m_0}(\Omega)} &\leq C_1 \text{tr}((K_1 \Lambda_1 K_1^T + K_2 \Lambda_2 K_2^T + \mu I_n)^{-2} (K_1 \Lambda_1 K_1^T + K_2 \Lambda_2 K_2^T)) \\ &\leq C_1 (\text{tr}((K_1 \Lambda_1 K_1^T + \mu I_n)^{-2} K_1 \Lambda_1 K_1^T)) + C_1 \mu^{-2} \text{tr}(K_2 \Lambda_2 K_2^T). \end{aligned} \quad (55)$$

Let $I_1 = \text{tr}((K_1 \Lambda_1 K_1^T + \mu I_n)^{-2} K_1 \Lambda_1 K_1^T)$. We have

$$I_1 = \sum_{i=1}^p \frac{\lambda_i(K_1 \Lambda_1 K_1^T)}{(\lambda_i(K_1 \Lambda_1 K_1^T) + \mu)^2} \leq \mu^{-2} p \leq \mu^{-2} n^{\frac{d}{2m_0}}, \quad (56)$$

where $\lambda_i(K_1\Lambda_1K_1^T)$ denote the i -th eigenvalue of $K_1\Lambda_1K_1^T$.

Combining (54), (55), and (56), we find that $\|I\|_{H^{m_0}(\Omega)} \leq C_9 n^{\frac{d}{2m_0}}$.

Together with Lemma 28, we have

$$\|I\|_n \leq C_{10}(h_n^{m_0}\|I\|_{H^{m_0}(\Omega)} + \|I\|_{L_2(\Omega)}) \leq C_{11}(n^{\frac{d}{2m_0} - \frac{m_0}{d}} + \|I\|_{L_2(\Omega)}). \quad (57)$$

Let $I_n = \text{tr}(R_K^2(R_K + \mu I_n)^{-2})$. Note that $\lambda_i(K_1\Lambda_1K_1^T) = \lambda_i(K_1^T K_1\Lambda_1)$ for $i = 1, \dots, p$, because if v_i is eigenvector corresponding to i -th eigenvalue of $K_1\Lambda_1K_1^T$, then

$$K_1\Lambda_1K_1^T v_i = \lambda_i v_i \Rightarrow K_1^T K_1\Lambda_1K_1^T v_i = \lambda_i K_1^T v_i.$$

By Lemma 23 and $R_K = K_1\Lambda_1K_1^T + K_2\Lambda_2K_2^T$, it can be shown that

$$\begin{aligned} I_n &\geq \text{tr}((K_1\Lambda_1K_1^T)^2(K_1\Lambda_1K_1^T + \mu I)^{-2}) \\ &= \sum_{i=1}^p \left(\frac{\lambda_i(K_1\Lambda_1K_1^T)}{\lambda_i(K_1\Lambda_1K_1^T) + \mu} \right)^2 \\ &= \sum_{i=1}^p \left(\frac{\lambda_i(\Lambda_1K_1^T K_1)}{\lambda_i(\Lambda_1K_1^T K_1) + \mu} \right)^2, \end{aligned}$$

which implies

$$I_n \geq \text{tr}((\Lambda_1K_1^T K_1)^2(\Lambda_1K_1^T K_1 + \mu I)^{-2}) \geq \text{tr}(\Lambda_1^2(\Lambda_1 + \mu(K_1^T K_1)^{-1})^{-2}). \quad (58)$$

Combining (53) with (58), we conclude that

$$I_n \geq \text{tr}(\Lambda_1^2(\Lambda_1 + C_{12}I_p)^{-2}) \geq \sum_{k=1}^p \frac{\lambda_k^2}{(\lambda_k + C_{12}/n)^2} \geq C_{13}p \geq C_{14}n^{d/(2m_0)}, \quad (59)$$

where the third inequality is by Lemma 24. It follows the Cauchy-Schwarz inequality that

$$\|I\|_n = \sqrt{\frac{1}{n} \sum_{k=1}^n (u(x_k)^T u(x_k))^2} \geq \frac{1}{n} \sum_{k=1}^n u(x_k)^T u(x_k) = I_n/n \geq C_{14}n^{d/(2m_0)-1}.$$

By (57), we have

$$\|I\|_{L_2(\Omega)} \geq \frac{1}{C_{10}}\|I\|_n - n^{d/(2m_0) - \frac{m_0}{d}} \geq C_{15}n^{d/(2m_0)-1} - n^{d/(2m_0) - \frac{m_0}{d}} \gtrsim n^{d/(2m_0)-1},$$

for some $n > N_1$ such that $C_{15}n^{d/(2m_0)-1} > 2n^{d/(2m_0) - \frac{m_0}{d}}$, which can be done since $m_0 > d$. Thus, for $n > \max(N_0, N_1)$, we have $\mathbb{E}\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \gtrsim n^{d/(2m_0)-1}$. But for $n \leq \max(N_0, N_1)$, taking $C_{16} = \inf_{n \leq \max(N_0, N_1)} n^{d/(2m_0)-1}/\mathbb{E}\|Z - \hat{f}_G\|_{L_2(\Omega)}^2$ (which is clearly larger than zero), we can see that $\mathbb{E}\|Z - \hat{f}_G\|_{L_2(\Omega)}^2 \geq C_{16}n^{d/(2m_0)-1}$ for all $n \leq \max(N_0, N_1)$. This finishes the proof.

Appendix H. Proof of Lemma 13

In this section, we set $m_g := m_0(g)$ for notational simplicity. Since $g \notin H^{m_g}(\mathbb{R}^d)$, we have

$$\int_{\mathbb{R}^d} |\mathcal{F}(g)(\omega)|^2 (1 + \|\omega\|^2)^{m_g} d\omega = \infty, \quad (60)$$

$$\text{and } \int_{\mathbb{R}^d} |\mathcal{F}(g)(\omega)|^2 (1 + \|\omega\|^2)^{m_g - \delta} d\omega < \infty, \forall \delta > 0. \quad (61)$$

Using the hyperspherical coordinate transformation, we can represent ω by a radial coordinate r , and $d - 1$ angular coordinates $\phi_1, \phi_2, \dots, \phi_d$. Let $\phi = (\phi_1, \phi_2, \dots, \phi_d)^T$, and the Jacobian of the transformation be J . We can rewrite the left-hand side in (60) as

$$\int_0^\infty \int_{[0, 2\pi]^{d-1}} |\mathcal{F}(g)(r, \phi)|^2 (1 + r^2)^{m_g} |\det(J)| d\phi dr.$$

Let $g_1(r) = (1 + r^2)^{m_g} \int_{[0, 2\pi]^{d-1}} |\mathcal{F}(g)(r, \phi)|^2 |\det(J)| d\phi$. Therefore, (60) is equal to $\int_0^\infty g_1(r) dr$, which is infinite. It suffices to find an increasing function $Q(r)$ satisfying

$$\int_0^\infty \frac{g_1(r)}{Q(r)} dr \leq C_0 \quad (62)$$

and

$$\lim_{r \rightarrow +\infty} \frac{\log Q(r)}{\log r} = 0, \quad (63)$$

where C_0 is a constant. This is because by (63), we naturally have

$$\int_{\mathbb{R}^d} \frac{|\mathcal{F}(g)(\omega)|^2 (1 + \|\omega\|_2^2)^{m_g + \delta_1}}{Q(\|\omega\|_2)} d\omega = \infty \quad (64)$$

for any $\delta_1 > 0$, and more specifically, if (64) is false, then there exists $\delta_1 > 0$ such that

$$\int_{\mathbb{R}^d} \frac{|\mathcal{F}(g)(\omega)|^2 (1 + \|\omega\|_2^2)^{m_g + \delta_1}}{Q(\|\omega\|_2)} d\omega < \infty. \quad (65)$$

By (63), there exists a constant C such that for $r > C$, $\frac{\log Q(r)}{\log r} < \delta_1/4$, which is the same as $Q(r) < r^{\delta_1/4}$. This implies that there exists a constant C_0 such that $Q(r) < C_0(1 + r^2)^{\delta_1/2}$ for all $r \geq 0$. Therefore, (65) yields

$$\begin{aligned} \infty &> \int_{\mathbb{R}^d} \frac{|\mathcal{F}(g)(\omega)|^2 (1 + \|\omega\|^2)^{m_g + \delta_1}}{Q(\|\omega\|)} d\omega \\ &> C_0 \int_{\mathbb{R}^d} |\mathcal{F}(g)(\omega)|^2 (1 + \|\omega\|^2)^{m_g + \delta_1/2} d\omega = \infty, \end{aligned}$$

which leads to a contradiction.

We construct $Q(r)$ by the following recurrence way. Let $\alpha_i = 2^{-i}$ for $i \in \mathbb{N}_+$, $\alpha_0 = 1$, $x_0 = 0$, and $x_1 = 1$. Let $Q(r) = 1$ for $0 \leq r < x_1$. Since (61) implies that $\int_0^\infty g_1(r) r^{-\alpha} dr < \infty$

for any $\alpha > 0$, there exists $x_2 > x_1^{x_1}$ such that $\int_{x_2}^{\infty} g_1(r)r^{-\alpha_1}dr < 1$. Let $Q(r) = x_1^{-\alpha_i}r^{\alpha_i}$ for $r \in (x_1, x_2]$. Suppose we have specified $Q(r)$ for $r \in (x_{i-1}, x_i]$. Clearly there exists an $x_{i+1} > x_i^{x_i}$ such that $\int_{x_{i+1}}^{\infty} g_1(r)r^{-\alpha_i}dr < 2^{-i}$. Take $Q(r) = Q(x_i)x_i^{-\alpha_i}r^{\alpha_i}$ for $r \in (x_i, x_{i+1}]$. It can be seen that

$$Q(r) = \left[\prod_{j=1}^i x_j^{\alpha_{j-1} - \alpha_j} \right] r^{\alpha_i}$$

and $Q(r)$ is an increasing function. To show that $Q(r)$ satisfies (62), we note that

$$\int_0^{\infty} \frac{g_1(r)}{Q(r)} dr = \sum_{i=1}^{\infty} \int_{x_{i-1}}^{x_i} \frac{g_1(r)}{Q(r)} dr \leq \sum_{i=1}^{\infty} \int_{x_{i-1}}^{\infty} \frac{g_1(r)}{Q(r)} dr \leq \int_0^1 g_1(r) dr + \sum_{i=2}^{\infty} 2^{-i} \leq C_1,$$

where the second inequality is because of the choice of x_i 's and $Q(r) \geq r^{\alpha_i}$ for $r \in (x_i, x_{i+1}]$.

Next, we show $Q(r)$ satisfies (63). For any $\delta > 0$, there exists an integer N such that for all $r > x_N$, $r \in (x_M, x_{M+1}]$ for some $M > 0$,

$$\begin{aligned} \frac{\log Q(r)}{\log r} &= \frac{(\sum_{i=1}^{M-1} (\alpha_{i-1} - \alpha_i) \log x_i) + (\alpha_{M-1} - \alpha_M) \log x_M + \alpha_M \log r}{\log r} \\ &= \frac{(\sum_{i=1}^{M-1} (\alpha_{i-1} - \alpha_i) \log x_i)}{\log r} + \frac{(\alpha_{M-1} - \alpha_M) \log x_M + \alpha_M \log r}{\log r} \\ &< \frac{(\sum_{i=1}^{M-1} (\alpha_{i-1} - \alpha_i) \log x_{M-1})}{\log r} + \frac{\alpha_{M-1} \log x_M}{\log r} + \alpha_M \\ &< \frac{1}{x_{M-1}} + \alpha_{M-1} + \alpha_M < \frac{1}{x_{N-1}} + 2\alpha_{N-1} < \delta, \end{aligned}$$

where the second inequality is because $r \geq x_M \geq x_{M-1}^{x_{M-1}}$, and the last inequality is because $x_{N-1} \rightarrow \infty$ and $\alpha_{N-1} \rightarrow 0$.

Appendix I. Proof of Theorem 15

In this section, we set $m_0 := m_0(f)$ for notational simplicity. We prove more general results of Theorem 15, as follows. Note that in Theorem 29, $H^{m_0}(\Omega)$ coincides with $\mathcal{N}_{\Psi}(\Omega)$.

Theorem 29 *Suppose the conditions of Theorem 15 hold. Suppose $\lambda_m = o(1)$ if $f \in \mathcal{N}_{\Psi}(\Omega)$, and $\lambda_m = o(Q(n)^{-m/m_0})$ if $f \notin \mathcal{N}_{\Psi}(\Omega)$, where $Q(n)$ is as in Lemma 13 with $g = f$.*

Furthermore, suppose $\lambda_m \gtrsim n^{-\frac{2m^2}{d(2m-m_0)}}$. If f has smoothness m_0 and $f \in \mathcal{N}_{\Psi}(\Omega)$, for all $t > C_0$ and n , with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\|f - \hat{f}_m\|_{L_2(\Omega)}^2 \leq CT, \quad \text{and} \quad \|\hat{f}_m\|_{\mathcal{N}_{\Psi}(\Omega)}^2 \leq C\lambda_m^{-1}T, \quad (66)$$

where

$$\begin{aligned} T &= \max \left\{ t^{\frac{4m}{2m+d}} n^{-\frac{2m}{2m+d}} \lambda_m^{\frac{d(m_0-m)}{m(2m+d)}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^{\frac{2d}{2m+d}}, \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2 + 4tn^{-\frac{1}{2}} \lambda_m^{\frac{2m_0-d}{4m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}, \right. \\ &\quad \left. t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{\frac{4mm_0-2m_0d-2md}{2m(4m-d)}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^{\frac{2(2m-d)}{4m-d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}} \right\}. \end{aligned}$$

If f has smoothness m_0 but $f \notin \mathcal{N}_\Psi(\Omega)$, for all $t > C_0$, with probability at least $1 - C_1 \exp(-C_2 t^2)$, we can obtain that

$$\|f - \hat{f}_m\|_{L_2(\Omega)}^2 \leq CT, \text{ and } \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C\lambda_m^{-1}T, \quad (67)$$

where

$$T = \max\left\{t^{\frac{4m}{2m+d}}n^{-\frac{2m}{2m+d}}\lambda_m^{\frac{d(m_0-m)}{m(2m+d)}}Q(n)^{\frac{d}{2m+d}}, \lambda_m^{\frac{m_0}{m}}Q(n) + 4tn^{-\frac{1}{2}}\lambda_m^{\frac{2m_0-d}{4m}}Q(n)^{1/2}, \right. \\ \left. t^{\frac{4m}{4m-d}}n^{-\frac{2m}{4m-d}}\lambda_m^{\frac{4mm_0-2m_0d-2md}{2m(4m-d)}}Q(n)^{\frac{2m-d}{4m-d}}, t^2n^{-1}\lambda_m^{-\frac{d}{2m}}\right\}.$$

Note that Theorem 15 can be obtained by taking $\lambda_m \asymp n^{-\frac{2m}{2m_0+d}}$ in Theorem 29.

Now we begin to prove Theorem 29. The following lemmas are used. Lemma 30 is Lemma A.1 in Tuo et al. (2020), which states that the inner product $\langle \epsilon, g \rangle_n$ is small; also see Lemma 8.4 of van de Geer (2000).

Lemma 30 *Suppose Condition (C5) holds. Let K be a kernel function, which is stationary, positive definite and intergrable on \mathbb{R}^d . Suppose there exist constants $c_2 \geq c_1 > 0$ and $m > d/2$ such that, for all $\omega \in \mathbb{R}^d$,*

$$c_1(1 + \|\omega\|_2^2)^{-m} \leq \mathcal{F}(K)(\omega) \leq c_2(1 + \|\omega\|_2^2)^{-m}.$$

Then for all $t > C$, with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\sup_{g \in \mathcal{N}_K(\Omega)} \frac{|\langle \epsilon, g \rangle_n|}{\|g\|_n^{1-\frac{d}{2m}} \|g\|_{\mathcal{N}_K(\Omega)}^{\frac{d}{2m}}} \leq tn^{-\frac{1}{2}}.$$

Lemma 31 states the solution to the expectation version of (13) obtained by replacing $\|\cdot\|_n$ with $\|\cdot\|_{L_2(\Omega)}$, denoted by f^* , can approximate f well. The proof of Lemma 31 can be found in Appendix L.3.

Lemma 31 *Suppose the conditions in Theorem 29 hold. Let f^* be the solution to the optimization problem*

$$\min_{\tilde{f} \in \mathcal{N}_\Phi(\Omega)} \|f - \tilde{f}\|_{L_2(\Omega)}^2 + \lambda_m \|\tilde{f}\|_{\mathcal{N}_\Phi(\Omega)}^2. \quad (68)$$

If $f \in H^{m_0}(\Omega)$, then

$$\|f - f^*\|_{L_2(\Omega)}^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C\lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2,$$

where C is a constant only depending on Ω , Φ , and Ψ including m and m_0 . In particular, we have

$$\|f - f^*\|_{L_2}^2 \leq C\lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \text{ and } \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C\lambda_m^{\frac{m_0-m}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2. \quad (69)$$

If $f \notin H^{m_0}(\Omega)$, then there exists an increasing $Q : \mathbb{R}_+ \mapsto \mathbb{R}_+$ such that

$$\|f - f^*\|_{L_2(\Omega)}^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C \lambda_m^{\frac{m_0}{m}} Q(n),$$

where C is a constant only depending on Ω , Φ , and Ψ including m and m_0 . In particular, we have

$$\|f - f^*\|_{L_2}^2 \leq C \lambda_m^{\frac{m_0}{m}} Q(n), \text{ and } \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C \lambda_m^{\frac{m_0-m}{m}} Q(n). \quad (70)$$

Proof of Theorem 29. The proof of Theorem 29 consists of two parts, according to f lies in $\mathcal{N}_\Psi(\Omega)$ or not.

Case 1: f has smoothness m_0 and $f \in \mathcal{N}_\Psi(\Omega)$.

We first consider the case that f has smoothness m_0 and $f \in \mathcal{N}_\Psi(\Omega)$. Let f^* be as in Lemma 31. Because \hat{f}_m is the solution to (13), we have

$$\|y - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq \|y - f^*\|_n^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2, \quad (71)$$

where $y = (y_1, \dots, y_n)^T$. By rearrangement, (71) yields the *basic inequality*

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq \|f - f^*\|_n^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 + 2\langle \epsilon, \hat{f}_m - f^* \rangle_n. \quad (72)$$

We apply Lemma 30 to $\langle \epsilon, \hat{f}_m - f^* \rangle_n$ and obtain that with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\langle \epsilon, \hat{f}_m - f^* \rangle_n \leq t n^{-\frac{1}{2}} \|\hat{f}_m - f^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}. \quad (73)$$

Plugging (73) into (72), the inequality

$$\begin{aligned} & \|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \\ & \leq \|f - f^*\|_n^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 + 2t n^{-\frac{1}{2}} \|\hat{f}_m - f^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ & \leq \|f - f^*\|_n^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 + 2t n^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ & \quad + 2t n^{-\frac{1}{2}} \|f - f^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \end{aligned} \quad (74)$$

holds with probability at least $1 - C_1 \exp(-C_2 t^2)$. The last inequality in (74) is because of the triangle inequality and the basic inequality $(a + b)^q \leq a^q + b^q$ for any $a, b \geq 0$ and $q \in [0, 1]$.

By the Gagliardo–Nirenberg interpolation inequality,

$$\|f^*\|_{\mathcal{N}_\Psi(\Omega)} \lesssim \|f^*\|_{H^{m_0}(\Omega)} \lesssim \|f^*\|_{L_2(\Omega)}^{\frac{m-m_0}{m}} \|f^*\|_{H^m(\Omega)}^{\frac{m_0}{m}} \lesssim \|f^*\|_{L_2(\Omega)}^{\frac{m-m_0}{m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{m_0}{m}}, \quad (75)$$

where the first and last inequalities are because $\|\cdot\|_{\mathcal{N}_\Psi(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_\Phi(\Omega)}$ are equivalent to $\|\cdot\|_{H^{m_0}(\Omega)}$ and $\|\cdot\|_{H^m(\Omega)}$, respectively. It can be seen from (75) that $f - f^* \in \mathcal{N}_\Psi(\Omega)$,

which is equivalent to $f - f^* \in H^{m_0}(\Omega)$. By Lemma 28, we have

$$\begin{aligned} \|f - f^*\|_n &\lesssim h_n^{m_0} \|f - f^*\|_{N_\Psi(\Omega)} + \|f - f^*\|_{L_2(\Omega)} \\ &\lesssim h_n^{m_0} \|f\|_{N_\Psi(\Omega)} + h_n^{m_0} \|f^*\|_{N_\Psi(\Omega)} + \|f - f^*\|_{L_2(\Omega)} \\ &\lesssim h_n^{m_0} \|f\|_{N_\Psi(\Omega)} + h_n^{m_0} \|f^*\|_{L_2(\Omega)}^{\frac{m-m_0}{m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{m_0}{m}} + \|f - f^*\|_{L_2(\Omega)}, \end{aligned} \quad (76)$$

where the second inequality is because of the triangle inequality, and the third inequality is because of (75).

The reproducing property (Wendland, 2004) implies that for any $x \in \Omega$,

$$|f(x)| = |\langle f, \Psi(x - \cdot) \rangle_{\mathcal{N}_\Psi(\Omega)}| \leq \|f\|_{\mathcal{N}_\Psi(\Omega)} \Psi(x - x), \quad (77)$$

which implies $\|f\|_{L_2(\Omega)} \lesssim \|f\|_{L_\infty(\Omega)} \lesssim \|f\|_{\mathcal{N}_\Psi(\Omega)}$. By Lemma 31, we obtain

$$\|f^*\|_{L_2(\Omega)} \leq \|f\|_{L_2(\Omega)} + \|f - f^*\|_{L_2(\Omega)} \lesssim \|f\|_{L_2(\Omega)} \lesssim \|f\|_{\mathcal{N}_\Psi(\Omega)},$$

which, together with (69) and (76), yields

$$\begin{aligned} \|f - f^*\|_n &\lesssim h_n^{m_0} \|f\|_{N_\Psi(\Omega)} + h_n^{m_0} (C \lambda_m^{\frac{m_0-m}{2m}})^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} \\ &\lesssim (h_n^{m_0} + h_n^{m_0} \lambda_m^{\frac{(m_0-m)m_0}{2m^2}} + \lambda_m^{\frac{m_0}{2m}}) \|f\|_{\mathcal{N}_\Psi(\Omega)} \\ &\lesssim (h_n^{m_0} \lambda_m^{\frac{(m_0-m)m_0}{2m^2}} + \lambda_m^{\frac{m_0}{2m}}) \|f\|_{\mathcal{N}_\Psi(\Omega)}, \end{aligned} \quad (78)$$

where the second inequality is because $\lambda_m \leq C_3$ and $m \geq m_0$. By Condition (C4) and the condition $\lambda_m \gtrsim n^{-\frac{2m^2}{d(2m-m_0)}}$, it can be checked that $h_n^{m_0} \lambda_m^{\frac{(m_0-m)m_0}{2m^2}} \lesssim \lambda_m^{\frac{m_0}{2m}}$. Therefore, (78) can be further bounded by

$$\|f - f^*\|_n \lesssim (h_n^{m_0} \lambda_m^{\frac{(m_0-m)m_0}{2m^2}} + \lambda_m^{\frac{m_0}{2m}}) \|f\|_{\mathcal{N}_\Psi(\Omega)} \lesssim \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}. \quad (79)$$

Plugging (79) into (74), we have that with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\begin{aligned} &\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \\ &\lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 + 2tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\quad + 2tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + C \lambda_m \lambda_m^{\frac{m_0-m}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + 2tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\quad + 2tn^{-\frac{1}{2}} (C \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + 2tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\quad + 2tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} + 2tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\quad + 2tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}, \end{aligned} \quad (80)$$

where the second inequality is because of Lemma 31, and the third inequality is because of the triangle inequality $\|\hat{f}_m - f^*\|_{\mathcal{N}_\Phi(\Omega)} \leq \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + \|f^*\|_{\mathcal{N}_\Phi(\Omega)}$ and the basic inequality $(a+b)^q \leq a^q + b^q$ for any $a, b \geq 0$ and $q \in [0, 1]$.

Next, we consider two subcases.

Case 1.1: $\|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} \leq \|f^*\|_{\mathcal{N}_\Phi(\Omega)}$. Then (80) implies

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + 4tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\quad + 4tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}, \end{aligned}$$

which implies either

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}, \quad (81)$$

or

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\lesssim tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} (\lambda_m^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{\frac{d}{2m}}. \end{aligned} \quad (82)$$

By Lemma 31, (81) implies

$$\begin{aligned} &\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \\ &\lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} (\lambda_m^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{\frac{d}{2m}} \\ &= \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + tn^{-\frac{1}{2}} \lambda_m^{\frac{2m_0-d}{4m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}. \end{aligned} \quad (83)$$

Solving (82) leads to

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 &\lesssim t^{\frac{4m}{2m+d}} n^{-\frac{2m}{2m+d}} \lambda_m^{\frac{d(m_0-m)}{m(2m+d)}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2d}{2m+d}}, \\ \text{and } \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim t^{\frac{4m}{2m+d}} n^{-\frac{2m}{2m+d}} \lambda_m^{\frac{d(m_0-m)(2m-d)}{4m^2(2m+d)} - 1} \lambda_m^{\frac{d(m_0-m)}{4m^2}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2d}{2m+d}}, \\ &= t^{\frac{4m}{2m+d}} n^{-\frac{2m}{2m+d}} \lambda_m^{\frac{d(m_0-m)}{m(2m+d)} - 1} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2d}{2m+d}}. \end{aligned} \quad (84)$$

It can be seen that (83) yields

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 &\lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + tn^{-\frac{1}{2}} \lambda_m^{\frac{2m_0-d}{4m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}, \\ \text{and } \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim \lambda_m^{\frac{m_0-m}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + tn^{-\frac{1}{2}} \lambda_m^{\frac{2m_0-d-4m}{4m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}. \end{aligned} \quad (85)$$

Case 1.2: $\|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} > \|f^*\|_{\mathcal{N}_\Phi(\Omega)}$. Then (80) implies

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + 4tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ &\quad + 4tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}, \end{aligned}$$

which implies either

$$\begin{aligned} & \|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \\ & \lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + 4tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}, \end{aligned} \quad (86)$$

or

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}. \quad (87)$$

It can be seen that (86) implies either

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 \quad (88)$$

or

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim tn^{-\frac{1}{2}} (\lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{1-\frac{d}{2m}} \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}. \quad (89)$$

Solving (88) leads to

$$\|f - \hat{f}_m\|_n^2 \lesssim \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \quad \text{and} \quad \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim \lambda_m^{\frac{m_0-m}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2. \quad (90)$$

Solving (89) yields

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 & \lesssim \lambda_m^{-\frac{2mm_0-m_0d-md}{(4m-d)m}} t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2(2m-d)}{4m-d}}, \\ \text{and } \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} & \lesssim \lambda_m^{-\frac{2mm_0-m_0d-md}{(4m-d)m}-1} t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2(2m-d)}{4m-d}}. \end{aligned} \quad (91)$$

Solving (87) yields

$$\|f - \hat{f}_m\|_n \lesssim tn^{-\frac{1}{2}} \lambda_m^{-\frac{d}{4m}} \quad \text{and} \quad \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} \lesssim tn^{-\frac{1}{2}} \lambda_m^{-\frac{2m+d}{4m}}. \quad (92)$$

Combining all the cases listed in (84), (85), (90), (91) and (92), we have

$$\|f - \hat{f}_m\|_n^2 \lesssim T, \quad \text{and} \quad \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim \lambda_m^{-1} T, \quad (93)$$

where

$$\begin{aligned} T = \max \{ & t^{\frac{4m}{2m+d}} n^{-\frac{2m}{2m+d}} \lambda_m^{\frac{d(m_0-m)}{m(2m+d)}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2d}{2m+d}}, \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + tn^{-\frac{1}{2}} \lambda_m^{\frac{2m_0-d}{4m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}, \\ & t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{\frac{2mm_0-m_0d-md}{m(4m-d)}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2(2m-d)}{4m-d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}} \}. \end{aligned}$$

It remains to bound the difference between $\|f - \hat{f}_m\|_n$ and $\|f - \hat{f}_m\|_{L_2(\Omega)}$, which can be done by applying Lemma 26. To this end, note that $f^* - \hat{f}_m \in \mathcal{N}_\Phi(\Omega)$, which is equivalent

to $f^* - \hat{f}_m \in H^m(\Omega)$. By the triangle inequality and Lemma 31,

$$\begin{aligned}
 \|f - \hat{f}_m\|_{L_2(\Omega)} &\leq \|f - f^*\|_{L_2(\Omega)} + \|f^* - \hat{f}_m\|_{L_2(\Omega)} \\
 &\lesssim \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^m \|f^* - \hat{f}_m\|_{H^m(\Omega)} + \|f^* - \hat{f}_m\|_n \\
 &\lesssim \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^m \|f^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + \|f^* - \hat{f}_m\|_n \\
 &\lesssim \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^m \|f^*\|_{\mathcal{N}_\Phi(\Omega)} + h_n^m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + \|f - f^*\|_n + \|f - \hat{f}_m\|_n \\
 &\lesssim \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^m \lambda_m^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + \|f - \hat{f}_m\|_n \\
 &\lesssim \lambda_m^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^m \lambda_m^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^m \lambda_m^{-1/2} T^{1/2} + T^{1/2} \\
 &\lesssim T^{1/2}.
 \end{aligned} \tag{94}$$

The second inequality is by Lemma 31; the third inequality is by the equivalence of $H^m(\Omega)$ and $\mathcal{N}_\Phi(\Omega)$; the fourth inequality is by the triangle inequality; the fifth inequality is by Lemma 31 and (79); the sixth inequality is by (93); the last inequality is because of Condition (C4) and the condition $\lambda_m \gtrsim n^{-\frac{2m^2}{d(2m-m_0)}} \geq n^{-\frac{2m}{d}}$. Then the desired results of Case 1 follow from (93) and (94).

Case 2: f has smoothness m_0 and $f \notin \mathcal{N}_\Psi(\Omega)$.

Let f^* be as in Lemma 31. Let $\delta = \frac{m_0^2(m_0-d/2)}{2(m_0+m)(m_0-d/2)+m_0^2} > 0$, we have $f \in H^{m_0-\delta}$ and $m_0 - \delta > d/2$. Similar to the proof in Case 1, we can change (76) to

$$\begin{aligned}
 \|f - f^*\|_n &\lesssim h_n^{m_0-\delta} \|f - f^*\|_{H^{m_0-\delta}(\Omega)} + \|f - f^*\|_{L_2(\Omega)} \\
 &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0-\delta} \|f^*\|_{H^{m_0-\delta}(\Omega)} + \|f - f^*\|_{L_2(\Omega)} \\
 &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0-\delta} \|f^*\|_{L_2(\Omega)}^{\frac{m-m_0+\delta}{m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{m_0-\delta}{m}} + \|f - f^*\|_{L_2(\Omega)},
 \end{aligned} \tag{95}$$

where the second inequality is by the triangle inequality, and last inequality is because of the Gagliardo–Nirenberg interpolation inequality. The Sobolev embedding theorem suggests that $\|f\|_{L_2(\Omega)} \leq C_3 \|f\|_{H^{m_0-\delta}(\Omega)}$. Therefore, Lemma 31 gives us

$$\|f^*\|_{L_2(\Omega)} \lesssim \|f\|_{L_2(\Omega)} + \|f - f^*\|_{L_2(\Omega)} \lesssim \|f\|_{L_2(\Omega)} \lesssim \|f\|_{H^{m_0-\delta}(\Omega)}, \tag{96}$$

where the second inequality is because $\lambda_m = o(Q(n)^{-m/m_0})$ yields $\|f - f^*\|_{L_2(\Omega)} \rightarrow 0$, which implies $\|f - f^*\|_{L_2(\Omega)} \leq (C - 1) \|f\|_{L_2(\Omega)}$ for some $C > 0$.

By (70), (95), and (96), we have

$$\begin{aligned}
 \|f - f^*\|_n &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0-\delta} \|f^*\|_{L_2(\Omega)}^{\frac{m-m_0+\delta}{m}} \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{m_0-\delta}{m}} + \|f - f^*\|_{L_2(\Omega)} \\
 &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0-\delta} (\|f\|_{H^{m_0-\delta}(\Omega)})^{\frac{m-m_0+\delta}{m}} (\lambda_m^{\frac{m_0-m}{2m}} Q(n)^{1/2})^{\frac{m_0-\delta}{m}} + \lambda_m^{\frac{m_0}{2m}} Q(n)^{1/2} \\
 &\lesssim (h_n^{m_0-\delta} \lambda_m^{\frac{(m_0-m)(m_0-\delta)}{2m^2}} + \lambda_m^{\frac{m_0}{2m}}) \max\{Q(n)^{1/2}, \|f\|_{H^{m_0-\delta}(\Omega)}\},
 \end{aligned} \tag{97}$$

where the last inequality is because $\lambda_m = o(Q(n)^{-m/m_0})$ and $m_0 \leq m$. Since Q is an increasing function and satisfies

$$\lim_{r \rightarrow +\infty} \frac{\log Q(r)}{\log r} = 0,$$

there exists a constant C_4 such that $Q(r) \leq C_4(1+r^2)^\delta$ for all $r \geq 0$. Therefore, by the extension theorem, there exists an extension of f_e such that $f = f_e|_\Omega$, and

$$\begin{aligned} \|f\|_{H^{m_0-\delta}(\Omega)}^2 &\lesssim \|f_e\|_{H^{m_0-\delta}(\mathbb{R}^d)}^2 = \int_{\mathbb{R}^d} (1 + \|\omega\|_2^2)^{m_0-\delta} |\mathcal{F}(f_e)(\omega)|^2 d\omega \\ &\leq C_5 \int_{\mathbb{R}^d} \frac{(1 + \|\omega\|_2^2)^{m_0} |\mathcal{F}(f_e)(\omega)|^2}{Q(\|\omega\|)} d\omega \leq C_5, \end{aligned}$$

which implies $\max\{Q(n)^{1/2}, \|f\|_{H^{m_0-\delta}(\Omega)}\} \lesssim Q(n)^{1/2}$. Noting that $h_n \lesssim n^{-1/d}$ because \mathcal{X} satisfies Condition (C4), we have $h_n^{m_0-\delta} \lambda_m^{\frac{(m_0-m)(m_0-\delta)}{2m^2}} \lesssim \lambda_m^{\frac{m_0}{2m}}$. Therefore, (97) can be further bounded by

$$\|f - f^*\|_n \lesssim \lambda_m^{\frac{m_0}{2m}} Q(n)^{1/2}. \quad (98)$$

Repeating the proof in the case of $f \in \mathcal{N}_\Psi(\Omega)$, we can obtain that

$$\|f - \hat{f}_m\|_n^2 \leq C_6 T, \text{ and } \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C_6 \lambda_m^{-1} T,$$

where

$$\begin{aligned} T = \max\{ &t^{\frac{4m}{2m+d}} n^{-\frac{2m}{2m+d}} \lambda_m^{\frac{d(m_0-m)}{m(2m+d)}} Q(n)^{\frac{d}{2m+d}}, \lambda_m^{\frac{m_0}{m}} Q(n) + t n^{-\frac{1}{2}} \lambda_m^{\frac{2m_0-d}{4m}} Q(n)^{1/2}, \\ &t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{\frac{4mm_0-2m_0d-2md}{2m(4m-d)}} Q(n)^{\frac{2m-d}{4m-d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}} \}. \end{aligned}$$

Similar to the proof of (94), we have

$$\begin{aligned} \|f - \hat{f}_m\|_{L_2(\Omega)} &\leq \|f - f^*\|_{L_2(\Omega)} + \|f^* - \hat{f}_m\|_{L_2(\Omega)} \\ &\lesssim \lambda_m^{\frac{m_0}{2m}} Q(n)^{1/2} + h_n^m \|f^* - \hat{f}_m\|_{H^m(\Omega)} + \|f^* - \hat{f}_m\|_n \\ &\lesssim \lambda_m^{\frac{m_0}{2m}} Q(n)^{1/2} + h_n^m \lambda_m^{\frac{m_0-m}{2m}} Q(n)^{1/2} + h_n^m \lambda_m^{-1} T + T \\ &\lesssim T, \end{aligned}$$

where the second inequality is by Lemma 31. This finishes the proof of the case $f \notin \mathcal{N}_\Psi(\Omega)$, thus finishes the proof of Theorem 29.

Appendix J. Proof of Theorem 16

In this section, we set $m_0 := m_0(f)$ for notational simplicity. We show a generalized version of Theorem 16 as follows. Recall that $H^{m_0}(\Omega)$ coincides with $\mathcal{N}_\Psi(\Omega)$.

Theorem 32 *Suppose conditions in Theorem 16 hold. Suppose $\lambda_m = o(1)$ if $f \in \mathcal{N}_\Psi$, and $\lambda_m = o(Q(n)^{-2m/m_0})$ if $f \notin \mathcal{N}_\Psi$. Furthermore, suppose $\lambda_m \gtrsim n^{-\frac{2m}{d}}$. If $f \in \mathcal{N}_\Psi(\Omega)$, let*

$$T = \max\left\{n^{-\frac{2m_0}{2m_0+d}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + \lambda_m n^{-\frac{2(m_0-m)}{2m_0+d}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \right. \\ \left. t^{\frac{4m}{4m-d}} n^{-\frac{8mm_0+2md-2m_0d}{(4m-d)(2m_0+d)}} \lambda_m^{-\frac{d}{4m-d}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^{\frac{2m-d}{4m-d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}}\right\}.$$

For all $t \geq C_0$ and n , with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\|f - \hat{f}_m\|_{L_2(\Omega)} \lesssim T^{1/2}.$$

If $f \notin \mathcal{N}_\Psi(\Omega)$, for all $t \geq C_0$ and n , with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\|f - \hat{f}_m\|_{L_2(\Omega)} \lesssim T_1^{1/2},$$

where

$$T_1 = \max\left\{n^{-\frac{2m_0}{2m_0+d}} Q(n) + \lambda_m n^{-\frac{2(m_0-m)}{2m_0+d}} Q(n), \right. \\ \left. t^{\frac{4m}{4m-d}} n^{-\frac{8mm_0+2md-2m_0d}{(4m-d)(2m_0+d)}} \lambda_m^{-\frac{d}{4m-d}} Q(n)^{\frac{2m-d}{8m-2d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}}\right\}.$$

We first show that Theorem 32 implies Theorem 16. The results of Theorem 16 under the case of $m_0/2 \leq m < m_0$ can be obtained by setting $\lambda_m \asymp n^{-\frac{2m}{2m_0+d}}$.

If $d/2 < m < m_0/2$, we have that $f \in H^{2m}(\Omega)$. Therefore, replacing m_0 by $2m$ and setting $\lambda_m \asymp n^{-\frac{2m}{4m+d}}$ in the case of $m_0/2 \leq m < m_0$, we obtain

$$\|f - \hat{f}_m\|_{L_2(\Omega)} \lesssim n^{-\frac{2m}{4m+d}}.$$

Therefore, we conclude that Theorem 32 implies Theorem 16.

Now we begin to prove Theorem 29. We need the following lemmas. Lemma 33 is Proposition 2.1 of Tuo and Wu (2016).

Lemma 33 *Each $h \in \mathcal{N}_\Phi(\Omega)$ has an extension $h \in \mathcal{N}_\Phi(\mathbb{R}^d)$ which defines an isometric map from $\mathcal{N}_\Phi(\Omega)$ to $\mathcal{N}_\Phi(\mathbb{R}^d)$. In other words, $h_e|_\Omega \in \mathcal{N}_\Phi(\Omega)$, and $\langle h_e, h'_e \rangle_{\mathcal{N}_\Phi(\mathbb{R}^d)} = \langle h, h' \rangle_{\mathcal{N}_\Phi(\Omega)}$ for all $h, h' \in \mathcal{N}_\Phi(\Omega)$, where $h_e|_\Omega$ denotes the restriction of h_e on the region Ω .*

Remark 34 *As shown in Tuo et al. (2020), the map is extended by the map from $F_\Phi(\Omega)$ defined in (15) to $F_\Phi(\mathbb{R}^d)$ given by*

$$\sum_{k=1}^n \beta_k \Phi(x - x_k), x \in \Omega \mapsto \sum_{k=1}^n \beta_k \Phi(x - x_k), x \in \mathbb{R}^d.$$

Lemma 35 is implied by the proof of Theorem 2.2 of Tuo et al. (2020).

Lemma 35 *Let Φ satisfy Condition (C3) and $f \in \mathcal{N}_\Phi(\Omega)$. Let f_e be an extended function by the map in Lemma 33. Suppose $f_e \in H^{2m}(\mathbb{R}^d)$, then the integral equation*

$$f(x) = \int_{\Omega} \Phi(x-y)v(y)dy, \quad x \in \Omega,$$

has a solution $v = h_f|_{\Omega} \in L_2(\Omega)$, where $h_f = \mathcal{F}^{-1}(\mathcal{F}(f_e)/\mathcal{F}(\Phi))$.

The proof has three steps. In Step 1, we establish an *improved basic inequality*. In Step 2, we prove the results under the scenario that $f \in \mathcal{N}_\Psi(\Omega)$. In Step 3, we prove the results under the scenario that $f \notin \mathcal{N}_\Psi(\Omega)$.

Step 1: Establish the improved basic inequality.

Let

$$\Psi_{2m}(x) = \frac{1}{\Gamma(2m-d/2)2^{2m-d/2-1}} \|x\|_2^{2m-d/2} K_{2m-d/2}(\|x\|_2),$$

i.e., Ψ_{2m} be the Matérn kernel function as in (8) with $\nu = 2m-d/2$ and $\phi = (2\sqrt{2m-d/2})^{-1}$. Therefore, (9) implies that there exist constants $C_2 \geq C_1 > 0$ such that

$$C_1(1 + \|\omega\|_2^2)^{-2m} \leq \mathcal{F}(\Psi_{2m})(\omega) \leq C_2(1 + \|\omega\|_2^2)^{-2m},$$

and $\mathcal{N}_{\Psi_{2m}}(\Omega)$ coincides with the Sobolev space $H^{2m}(\Omega)$.

Let f^* be the solution to the optimization problem

$$\min_{\tilde{f} \in \mathcal{N}_{\Psi_{2m}}(\Omega)} \|f - \tilde{f}\|_{L_2(\Omega)}^2 + \lambda_{2m} \|\tilde{f}\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2, \quad (99)$$

and f_n^* be the solution to the optimization problem

$$\min_{\tilde{f} \in \mathcal{N}_{\Psi_{2m}}(\Omega)} \|f - \tilde{f}\|_n^2 + \lambda_{2m} \|\tilde{f}\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2, \quad (100)$$

where $\lambda_{2m} = n^{-\frac{4m}{2m_0+d}}$ is a regularization parameter.

Because \hat{f}_m is the solution to (13), we have

$$\|y - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq \|y - f_n^*\|_n^2 + \lambda_m \|f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^2. \quad (101)$$

By rearrangement, (101) yields

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq \|f - f_n^*\|_n^2 + \lambda_m \|f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^2 + 2\langle \epsilon, \hat{f}_m - f_n^* \rangle_n. \quad (102)$$

Notice that

$$\|f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^2 - \|\hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 = 2\langle f_n^* - \hat{f}_m, f_n^* \rangle_{\mathcal{N}_\Phi(\Omega)} - \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2. \quad (103)$$

Plugging (103) into (102) gives us

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq \|f - f_n^*\|_n^2 + 2\lambda_m \langle f_n^* - \hat{f}_m, f_n^* \rangle_{\mathcal{N}_\Phi(\Omega)} + 2\langle \epsilon, \hat{f}_m - f_n^* \rangle_n. \quad (104)$$

Next, we consider the term $\langle f_n^* - \hat{f}_m, f_n^* \rangle_{\mathcal{N}_\Phi(\Omega)}$ in (104). By the representer theorem, the solution of (100) can be expressed by

$$f_n^*(x) = r_{2m}(x)^T (R_{2m} + n\lambda_{2m}I_n)^{-1} F,$$

where $r_{2m}(x) = (\Psi_{2m}(x - x_1), \dots, \Psi_{2m}(x - x_n))^T$, $R_{2m} = (\Psi_{2m}(x_j - x_k))_{jk}$, I_n is an identity matrix, and $F = (f(x_1), \dots, f(x_n))^T$. We can extend $f_n^*(x)$ from $\mathcal{N}_{\Psi_{2m}}(\Omega)$ to $\mathcal{N}_{\Psi_{2m}}(\mathbb{R}^d)$ by the map

$$f_n^*(x) = r_{2m}(x)^T (R_{2m} + n\lambda_{2m}I_n)^{-1} F, x \in \Omega \mapsto f_{n,e}^*(x) = r_{2m}(x)^T (R_{2m} + n\lambda_{2m}I_n)^{-1} F, x \in \mathbb{R}^d.$$

Clearly, $\|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)} = \|f_{n,e}^*\|_{\mathcal{N}_{\Psi_{2m}}(\mathbb{R}^d)}$. As explained in Remark 34, $f_{n,e}$ is the extension as in Lemma 33. By the equivalence of $\mathcal{N}_{\Psi_{2m}}(\mathbb{R}^d)$ and $H^{2m}(\mathbb{R}^d)$, we can apply Lemma 35 to f_n^* , and obtain

$$f_n^*(x) = \int_{\Omega} \Phi(x - y)v(y)dy, \quad x \in \Omega,$$

with $v = h_f|_{\Omega} \in L_2(\Omega)$, where $h_f = \mathcal{F}^{-1}(\mathcal{F}(f_{n,e}^*)/\mathcal{F}(\Phi))$. Proposition 10.28 of Wendland (2004) shows that for any function $g \in \mathcal{N}_\Phi(\Omega)$, $\langle g, f_n^* \rangle_{\mathcal{N}_\Phi(\Omega)} = \langle g, v \rangle_{L_2(\Omega)}$. Together with (104), we have

$$\begin{aligned} & \|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq \|f - f_n^*\|_n^2 + 2\lambda_m \langle f_n^* - \hat{f}_m, v \rangle_{L_2(\Omega)} + 2\langle \epsilon, \hat{f}_m - f_n^* \rangle_n \\ & \leq \|f - f_n^*\|_n^2 + 2\lambda_m \|f_n^* - \hat{f}_m\|_{L_2(\Omega)} \|v\|_{L_2(\Omega)} + 2\langle \epsilon, \hat{f}_m - f_n^* \rangle_n. \end{aligned} \quad (105)$$

We call (105) the *improved basic inequality*, which improves the basic inequality (72) in the oversmoothed case.

Step 2: Prove the results under the case $f \in \mathcal{N}_\Psi(\Omega)$.

Applying Lemma 30 to $\langle \epsilon, \hat{f}_m - f_n^* \rangle_n$, we obtain that for all $t \geq C_0$, with probability at least $1 - C_1 \exp(-C_2 t^2)$,

$$\langle \epsilon, \hat{f}_m - f_n^* \rangle_n \leq tn^{-\frac{1}{2}} \|\hat{f}_m - f_n^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}. \quad (106)$$

Plugging (106) into (105), we obtain

$$\begin{aligned} & \|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \\ & \leq \|f - f_n^*\|_n^2 + 2\lambda_m \|f_n^* - \hat{f}_m\|_{L_2(\Omega)} \|v\|_{L_2(\Omega)} + Ctn^{-\frac{1}{2}} \|\hat{f}_m - f_n^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\ & \leq \|f - f_n^*\|_n^2 + 2\lambda_m \|f - f_n^*\|_{L_2(\Omega)} \|v\|_{L_2(\Omega)} + 2\lambda_m \|f - \hat{f}_m\|_{L_2(\Omega)} \|v\|_{L_2(\Omega)} \\ & \quad + Ctn^{-\frac{1}{2}} \|f - f_n^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} + Ctn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}, \end{aligned} \quad (107)$$

where the second inequality is because of the triangle inequality $\|\hat{f}_m - f_n^*\|_n \leq \|f - \hat{f}_m\|_n + \|f - f_n^*\|_n$ and the basic inequality $(a + b)^q \leq a^q + b^q$ for any $a, b \geq 0$ and $q \in [0, 1]$.

Since $m_0/2 \leq m$, we have $2m \geq m_0$. Recall that f^* is the solution to (99). Lemma 31 gives us that

$$\|f - f^*\|_{L_2}^2 \lesssim \lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \text{ and } \|f^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2 \lesssim \lambda_{2m}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2. \quad (108)$$

As shown in (79), we have

$$\begin{aligned} \|f - f^*\|_n^2 &\lesssim (h_n^{m_0} \lambda_{2m}^{\frac{(m_0-2m)m_0}{8m^2}} + \lambda_{2m}^{\frac{m_0}{4m}})^2 \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 \\ &\lesssim (h_n^{2m_0} \lambda_{2m}^{\frac{(m_0-2m)m_0}{4m^2}} + \lambda_{2m}^{\frac{m_0}{2m}}) \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 \lesssim \lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \end{aligned} \quad (109)$$

where the second inequality is because of the Cauchy-Schwarz inequality, and the last inequality is because $h_n \lesssim n^{-1/d}$ and $\lambda_{2m} = n^{-\frac{4m}{2m_0+d}}$ (thus $h_n^{2m_0} \lambda_{2m}^{\frac{(m_0-2m)m_0}{4m^2}} \lesssim \lambda_{2m}^{\frac{m_0}{2m}}$).

Because f_n^* is the solution to (100), we have

$$\|f - f_n^*\|_n^2 + \lambda_{2m} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2 \leq \|f - f^*\|_n^2 + \lambda_{2m} \|f^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2. \quad (110)$$

Combining (108), (109), and (110) yields

$$\|f - f_n^*\|_n^2 + \lambda_{2m} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2 \lesssim \lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2,$$

which implies

$$\|f - f_n^*\|_n^2 \lesssim \lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \text{ and } \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2 \lesssim \lambda_{2m}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2. \quad (111)$$

Similar to (75), by the Gagliardo–Nirenberg interpolation inequality, we can show that

$$\|f_n^*\|_{\mathcal{N}_\Psi(\Omega)} \lesssim \|f_n^*\|_{H^{m_0}(\Omega)} \lesssim \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0}{2m}} \|f_n^*\|_{H^{2m}(\Omega)}^{\frac{m_0}{2m}} \lesssim \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0}{2m}}. \quad (112)$$

Applying Lemma 26 to $\|f - f_n^*\|_{L_2(\Omega)}$, it can be seen that

$$\begin{aligned} \|f - f_n^*\|_{L_2(\Omega)} &\lesssim h_n^{m_0} \|f - f_n^*\|_{H^{m_0}(\Omega)} + \|f - f_n^*\|_n \\ &\lesssim h_n^{m_0} \|f - f_n^*\|_{\mathcal{N}_\Psi(\Omega)} + \|f - f_n^*\|_n \\ &\lesssim h_n^{m_0} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^{m_0} \|f_n^*\|_{\mathcal{N}_\Psi(\Omega)} + \|f - f_n^*\|_n \\ &\lesssim h_n^{m_0} \|f\|_{\mathcal{N}_\Psi(\Omega)} + h_n^{m_0} \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0}{2m}} + \lambda_{2m}^{\frac{m_0}{4m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} \\ &\lesssim h_n^{m_0} \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0}{2m}} + \lambda_{2m}^{\frac{m_0}{4m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}, \end{aligned} \quad (113)$$

where the second inequality is because $\|\cdot\|_{H^{m_0}(\Omega)}$ is equivalent to $\|\cdot\|_{\mathcal{N}_\Psi(\Omega)}$, the third inequality is because of the triangle inequality, the fourth inequality is because of (111) and (112), and the last inequality is because $h_n^{m_0} \lesssim \lambda_{2m}^{\frac{m_0}{4m}}$.

Applying Lemma 26 to $\|f_n^*\|_{L_2(\Omega)}$ leads to

$$\begin{aligned} \|f_n^*\|_{L_2(\Omega)} &\lesssim h_n^{2m} \|f_n^*\|_{H^{2m}(\Omega)} + \|f_n^*\|_n \lesssim h_n^{2m} \|f_n^*\|_{N_{\Psi_{2m}}(\Omega)} + \|f_n^*\|_n \\ &\lesssim h_n^{2m} \|f_n^*\|_{N_{\Psi_{2m}}(\Omega)} + \|f\|_n + \|f - f^*\|_n \\ &\lesssim h_n^{2m} \lambda_{2m}^{\frac{m_0}{4m}-1/2} \|f\|_{\mathcal{N}_{\Psi}(\Omega)} + \|f\|_n + \lambda_{2m}^{\frac{m_0}{4m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)} \lesssim \|f\|_{\mathcal{N}_{\Psi}(\Omega)}, \end{aligned} \quad (114)$$

where the second inequality is because $\|\cdot\|_{H^{2m}(\Omega)}$ is equivalent to $\|\cdot\|_{N_{\Psi_{2m}}(\Omega)}$, the third inequality is because of the triangle inequality, the fourth inequality is because of (109) and (111), and the last inequality is because of $h_n \lesssim n^{-1/d}$ and (77).

Plugging (111) and (114) into (113), we have

$$\|f - f_n^*\|_{L_2(\Omega)} \lesssim h_n^{m_0} \lambda_{2m}^{\frac{m_0(m_0-2m)}{8m^2}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)} + \lambda_{2m}^{\frac{m_0}{4m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)} \lesssim \lambda_{2m}^{\frac{m_0}{4m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}, \quad (115)$$

where the last inequality is because $h_n^{m_0} \lambda_{2m}^{\frac{m_0(m_0-2m)}{8m^2}} \lesssim \lambda_{2m}^{\frac{m_0}{4m}}$, which can be checked by noting the fact $h_n \lesssim n^{-1/d}$ and $\lambda_{2m} = n^{-\frac{4m}{2m_0+d}}$.

The Plancherel theorem (Bracewell, 1986) implies that

$$\|v\|_{L_2(\Omega)}^2 \lesssim \|h_f\|_{L_2(\mathbb{R}^d)}^2 = \|\mathcal{F}(f_{n,e}^*)/\mathcal{F}(\Phi)\|_{L_2(\mathbb{R}^d)}^2 \lesssim \|f_{n,e}^*\|_{\mathcal{N}_{\Psi_{2m}}(\mathbb{R}^d)}^2 \lesssim \lambda_{2m}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2. \quad (116)$$

So far, we have provided upper bounds of $\|f - f_n^*\|_n$, $\|f - f_n^*\|_{L_2(\Omega)}$, and $\|v\|_{L_2(\Omega)}$. It remains to solve (107), which can be divided to several cases. Note that (107) implies that either

$$\|f - \hat{f}_n\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)}^2 \leq 2(\|f - f_n^*\|_n^2 + 2\lambda_m \|f - f_n^*\|_{L_2(\Omega)} \|v\|_{L_2(\Omega)}), \quad (117)$$

or

$$\begin{aligned} &\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)}^2 \\ &\leq 2(2\lambda_m \|f - \hat{f}_m\|_{L_2(\Omega)} \|v\|_{L_2(\Omega)} + Ctn^{-\frac{1}{2}} \|f - f_n^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f_n^*\|_{\mathcal{N}_{\Phi}(\Omega)}^{\frac{d}{2m}} \\ &\quad + Ctn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|f_n^* - \hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)}^{\frac{d}{2m}}). \end{aligned} \quad (118)$$

Plugging (111), (115), and (116) into (117) leads to

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)}^2 \lesssim \lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2 + \lambda_m \lambda_{2m}^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2,$$

which implies

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 &\lesssim \lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2 + \lambda_m \lambda_{2m}^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2, \\ \text{and } \|f_n^* - \hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)}^2 &\lesssim \lambda_m^{-1} \lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2 + \lambda_{2m}^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_{\Psi}(\Omega)}^2. \end{aligned} \quad (119)$$

Solving (118) is more complicated. By Lemma 26, it holds that

$$\begin{aligned}
 \|f - \hat{f}_m\|_{L_2(\Omega)} &\lesssim h_n^m \|f - \hat{f}_m\|_{H^m(\Omega)} + \|f - \hat{f}_m\|_n \\
 &\lesssim h_n^m \|f - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + \|f - \hat{f}_m\|_n \\
 &\lesssim h_n^m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + h_n^m \|f - f_n^*\|_{\mathcal{N}_\Phi(\Omega)} + \|f - \hat{f}_m\|_n, \tag{120}
 \end{aligned}$$

where the second inequality is by the equivalence of $\|\cdot\|_{H^m(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_\Phi(\Omega)}$, and the third inequality is by the triangle inequality.

By the Gagliardo–Nirenberg interpolation inequality, we have

$$\|f - f_n^*\|_{\mathcal{N}_\Phi(\Omega)} \lesssim \|f - f_n^*\|_{H^m(\Omega)} \lesssim \|f - f_n^*\|_{L_2(\Omega)}^{\frac{m_0-m}{m_0}} \|f - f_n^*\|_{H^{m_0}(\Omega)}^{\frac{m}{m_0}}, \tag{121}$$

where the first inequality is because of the equivalence of $\|\cdot\|_{H^m(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_\Phi(\Omega)}$. Using the Gagliardo–Nirenberg interpolation inequality again, we find that

$$\begin{aligned}
 \|f - f_n^*\|_{H^{m_0}(\Omega)} &\leq \|f\|_{H^{m_0}(\Omega)} + \|f_n^*\|_{H^{m_0}(\Omega)} \lesssim \|f\|_{H^{m_0}(\Omega)} + \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0}{2m}} \|f_n^*\|_{H^{2m}(\Omega)}^{\frac{m_0}{2m}} \\
 &\lesssim \|f\|_{\mathcal{N}_\Psi(\Omega)} + \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0}{2m}} \lesssim \|f\|_{\mathcal{N}_\Psi(\Omega)} + \lambda_{2m}^{\frac{(m_0-2m)m_0}{8m^2}} \|f\|_{\mathcal{N}_\Psi(\Omega)} \lesssim \lambda_{2m}^{\frac{(m_0-2m)m_0}{8m^2}} \|f\|_{\mathcal{N}_\Psi(\Omega)}, \tag{122}
 \end{aligned}$$

where the first inequality is by the triangle inequality, the third inequality is by the equivalence of $\|\cdot\|_{H^{m_0}(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_\Psi(\Omega)}$ and the equivalence of $\|\cdot\|_{H^{2m}(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}$, the fourth inequality is by (111) and (114), and the last inequality is because $\lambda_{2m} \lesssim 1$ and $m_0 \leq 2m$. Combining (115), (120), (121), and (122) leads to

$$\begin{aligned}
 \|f - \hat{f}_m\|_{L_2(\Omega)} &\lesssim h_n^m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + h_n^m \|f - f_n^*\|_{L_2(\Omega)}^{\frac{m_0-m}{m_0}} \|f - f_n^*\|_{H^{m_0}(\Omega)}^{\frac{m}{m_0}} + \|f - \hat{f}_m\|_n \\
 &\lesssim h_n^m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + h_n^m \lambda_{2m}^{\frac{3m_0-4m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + \|f - \hat{f}_m\|_n. \tag{123}
 \end{aligned}$$

Plugging (123) into (118) leads to

$$\begin{aligned}
 &\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \\
 &\lesssim h_n^m \lambda_m \|v\|_{L_2(\Omega)} \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + h_n^m \lambda_m \|v\|_{L_2(\Omega)} \lambda_{2m}^{\frac{3m_0-4m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + \lambda_m \|v\|_{L_2(\Omega)} \|f - \hat{f}_m\|_n \\
 &\quad + tn^{-\frac{1}{2}} \|f - f_n^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} + tn^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}} \\
 &= I_1 + I_2 + I_3 + I_4 + I_5. \tag{124}
 \end{aligned}$$

Depending on which I_k is equal to $\max\{I_1, I_2, \dots, I_5\}$, (124) implies one of the following case is true:

Case 1.1: $I_1 = \max\{I_1, I_2, \dots, I_5\}$. Under this case, we have

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim h_n^m \lambda_m \|v\|_{L_2(\Omega)} \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}. \tag{125}$$

For the conciseness of this proof, we only provide details on solving (125) in Case 1.1. The inequalities in other cases can be solved similarly.

Note that (125) implies that

$$\lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim h_n^m \lambda_m \|v\|_{L_2(\Omega)} \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)},$$

which implies

$$\|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim h_n^{2m} \|v\|_{L_2(\Omega)}^2 \lesssim h_n^{2m} \lambda_{2m}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \quad (126)$$

where the last inequality is because of (116). Together with (125), we have

$$\|f - \hat{f}_m\|_n^2 \lesssim h_n^m \lambda_m \|v\|_{L_2(\Omega)} \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} \lesssim h_n^{2m} \lambda_m \lambda_{2m}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2. \quad (127)$$

Case 1.2: $I_2 = \max\{I_1, I_2, \dots, I_5\}$. Under this case, we have

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim h_n^m \lambda_m \|v\|_{L_2(\Omega)} \lambda_{2m}^{\frac{3m_0-4m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}. \quad (128)$$

By (116), (128) yields

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 &\lesssim h_n^m \lambda_m \lambda_{2m}^{\frac{5m_0-8m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \\ \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim h_n^m \lambda_{2m}^{\frac{5m_0-8m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2. \end{aligned} \quad (129)$$

Case 1.3: $I_3 = \max\{I_1, I_2, \dots, I_5\}$. Under this case, we have

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim \lambda_m \|v\|_{L_2(\Omega)} \|f - \hat{f}_m\|_n. \quad (130)$$

Solving (130) leads to

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 &\lesssim \lambda_m^2 \lambda_{2m}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \\ \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim \lambda_m \lambda_{2m}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \end{aligned} \quad (131)$$

where we use (116) to bound $\|v\|_{L_2(\Omega)}$.

Case 1.4: $I_4 = \max\{I_1, I_2, \dots, I_5\}$. Under this case, we have

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim t n^{-\frac{1}{2}} \|f - f_n^*\|_n^{1-\frac{d}{2m}} \|\hat{f}_m - f_n^*\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}. \quad (132)$$

Solving (132) leads to

$$\begin{aligned} \|f - \hat{f}_m\|_n^2 &\lesssim t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{-\frac{d}{4m-d}} (\lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{\frac{2m-d}{4m-d}}, \\ \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 &\lesssim t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{-\frac{4m}{4m-d}} (\lambda_{2m}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)})^{\frac{2m-d}{4m-d}}, \end{aligned} \quad (133)$$

where we use (111) to bound $\|f - f_n^*\|_n$.

Case 1.5: $I_5 = \max\{I_1, I_2, \dots, I_5\}$. Under this case, we have

$$\|f - \hat{f}_m\|_n^2 + \lambda_m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim t n^{-\frac{1}{2}} \|f - \hat{f}_m\|_n^{1-\frac{d}{2m}} \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^{\frac{d}{2m}}. \quad (134)$$

Solving (134) leads to

$$\|f - \hat{f}_m\|_n^2 \lesssim t^2 n^{-1} \lambda_m^{-\frac{d}{2m}}, \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim t^2 n^{-1} \lambda_m^{-\frac{2m+d}{2m}}. \quad (135)$$

Combining (119), (126), (127), (129), (131), (133), and (135) we have

$$\|f - \hat{f}_m\|_n^2 \lesssim T, \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)}^2 \lesssim \lambda_m^{-1} T, \quad (136)$$

where

$$\begin{aligned} T &= \max\left\{\lambda_{\frac{2m}{2m}}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + \lambda_m \lambda_{\frac{2m}{2m}}^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, h_n^{2m} \lambda_m \lambda_{\frac{2m}{2m}}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \right. \\ &\quad h_n^m \lambda_m \lambda_{\frac{2m}{2m}}^{\frac{5m_0-8m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \lambda_m^2 \lambda_{\frac{2m}{2m}}^{\frac{m_0-2m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \\ &\quad \left. t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{-\frac{d}{4m-d}} \left(\lambda_{\frac{2m}{2m}}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}\right)^{\frac{2m-d}{4m-d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}}\right\} \\ &= \max\left\{\lambda_{\frac{2m}{2m}}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 + \lambda_m \lambda_{\frac{2m}{2m}}^{\frac{m_0-m}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \right. \\ &\quad \left. t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{-\frac{d}{4m-d}} \left(\lambda_{\frac{2m}{2m}}^{\frac{m_0}{2m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}\right)^{\frac{2m-d}{4m-d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}}\right\}, \end{aligned}$$

because $\lambda_m^2 \lambda_{\frac{2m}{2m}}^{\frac{m_0-2m}{2m}} \lesssim \lambda_m \lambda_{\frac{2m}{2m}}^{\frac{m_0-2m}{2m}}$, $h_n \lesssim n^{-1/d}$ and $\lambda_{2m} = n^{-\frac{4m}{2m_0+d}}$.

We finish Step 2 by bounding the difference between $\|f - \hat{f}_m\|_n^2$ and $\|f - \hat{f}_m\|_{L_2(\Omega)}^2$. By (115), (121), and (122), it can be seen that

$$\|f - f_n^*\|_{\mathcal{N}_\Phi(\Omega)} \lesssim \|f - f_n^*\|_{L_2(\Omega)}^{\frac{m_0-m}{m_0}} \|f - f_n^*\|_{H^{m_0}(\Omega)}^{\frac{m}{m_0}} \lesssim \lambda_{\frac{2m}{2m}}^{\frac{3m_0-4m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}. \quad (137)$$

By (120), (136), and (137), we have

$$\begin{aligned} \|f - \hat{f}_m\|_{L_2(\Omega)} &\lesssim h_n^m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + h_n^m \|f - f_n^*\|_{\mathcal{N}_\Phi(\Omega)} + \|f - \hat{f}_m\|_n \\ &\lesssim h_n^m \lambda_m^{-1/2} T^{1/2} + h_n^m \lambda_{\frac{2m}{2m}}^{\frac{3m_0-4m}{8m}} \|f\|_{\mathcal{N}_\Psi(\Omega)} + T^{1/2} \\ &\lesssim T^{1/2} + n^{-\frac{4m_0m+3m_0d-2md}{2d(2m_0+d)}} \lesssim T^{1/2}, \end{aligned}$$

where the second inequality is by $\lambda_m \gtrsim n^{-\frac{2m}{d}}$, the third inequality is by $h_n \lesssim n^{-1/d}$ and $\lambda_{2m} = n^{-\frac{4m}{2m_0+d}}$, and the last inequality is because the optimal convergence rate of T is $n^{-\frac{2m_0}{2m_0+d}}$, which is always larger than $n^{-\frac{4m_0m+3m_0d-2md}{d(2m_0+d)}}$. Therefore, we finish the proof of the case $f \in \mathcal{N}_\Psi(\Omega)$.

Step 3: Proof of the case $f \notin \mathcal{N}_\Psi(\Omega)$.

Let f^* be as in (99). We still set $\lambda_{2m} = n^{-\frac{4m}{2m_0+d}}$. If $f \notin \mathcal{N}_\Psi(\Omega)$, Lemma 31 gives us that

$$\|f - f^*\|_{L_2}^2 \leq C \lambda_{\frac{2m}{2m}}^{\frac{m_0}{2m}} Q(n), \text{ and } \|f^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2 \leq C \lambda_{\frac{2m}{2m}}^{\frac{m_0-2m}{2m}} Q(n), \quad (138)$$

where $Q: \mathbb{R}_+ \mapsto \mathbb{R}_+$ satisfies

$$\lim_{r \rightarrow +\infty} \frac{\log Q(r)}{\log r} = 0.$$

Let $\delta = \frac{m_0^2(m_0-d/2)}{2(m_0+2m)(m_0-d/2)+m_0^2} > 0$. Thus, $m_0 - \delta > d/2$. As shown in (98) (note that we replace m in (98) by $2m$ in (139)), we have

$$\|f - f^*\|_n \lesssim \lambda_{2m}^{\frac{m_0}{4m}} Q(n)^{1/2}. \quad (139)$$

Note that (110) is also valid under the case of $f \notin \mathcal{N}_{\Psi(\Omega)}$. Combining (139) with (110) and (138), yields

$$\|f - f_n^*\|_n^2 + \lambda_{2m} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^2 \lesssim \lambda_{2m}^{\frac{m_0}{2m}} Q(n). \quad (140)$$

By the Gagliardo–Nirenberg interpolation inequality, we have

$$\|f_n^*\|_{H^{m_0-\delta}(\Omega)} \lesssim \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0+\delta}{2m}} \|f_n^*\|_{H^{2m}(\Omega)}^{\frac{m_0-\delta}{2m}} \lesssim \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0+\delta}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0-\delta}{2m}}, \quad (141)$$

where the last inequality is because of the equivalence of $\|\cdot\|_{H^{2m}(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}$. By Lemma 26, it can be seen that

$$\begin{aligned} \|f - f_n^*\|_{L_2(\Omega)} &\lesssim h_n^{m_0-\delta} \|f - f_n^*\|_{H^{m_0-\delta}(\Omega)} + \|f - f_n^*\|_n \\ &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0} \|f_n^*\|_{H^{m_0-\delta}(\Omega)} + \|f - f_n^*\|_n \\ &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0-\delta} \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0+\delta}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0-\delta}{2m}} + \lambda_{2m}^{\frac{m_0}{4m}} Q(n)^{1/2}, \end{aligned} \quad (142)$$

where the second inequality is because of the triangle inequality, and the last inequality is because of (140) and (141).

Since $f_n^* \in \mathcal{N}_{\Psi_{2m}}(\Omega)$, $f_n^* \in H^{2m}(\Omega)$. Applying Lemma 26 to f_n^* leads to

$$\begin{aligned} \|f_n^*\|_{L_2(\Omega)} &\lesssim h_n^{2m} \|f_n^*\|_{H^{2m}(\Omega)} + \|f_n^*\|_n \\ &\lesssim h_n^{2m} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)} + \|f\|_n + \|f - f_n^*\|_n \\ &\lesssim h_n^{2m} \lambda_{2m}^{\frac{m_0-2m}{2m}} Q(n) + \|f\|_n + \lambda_{2m}^{\frac{m_0}{4m}} Q(n)^{1/2} \\ &\lesssim 1, \end{aligned} \quad (143)$$

where the second inequality is by the equivalence of $\|\cdot\|_{H^{2m}(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}$ and the triangle inequality, the third inequality is by (140), and the last inequality is because of (77) and $h_n^{2m} \lambda_{2m}^{\frac{m_0-2m}{2m}} Q(n) \lesssim n^{-\frac{2m(2m_0-d)+2m_0d}{(2m_0+d)d}} Q(n) \lesssim 1$.

Similar to the proof of Theorem 29, we have $\|f\|_{H^{m_0-\delta}(\Omega)} \lesssim Q(n)^{1/2}$. Plugging (143) into (142), we have

$$\begin{aligned} \|f - f_n^*\|_{L_2(\Omega)} &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0-\delta} \|f_n^*\|_{L_2(\Omega)}^{\frac{m-m_0+\delta}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0-\delta}{2m}} + \lambda_{2m}^{\frac{m_0}{4m}} Q(n)^{1/2} \\ &\lesssim h_n^{m_0-\delta} \|f\|_{H^{m_0-\delta}(\Omega)} + h_n^{m_0-\delta} (\lambda_{2m}^{\frac{m_0-2m}{4m}} Q(n)^{1/2})^{\frac{m_0-\delta}{2m}} + \lambda_{2m}^{\frac{m_0}{4m}} Q(n)^{1/2} \\ &\lesssim \lambda_{2m}^{\frac{m_0}{4m}} Q(n)^{1/2}, \end{aligned} \quad (144)$$

where the second inequality is by (140), and the last inequality is because $h_n^{m_0-\delta} \lambda_{2m}^{\frac{(m_0-2m)(m_0-\delta)}{8m^2}} \lesssim \lambda_{2m}^{\frac{m_0}{4m}}$ and $Q(n) \gtrsim 1$.

The Plancherel theorem (Bracewell, 1986) implies that

$$\|v\|_{L_2(\Omega)}^2 \lesssim \|h_f\|_{L_2(\mathbb{R}^d)}^2 = \|\mathcal{F}(f_{n,e}^*)/\mathcal{F}(\Phi)\|_{L_2(\mathbb{R}^d)}^2 \lesssim \|f_{n,e}^*\|_{\mathcal{N}_{\Psi_{2m}}(\mathbb{R}^d)}^2 \lesssim \lambda_{2m}^{\frac{m_0-2m}{2m}} Q(n).$$

Note that (107) also holds for $f \notin \mathcal{N}_{\Psi(\Omega)}$. Repeating the process of obtaining (119), (126), (127), (129), (131), (133), and (135), we have

$$\|f - \hat{f}_m\|_n^2 \lesssim T_1, \|f_n^* - \hat{f}_m\|_{\mathcal{N}_{\Phi}(\Omega)}^2 \lesssim \lambda_m^{-1} T_1, \quad (145)$$

where

$$T_1 = \max\left\{\lambda_{2m}^{\frac{m_0}{2m}} Q(n) + \lambda_m \lambda_{2m}^{\frac{m_0-m}{2m}} Q(n), t^{\frac{4m}{4m-d}} n^{-\frac{2m}{4m-d}} \lambda_m^{-\frac{d}{4m-d}} (\lambda_{2m}^{\frac{m_0}{2m}} Q(n))^{\frac{2m-d}{4m-d}}, t^2 n^{-1} \lambda_m^{-\frac{d}{2m}}\right\}.$$

It remains to bound the difference between $\|f - \hat{f}_m\|_n^2$ and $\|f - \hat{f}_m\|_{L_2(\Omega)}^2$. Using the Gagliardo–Nirenberg interpolation inequality, for $\delta_1 = \min\{m_0 - m, \frac{m_0^2 d + 2mm_0(2m_0 - d)}{8mm_0 + 4md}\} > 0$, we find that

$$\begin{aligned} \|f - f_n^*\|_{H^{m_0-\delta_1}(\Omega)} &\leq \|f\|_{H^{m_0-\delta_1}(\Omega)} + \|f_n^*\|_{H^{m_0-\delta_1}(\Omega)} \\ &\lesssim \|f\|_{H^{m_0-\delta_1}(\Omega)} + \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0+\delta_1}{2m}} \|f_n^*\|_{H^{\frac{m_0-\delta_1}{2m}}(\Omega)} \\ &\lesssim \|f\|_{H^{m_0-\delta_1}(\Omega)} + \|f_n^*\|_{L_2(\Omega)}^{\frac{2m-m_0+\delta_1}{2m}} \|f_n^*\|_{\mathcal{N}_{\Psi_{2m}}(\Omega)}^{\frac{m_0-\delta_1}{2m}} \\ &\lesssim \|f\|_{H^{m_0-\delta_1}(\Omega)} + (\lambda_{2m}^{\frac{m_0-2m}{4m}} Q(n))^{1/2} \frac{m_0-\delta_1}{2m} \\ &\lesssim (\lambda_{2m}^{\frac{m_0-2m}{4m}} Q(n))^{1/2} \frac{m_0-\delta_1}{2m}, \end{aligned} \quad (146)$$

where the first inequality is by the triangle inequality, the third inequality is by the equivalence of $\|\cdot\|_{H^{2m}(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_{\Psi_{2m}}}$, the fourth inequality is by (140) and (143), and the last inequality is by $\|f\|_{H^{m_0-\delta_1}(\Omega)} \lesssim Q(n)^{1/2}$ (which can be shown similarly as showing $\|f\|_{H^{m_0-\delta}(\Omega)} \lesssim Q(n)^{1/2}$), and $Q(n)^{\frac{2m-m_0}{4m}} \lesssim \lambda_{2m}^{\frac{m_0(m_0-2m)}{8m^2}}$.

By the Gagliardo–Nirenberg interpolation inequality, we have

$$\begin{aligned} \|f - f_n^*\|_{\mathcal{N}_{\Phi}(\Omega)} &\lesssim \|f - f_n^*\|_{H^m(\Omega)} \lesssim \|f - f_n^*\|_{L_2(\Omega)}^{\frac{m_0-\delta_1-m}{m_0-\delta_1}} \|f - f_n^*\|_{H^{\frac{m_0-\delta_1}{m_0-\delta_1}}(\Omega)} \\ &\lesssim (\lambda_{2m}^{\frac{m_0}{4m}} Q(n))^{1/2} \frac{m_0-\delta_1-m}{m_0-\delta_1} ((\lambda_{2m}^{\frac{m_0-2m}{4m}} Q(n))^{1/2} \frac{m_0-\delta_1}{2m})^{\frac{m}{m_0-\delta_1}} \\ &= \lambda_{2m}^{\frac{3m_0^2-3m_0\delta_1-4mm_0+2m\delta_1}{8m(m_0-\delta_1)}} Q(n)^{\frac{3m_0-2m-3\delta_1}{4(m_0-\delta_1)}}, \end{aligned} \quad (147)$$

where the first inequality is because of the equivalence of $\|\cdot\|_{H^m(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_{\Phi}(\Omega)}$, and third inequality is by (144) and (146).

By Lemma 26, we have

$$\begin{aligned}
 \|f - \hat{f}_m\|_{L_2(\Omega)} &\lesssim h_n^m \|f - \hat{f}_m\|_{H^m(\Omega)} + \|f - \hat{f}_m\|_n \\
 &\lesssim h_n^m \|f - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + \|f - \hat{f}_m\|_n \\
 &\lesssim h_n^m \|f_n^* - \hat{f}_m\|_{\mathcal{N}_\Phi(\Omega)} + h_n^m \|f - f_n^*\|_{\mathcal{N}_\Phi(\Omega)} + \|f - \hat{f}_m\|_n \\
 &\lesssim h_n^m \lambda_m^{-1/2} T_1^{1/2} + h_n^m \lambda_{2m}^{\frac{3m_0^2 - 3m_0\delta_1 - 4mm_0 + 2m\delta_1}{8m(m_0 - \delta_1)}} Q(n)^{\frac{3m_0 - 2m - 3\delta_1}{4(m_0 - \delta_1)}} + T_1^{1/2} \\
 &\lesssim T_1^{1/2},
 \end{aligned}$$

where the second inequality is by the equivalence of $\|\cdot\|_{H^m(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_\Phi(\Omega)}$, the third inequality is by the triangle inequality. The fourth inequality is by (136), (145), (146) and (147), and the last inequality is by the facts that $\lambda_m \gtrsim n^{-\frac{2m}{d}}$, $h_n \lesssim n^{-1/d}$, $\lambda_{2m} = n^{-\frac{4m}{2m_0+d}}$, and that since T_1 is always larger than $n^{-\frac{2m_0}{2m_0+d}}$, it can be checked that $T_1^{1/2}$ is always larger than $h_n^m \lambda_{2m}^{\frac{3m_0^2 - 3m_0\delta_1 - 4mm_0 + 2m\delta_1}{8m(m_0 - \delta_1)}} Q(n)^{\frac{3m_0 - 2m - 3\delta_1}{4(m_0 - \delta_1)}}$, which is also because of our choice of δ_1 . Therefore, we finish the proof.

Appendix K. Proof of Proposition 17

Let $u = (u_1, \dots, u_n)^T = (R_m + \mu_m I_n)^{-1} r_m(x)$. By the representer theorem,

$$\hat{f}_m(x) = u^T Y = u^T F + u^T \epsilon,$$

where $F = (f(x_1), \dots, f(x_n))^T$ and $\epsilon = (\epsilon_1, \dots, \epsilon_n)^T$. Therefore,

$$\mathbb{E}(f(x) - \hat{f}_m(x))^2 = (f(x) - u^T F)^2 + \sigma_\epsilon^2 u^T u, \quad (148)$$

where σ_ϵ^2 is the variance of ϵ_j . The Fourier inverse theorem implies

$$\begin{aligned}
 &(f(x) - \sum_{j=1}^n u_j f(x_j))^2 \\
 &= \left| \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left(\sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right) \mathcal{F}(f)(\omega) d\omega \right|^2 \\
 &\leq \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{|\mathcal{F}(f)(\omega)|^2}{\mathcal{F}(\Psi)(\omega)} d\omega \\
 &= \left(\Psi(x - x) - 2 \sum_{j=1}^n u_j \Psi(x - x_j) + \sum_{j=1}^n \sum_{k=1}^n u_k u_j \Psi(x_k - x_j) \right) \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \quad (149)
 \end{aligned}$$

where the inequality is by the Cauchy-Schwarz inequality.

Now consider $\mathbb{E}(Z(x) - \hat{f}_G(x))^2$. Direct computation shows that

$$\mathbb{E}(Z(x) - \hat{f}_G(x))^2 = \left(\Psi(x - x) - 2 \sum_{j=1}^n u_j \Psi(x - x_j) + \sum_{j=1}^n \sum_{k=1}^n u_k u_j \Psi(x_k - x_j) \right) + \sigma_\epsilon^2 u^T u. \quad (150)$$

Plugging (149) into (148), we have

$$\begin{aligned}
 \mathbb{E}(f(x) - \hat{f}_m(x))^2 &\leq \left(\Psi(x-x) - 2 \sum_{j=1}^n u_j \Psi(x-x_j) + \sum_{j=1}^n \sum_{j=1}^n u_k u_j \Psi(x_k - x_j) \right) \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 \\
 &\quad + \sigma_\epsilon^2 u^T u \\
 &\leq C \left(\Psi(x-x) - 2 \sum_{j=1}^n u_j \Psi(x-x_j) + \sum_{j=1}^n \sum_{j=1}^n u_k u_j \Psi(x_k - x_j) + \sigma_\epsilon^2 u^T u \right) \\
 &= C \mathbb{E}(Z(x) - \hat{f}_G(x))^2,
 \end{aligned}$$

where $C = \max\{1, \|f\|_{\mathcal{N}_\Psi(\Omega)}^2\}$, and the last equality is by (150). This finishes the proof.

Appendix L. Proof of auxiliary lemmas

L.1 Proof of Lemma 22

We first state some lemmas used in this proof. Lemma 36 can be obtained by repeating the arguments used to establish Theorem 2.2 of Narcowich et al. (1994); also see Equation (4) in Narcowich et al. (2006). Lemma 37 is Lemma 3.2 of Narcowich et al. (2006). Lemma 38 can be obtained by elementary mathematical analysis, and the proof is in Appendix L.4.

Lemma 36 *Let Ψ be a Matérn correlation function satisfying Condition (C2). Suppose the design points $X = \{x_1, \dots, x_n\}$. Let Λ_X be the maximum eigenvalue of matrix $(\Psi(x_j - x_k))_{jk}$. Then*

$$\Lambda_X \leq \Psi(0) + \sum_{k=1}^{\infty} 3d(k+2)^{d-1} \Psi(kq_X),$$

where q_X is the separation radius of X .

Lemma 37 *Let Ψ be a Matérn correlation function satisfying Condition (C2). Then we have that Ψ is positive definite, decreasing on $[0, \infty)$, and satisfies the bound*

$$\Psi(x) \leq \sqrt{2\pi c_{m_0}} r^{\nu-1/2} e^{-r+\nu^2/2r}, \quad r = \|x\|_2 > 0,$$

where $\nu = m_0 - d/2$.

Lemma 38 *Define function g as*

$$g(x) = x^{d/2+m_0-3/2} e^{-x}, \quad x \geq 1.$$

We have $g(x) \leq C e^{-x/2}$ for all $x \geq 1$, where $C = (d + 2m_0)^{d/2+m_0}$.

Now we begin to prove Lemma 22. Note that $k + 2 \leq 3k$ for $k \geq 1$, which, together with Lemma 36, leads to

$$\begin{aligned}
 \Lambda_X &\leq \Psi(0) + \sum_{k=1}^{\infty} 3d(k+2)^{d-1}\Psi(kq_X) \\
 &\leq \Psi(0) + 3^d d \sum_{k=1}^{\infty} k^{d-1}\Psi(kq_X) \\
 &= \Psi(0) + 3^d d \sum_{k=1}^{\lfloor 1/q_X \rfloor} k^{d-1}\Psi(kq_X) + 3^d d \sum_{k=\lfloor 1/q_X \rfloor+1}^{\infty} k^{d-1}\Psi(kq_X) \\
 &= \Psi(0) + I_1 + I_2,
 \end{aligned} \tag{151}$$

where $\lfloor a \rfloor$ is the integer part of $a \in \mathbb{R}_+$. Since $\Psi(x)$ is a decreasing function, the first term I_1 can be bounded by

$$I_1 \leq 3^d d \sum_{k=1}^{\lfloor 1/q_X \rfloor} k^{d-1}\Psi(0) \leq C_1 3^d d \Psi(0) (\lfloor 1/q_X \rfloor)^d \leq C_1 3^d d \Psi(0) (1/q_X)^d, \tag{152}$$

where we utilize the basic inequality $\sum_{k=1}^m k^{d-1} \leq C_1 m^d$.

Using Lemma 37, the second term I_2 can be bounded by

$$I_2 \leq 3^d d \sum_{k=\lfloor 1/q_X \rfloor+1}^{\infty} k^{d-1}\Psi(kq_X) \leq C_2 \sum_{k=\lfloor 1/q_X \rfloor+1}^{\infty} k^{d-1} (kq_X)^{m_0-d/2-1/2} e^{-kq_X + (m_0-d/2)^2/(2kq_X)}.$$

Clearly, $kq_X \geq 1$ for $k \geq \lfloor 1/q_X \rfloor + 1$, which implies $e^{(m_0-d/2)^2/(2kq_X)} \leq e^{(m_0-d/2)^2/2}$. Therefore, I_2 can be further bounded by

$$\begin{aligned}
 I_2 &\leq C_2 e^{(m_0-d/2)^2/2} q_X^{-d+1} \sum_{k=\lfloor 1/q_X \rfloor+1}^{\infty} (kq_X)^{d-1} (kq_X)^{m_0-d/2-1/2} e^{-kq_X} \\
 &= C_2 e^{(m_0-d/2)^2/2} q_X^{-d+1} \sum_{k=\lfloor 1/q_X \rfloor+1}^{\infty} (kq_X)^{m_0+d/2-3/2} e^{-kq_X} \\
 &= C_2 e^{(m_0-d/2)^2/2} q_X^{-d+1} I_3,
 \end{aligned} \tag{153}$$

where

$$I_3 = \sum_{k=\lfloor 1/q_X \rfloor+1}^{\infty} (kq_X)^{d/2+m_0-3/2} e^{-kq_X}.$$

Consider function $g(x) = x^{d/2+m_0-3/2} e^{-x}$, $x \geq 1$. By Lemma 38, we have $g(x) \leq C_3 e^{-x/2}$, where $C_3 = (d+2m_0)^{d/2+m_0}$. This implies that I_3 can be bounded by

$$\begin{aligned}
 I_3 &\leq C_3 \sum_{k=\lfloor 1/q_X \rfloor+1}^{\infty} e^{-kq_X/2} \leq C_3 \sum_{k=0}^{\infty} e^{-kq_X/2} \\
 &= \frac{C_3}{1 - e^{-q_X/2}} \leq C_3 \frac{q_X/2 + 1}{q_X/2} \lesssim q_X^{-1},
 \end{aligned} \tag{154}$$

where third inequality is because of the basic inequality $1 - e^{-x} > \frac{x}{x+1}$ for $x > 0$, and the last equality is because $q_X \lesssim 1$. Plugging (154) into (153), we have $I_2 \leq C_4 q_X^{-d}$. Together with (152) and (151), we can see the desired result holds.

L.2 Proof of Lemma 25

Let $u = (u_1, \dots, u_n)^T = (R + \mu I_n)^{-1} r(x)$, where R , r and μ are as in (2). The Fourier inversion theorem implies that

$$\begin{aligned}
 & K(x-x) - r_K(x)^T (R_K + \mu I_n)^{-1} r_K(x) \\
 & \leq K(x-x) - 2 \sum_{j=1}^n u_j K(x-x_j) + \sum_{j=1}^n \sum_{k=1}^n u_j u_k K(x_j-x_k) + \mu \|u\|_2^2 \\
 & = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(K)(\omega) d\omega + \mu \|u\|_2^2 \\
 & \leq A_0 \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + \mu \|u\|_2^2 \\
 & \leq \max\{A_0, 1\} \left(\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left| \sum_{j=1}^n u_j e^{-i\langle x_j, \omega \rangle} - e^{-i\langle x, \omega \rangle} \right|^2 \mathcal{F}(\Psi)(\omega) d\omega + \mu \|u\|_2^2 \right) \\
 & = \max\{A_0, 1\} (\Psi(x-x) - r(x)^T (R + \mu I_n)^{-1} r(x)),
 \end{aligned}$$

where r and R are as in (2). This finishes the proof.

L.3 Proof of Lemma 31

In this section, we set $m_0 := m_0(f)$ for notational simplicity. Since Ω has Lipschitz boundary, there exists an extension operator from $L_2(\Omega)$ to $L_2(\mathbb{R}^d)$, such that the smoothness of each function is maintained (DeVore and Sharpley, 1993; Rychkov, 1999). Therefore, there exist constants $0 < C_1 \leq C_2$ such that for any functions $h_1 \in H^m(\Omega)$ and $h_2 \in H^{m_0}(\Omega)$, there exist $h_{1,e} \in H^m(\mathbb{R}^d)$ and $h_{2,e} \in H^{m_0}(\mathbb{R}^d)$ satisfying

$$C_1 \|h_{1,e}\|_{H^m(\mathbb{R}^d)} \leq \|h_1\|_{H^m(\Omega)} \leq C_2 \|h_{1,e}\|_{H^m(\mathbb{R}^d)}, \quad (155)$$

$$C_1 \|h_{2,e}\|_{H^{m_0}(\mathbb{R}^d)} \leq \|h_2\|_{H^{m_0}(\Omega)} \leq C_2 \|h_{2,e}\|_{H^{m_0}(\mathbb{R}^d)}, \quad (156)$$

and $h_{1,e}(x) = h_1(x)$ and $h_{2,e}(x) = h_2(x)$ for any $x \in \Omega$. Let f_1 be the solution to the optimization problem

$$\min_{\tilde{f} \in H^m(\mathbb{R}^d)} \|f_e - \tilde{f}\|_{L_2(\mathbb{R}^d)}^2 + \lambda_m \|\tilde{f}\|_{H^m(\mathbb{R}^d)}^2, \quad (157)$$

where f_e is the extension of f satisfying (156) with $h_2 = f$.

Because Φ satisfies Condition (C3), $\mathcal{N}_\Phi(\Omega)$ coincides with $H^m(\Omega)$. Since f^* is the solution to (68), by (155), we have

$$\begin{aligned} & \|f - f^*\|_{L_2(\Omega)}^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq \|f - f_{1,r}\|_{L_2(\Omega)}^2 + \lambda_m \|f_{1,r}\|_{\mathcal{N}_\Phi(\Omega)}^2 \\ & \leq C_3 \left(\|f - f_{1,r}\|_{L_2(\Omega)}^2 + \lambda_m \|f_{1,r}\|_{H^m(\Omega)}^2 \right) \leq C_4 \left(\|f_e - f_1\|_{L_2(\mathbb{R}^d)}^2 + \lambda_m \|f_1\|_{H^m(\mathbb{R}^d)}^2 \right), \end{aligned} \quad (158)$$

where $f_{1,r}$ is the restriction of f_1 onto Ω .

By the Fourier transform and the Plancherel theorem (Bracewell, 1986), we have

$$\begin{aligned} & \|f_e - f_1\|_{L_2(\mathbb{R}^d)}^2 + \lambda_m \|f_1\|_{H^m(\mathbb{R}^d)}^2 \\ & = \int_{\mathbb{R}^d} |\mathcal{F}(f_e)(\omega) - \mathcal{F}(f_1)(\omega)|^2 d\omega + \lambda_m \int_{\mathbb{R}^d} |\mathcal{F}(f_1)(\omega)|^2 (1 + \|\omega\|_2^2)^m d\omega \\ & = \int_{\mathbb{R}^d} (|\mathcal{F}(f_e)(\omega) - \mathcal{F}(f_1)(\omega)|^2 + \lambda_m |\mathcal{F}(f_1)(\omega)|^2 (1 + \|\omega\|_2^2)^m) d\omega \\ & = \int_{\mathbb{R}^d} \frac{\lambda_m (1 + \|\omega\|_2^2)^m}{1 + \lambda_m (1 + \|\omega\|_2^2)^m} |\mathcal{F}(f_e)(\omega)|^2 d\omega \\ & = \int_{\Omega_1} \frac{\lambda_m (1 + \|\omega\|_2^2)^m}{1 + \lambda_m (1 + \|\omega\|_2^2)^m} |\mathcal{F}(f_e)(\omega)|^2 d\omega + \int_{\Omega_1^C} \frac{\lambda_m (1 + \|\omega\|_2^2)^m}{1 + \lambda_m (1 + \|\omega\|_2^2)^m} |\mathcal{F}(f_e)(\omega)|^2 d\omega \\ & \leq \int_{\Omega_1} \lambda_m (1 + \|\omega\|_2^2)^m |\mathcal{F}(f_e)(\omega)|^2 d\omega + \int_{\Omega_1^C} |\mathcal{F}(f_e)(\omega)|^2 d\omega, \end{aligned} \quad (159)$$

where $\Omega_1 = \{\omega : \lambda_m (1 + \|\omega\|_2^2)^m < 1\}$, $\Omega_1^C = \mathbb{R}^d \setminus \Omega_1$, and the third equality follows that f_1 is the solution to (157).

On the set Ω_1 , since $\lambda_m (1 + \|\omega\|_2^2)^m < 1$ and $m \geq m_0$, it can be verified that $\lambda_m (1 + \|\omega\|_2^2)^m \leq \lambda_m^{\frac{m_0}{m}} (1 + \|\omega\|_2^2)^{m_0}$. On the other hand, since $\lambda_m (1 + \|\omega\|_2^2)^m \geq 1$ on the set Ω_1^C , we have $\lambda_m^{\frac{m_0}{m}} (1 + \|\omega\|_2^2)^{m_0} \geq 1$. Together with (159), we obtain

$$\begin{aligned} & \|f_e - f_1\|_{L_2(\mathbb{R}^d)}^2 + \lambda_m \|f_1\|_{H^m(\mathbb{R}^d)}^2 \\ & \leq \int_{\Omega_1} \lambda_m (1 + \|\omega\|_2^2)^m |\mathcal{F}(f_e)(\omega)|^2 d\omega + \int_{\Omega_1^C} |\mathcal{F}(f_e)(\omega)|^2 d\omega \\ & \leq \lambda_m^{\frac{m_0}{m}} \int_{\Omega_1} (1 + \|\omega\|_2^2)^{m_0} |\mathcal{F}(f_e)(\omega)|^2 d\omega + \lambda_m^{\frac{m_0}{m}} \int_{\Omega_1^C} (1 + \|\omega\|_2^2)^{m_0} |\mathcal{F}(f_e)(\omega)|^2 d\omega \\ & = \lambda_m^{\frac{m_0}{m}} \|f_e\|_{H^{m_0}(\mathbb{R}^d)}^2 \leq C_5 \lambda_m^{\frac{m_0}{m}} \|f\|_{H^{m_0}(\Omega)}^2 \leq C_6 \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2, \end{aligned} \quad (160)$$

where the third inequality follows from (156) and the last inequality is because of the equivalence of $\|\cdot\|_{H^{m_0}(\Omega)}$ and $\|\cdot\|_{\mathcal{N}_\Psi(\Omega)}$.

Combining (158) and (160) yields

$$\|f - f^*\|_{L_2(\Omega)}^2 + \lambda_m \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C_6 \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2,$$

which implies

$$\|f^* - f\|_{L_2(\Omega)}^2 \leq C_6 \lambda_m^{\frac{m_0}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2 \quad \text{and} \quad \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C_6 \lambda_m^{\frac{m_0-m}{m}} \|f\|_{\mathcal{N}_\Psi(\Omega)}^2.$$

Next, we consider the case $f \notin H^{m_0}(\Omega)$. If $f \notin H^{m_0}(\Omega)$, by Lemma 13, there exists a function $Q : \mathbb{R}_+ \mapsto \mathbb{R}_+$ such that

$$\int_{\mathbb{R}^d} \frac{|\mathcal{F}(f)(\omega)|^2 (1 + \|\omega\|_2^2)^{m_0}}{Q(\|\omega\|_2)} d\omega \leq 1, \text{ and } \lim_{r \rightarrow +\infty} \frac{\log Q(r)}{\log r} = 0.$$

Therefore, (159) can be changed to

$$\begin{aligned} & \|f_e - f_1\|_{L_2(\mathbb{R}^d)}^2 + \lambda_m \|f_1\|_{H^m(\mathbb{R}^d)}^2 \\ &= \int_{\mathbb{R}^d} \frac{\lambda_m (1 + \|\omega\|_2^2)^m}{1 + \lambda_m (1 + \|\omega\|_2^2)^m} |\mathcal{F}(f)(\omega)|^2 d\omega \\ &= \int_{\Omega_2} \frac{\lambda_m (1 + \|\omega\|_2^2)^m}{1 + \lambda_m (1 + \|\omega\|_2^2)^m} |\mathcal{F}(f)(\omega)|^2 d\omega + \int_{\Omega_2^C} \frac{\lambda_m (1 + \|\omega\|_2^2)^m}{1 + \lambda_m (1 + \|\omega\|_2^2)^m} |\mathcal{F}(f)(\omega)|^2 d\omega \\ &\leq \int_{\Omega_2} \lambda_m (1 + \|\omega\|_2^2)^m |\mathcal{F}(f)(\omega)|^2 d\omega + \int_{\Omega_2^C} |\mathcal{F}(f)(\omega)|^2 d\omega \\ &\leq C_7 \left(\lambda_m^{\frac{m_0}{m}} Q_1(n) \int_{\Omega_2} (1 + \|\omega\|_2^2)^{m_0} \frac{|\mathcal{F}(f)(\omega)|^2}{Q(\|\omega\|_2)} d\omega + \lambda_m^{\frac{m_0}{m}} \int_{\Omega_2^C} (1 + \|\omega\|_2^2)^{m_0} \frac{|\mathcal{F}(f)(\omega)|^2}{Q(\|\omega\|_2)} d\omega \right) \\ &\leq C_8 \lambda_m^{\frac{m_0}{m}} Q_1(n), \end{aligned} \tag{161}$$

where $\Omega_2 = \{\omega : \lambda_m (1 + \|\omega\|_2^2)^m < Q(\|\omega\|_2)^{m/m_0}\}$, $\Omega_2^C = \mathbb{R}^d \setminus \Omega_2$, and $Q_1 : \mathbb{R}_+ \mapsto \mathbb{R}_+$ is a function such that $\sup_{\omega \in \Omega_2} Q(\omega)^{m/m_0} = Q_1(n)$, since we assume $\lambda_m \asymp n^\alpha$ for some α . It can be seen that Q_1 satisfies

$$\lim_{r \rightarrow +\infty} \frac{\log Q_1(r)}{\log r} = 0.$$

The second inequality of (161) follows from the fact that if $\omega \in \Omega_2$,

$$\frac{\lambda_m (1 + \|\omega\|_2^2)^m}{Q(\|\omega\|_2)^{m/m_0}} < \left(\frac{\lambda_m (1 + \|\omega\|_2^2)^m}{Q(\|\omega\|_2)^{m/m_0}} \right)^{m_0/m},$$

and otherwise

$$\left(\frac{\lambda_m (1 + \|\omega\|_2^2)^m}{Q(\|\omega\|_2)^{m/m_0}} \right)^{m_0/m} > C_9 > 0.$$

Note that (158) also holds for $f \notin \mathcal{N}_\Psi(\Omega)$. Therefore, it can be seen that (158) and (161) imply that

$$\|f^* - f\|_{L_2(\Omega)}^2 \leq C_8 \lambda_m^{\frac{m_0}{m}} Q_1(n) \text{ and } \|f^*\|_{\mathcal{N}_\Phi(\Omega)}^2 \leq C_8 \lambda_m^{\frac{m_0-m}{m}} Q_1(n).$$

This finishes the proof of Lemma 31.

L.4 Proof of Lemma 38

The result is implied by

$$x^{d/2+m_0-3/2}e^{-x} \leq Ce^{-x/2} \Leftrightarrow x^{d/2+m_0-3/2} \leq Ce^{x/2} \Leftrightarrow (d/2 + m_0 - 3/2) \log x \leq \log C + \frac{x}{2}.$$

Consider function $h(x) = \log C + \frac{x}{2} - (\frac{d}{2} + m_0 - \frac{3}{2}) \log x$. The first order derivative of $h(x)$ is

$$\frac{dh(x)}{dx} = \frac{1}{2} - \frac{d/2 + m_0 - 3/2}{x}.$$

If $d/2 + m_0 - 3/2 \leq 1/2$, then $h(x)$ is an increasing function on $[1, \infty)$, which implies $h(x) \geq h(1) > 0$, and the result of Lemma 38 holds. If $d/2 + m_0 - 3/2 > 1/2$, then h decreases on $[1, d + 2m_0 - 3)$, and increases on $[d + 2m_0 - 3, \infty)$, which implies that h takes the minimum at $x = d + 2m_0 - 3$. Since $h(x) \geq h(d + 2m_0 - 3)$ for all $x \geq 1$ and $h(d + 2m_0 - 3) > 0$, we finish the proof of Lemma 38.

Appendix M. Proof of statements in Example 2

Direct computation shows that the Fourier transform of f is

$$\mathcal{F}(f)(\omega) = \frac{4 \sin^2(\omega/2)}{\sqrt{2\pi}\omega^2}, \quad \omega \in \mathbb{R}.$$

It can be seen that

$$\begin{aligned} & \int_{\mathbb{R}} |\mathcal{F}(f)(\omega)|^2 (1 + |\omega|^2)^{3/2} d\omega \\ & \geq \int_{\mathbb{R}} |\mathcal{F}(f)(\omega)|^2 (1 + |\omega|^3) d\omega = \int_{\mathbb{R}} \frac{2(1 - \cos(\omega))^2}{\pi\omega^4} (1 + |\omega|^3) d\omega \\ & \geq \int_{\pi/2}^{\infty} \frac{2(1 - \cos(\omega))^2}{\pi\omega} d\omega = \int_0^{\infty} \frac{2(1 - \sin(t))^2}{\pi(t + \pi/2)} dt \\ & \geq \int_0^{\infty} \frac{2}{\pi(t + \pi/2)} dt - \int_0^{\infty} \frac{4 \sin(t)}{\pi(t + \pi/2)} dt \\ & \geq \int_0^{\infty} \frac{2}{\pi(t + \pi/2)} dt - \int_0^{\infty} \frac{4 \sin(t)}{\pi t} dt. \end{aligned}$$

Note that $\int_0^{\infty} \frac{2}{\pi(t + \pi/2)} dt = \infty$ and $\int_0^{\infty} \frac{4 \sin(t)}{\pi t} dt = 2$ (Bartle and Sherbert, 2000), which implies $\int_{\mathbb{R}} |\mathcal{F}(f)(\omega)|^2 (1 + |\omega|)^{3/2} d\omega = \infty$. This implies f does not belong to the Sobolev space $H^{3/2}(\mathbb{R})$. By checking that

$$\begin{aligned} & \int_{\mathbb{R}} |\mathcal{F}(f)(\omega)|^2 (1 + |\omega|^2)^{3/2 - \delta/2} d\omega \\ & \leq \int_{\mathbb{R}} |\mathcal{F}(f)(\omega)|^2 (1 + |\omega|)^{3 - \delta} d\omega = \int_{\mathbb{R}} \frac{2(1 - \cos(\omega))^2}{\pi\omega^4} (1 + |\omega|)^{3 - \delta} d\omega \\ & \leq \int_{-1}^1 \frac{2(1 - \cos(\omega))^2}{\pi\omega^4} (1 + |\omega|)^{3 - \delta} d\omega + \int_{\mathbb{R} \setminus [-1, 1]} \frac{8}{\pi\omega^4} (1 + |\omega|)^{3 - \delta} d\omega < \infty, \quad \forall \delta > 0, \end{aligned}$$

we can conclude that f has smoothness $3/2$. It is easily seen that, the function $Q(t) := C \log^2(1+t)$ defined on \mathbb{R}_+ with C an appropriate constant satisfies $\int_{\mathbb{R}} \frac{|\mathcal{F}(f)(\omega)|^2}{Q(|\omega|)} (1 + |\omega|^2)^{3/2} d\omega \leq 1$.