Optimal degree of smoothness to exploit in nonparametric regressions*

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Abstract

When the unknown regression function of a single variable is known to have derivatives up to the \((\gamma + 1)\)th order bounded in absolute values by a common constant everywhere or a.e., the classical minimax optimal rate of the mean integrated squared error (MISE) \(\left(\frac{1}{n}\right)^{\frac{2\gamma+2}{2\gamma+3}}\) leads one to conclude that, as \(\gamma\) gets larger, the rate gets closer to \(\frac{1}{n}\). This paper shows that: (i) if \(n \leq \frac{1}{(\gamma + 1)^{\gamma+3}}\), the minimax optimal MISE rate is roughly \(\frac{\log n}{n}\) and the optimal degree of smoothness to exploit is roughly \(\left\lceil \frac{\log n}{2} \right\rceil - 2\); (ii) if \(n > \frac{1}{(\gamma + 1)^{\gamma+3}}\), the minimax optimal MISE rate is \(\left(\frac{1}{n}\right)^{\frac{2\gamma+2}{2\gamma+3}}\) and the optimal degree of smoothness to exploit is \(\gamma + 1\).

The building blocks of our minimax optimality results are a set of metric entropy bounds we develop in this paper for smooth function classes. Some of our bounds are original, and some of them improve and/or generalize the ones in the literature. Our metric entropy bounds allow us to explore the minimax optimal MISE rates associated with some commonly seen smoothness classes and also several non-standard smoothness classes, and can also be of independent interest even if one does not care about the nonparametric regressions.

1 Introduction

Estimation of an unknown univariate function \(f\) from the nonparametric regression model

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y_i = f(x_i) + \varepsilon_i, \quad i = 1, ..., n
\]

has been a central research topic in econometrics, machine learning, numerical analysis and statistics. Many semiparametric estimators involve nonparametric regressions as an intermediate step, and some of the classical examples in economics can be found in several Handbook of Econometrics chapters such as Powell (1994), Chen (2007), and Ichimura and Todd (2007). The typical assumption about \(f\) in (1) is that it has derivatives up to a given \((\gamma + 1)\)th order bounded in absolute values by a common constant everywhere or almost everywhere (a.e.). Given an estimator of \(f\), an important object of interest is the convergence rate of the mean integrated squared error (MISE) of this estimator and the minimax optimality property of the MISE rate, which tells one how fast

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the population mean squared distance between the estimator and \( f \) shrinks to zero uniformly when \( f \) ranges over a smoothness class, as the sample size \( n \) increases. In particular, MISE is a global mean squared error criterion by integrating over all possible input \((x)\) values and noise values with respect to some underlying distribution (see Pagan and Ulla, 1999).

When \( \gamma \) is finite and the sample size \( n \to \infty \), existing results show that the minimax optimal MISE rate is \((\frac{1}{n})^\frac{2\gamma+2}{2\gamma+3}\) which decreases as \( \gamma \) increases.\[1\] The classical results give rise to the so called “blessing of smoothness” folklore (i.e., the more smoothness one can exploit, the better). Empirical researchers are advised to exploit higher degree smoothness assumptions if they are facing a small sample size. This suggestion is particularly common in economic applications where researchers need to perform subsample analyses and in these applications, \( n \) often ranges from several hundreds to a thousand (see, studies on intergenerational mobility such as Durlauf, et. al, 2022 and Maasoumi, et. al, 2022).

The classical minimax optimal rate \((\frac{1}{n})^\frac{2\gamma+2}{2\gamma+3}\) leads one to conclude that, as \( \gamma \) gets larger, the rate gets closer to \( \frac{1}{n} \). In this paper, by studying the minimax optimal MISE under two regimes \( n \leq (\gamma + 1)^{2\gamma+3} \) and \( n > (\gamma + 1)^{2\gamma+3} \), we show that one may not obtain a rate getting closer to \( \frac{1}{n} \) as \( \gamma \) gets larger. Based on the minimax optimality literature, a rate is said to be minimax optimal in our problem if we can show: (1) the MISE for \textit{any} estimators (by taking the supremum over all estimators) in the worst case scenario (by taking the supremum over a \((\gamma + 1)\)th degree smoothness class) is bounded from below, and such a bound is called a minimax lower bound; (2) there exists an estimator such that its MISE in the worst case scenario has an upper bound that matches the lower bound up to some universal constant independent of \( n \) (and in our interest, also independent of \( \gamma \)), the so-called achievability result; that is, apart from the universal constants, the upper bound matches the lower bound and the matching part is the minimax optimal rate.

In terms of the minimax optimal MISE rates associated with the standard \((\gamma + 1)\)th degree smoothness classes, we show the following results: (i) if \( n \leq (\gamma + 1)^{2\gamma+3} \), the minimax optimal MISE rate is roughly \( \frac{\log n}{n} \) and the optimal degree of smoothness to exploit is roughly \( \frac{\log n}{2n} - 2 \).\[2\]

(ii) if \( n > (\gamma + 1)^{2\gamma+3} \) (which clearly includes the degenerate case of \( \gamma \) being finite and \( n \) tending to infinity), the minimax optimal MISE rate is \((\frac{1}{n})^\frac{2\gamma+2}{2\gamma+3}\) and the optimal degree of smoothness to exploit is \( \gamma + 1 \). To our knowledge, this paper is the first in the literature to show the minimax optimal rate in the small sample regime and the sample size (i.e., \((\gamma + 1)^{2\gamma+3}\)) at which the minimax optimal rate transitions from roughly \( \frac{\log n}{n} \) to \((\frac{1}{n})^\frac{2\gamma+2}{2\gamma+3}\).

Particularly, we show in this paper that, if the maximum smoothness degree of \( f \) is \((\gamma + 1)\), estimators which minimize the sum of squared residuals and are constrained to exploit the optimal degree of smoothness achieve the abovementioned minimax optimal MISE rates. These estimators will be referred to as the constrained nonparametric least squares estimator (CNLS) in the following. CNLS estimators constrained to be in a Sobolev class associated with a Reproducing Kernel Hilbert Space (RKHS) radius have nice closed form expressions via kernel functions and are easy to implement in the regularized form, often referred to as the kernel ridge regression (KRR) estimators (among the most popular nonparametric estimators) in machine learning. There is a

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1 See Tsybakov (2009) for a comprehensive review of the literature that show the classical asymptotic minimax optimal rate \((\frac{1}{n})^\frac{2\gamma}{2\gamma+3}\) under the assumption of \( \gamma \) being finite and \( n \) tending to infinity.

2 In this paper, a \textit{standard} \((\gamma + 1)\)th degree smoothness class refers to one that consists of functions with derivatives belonging to a ball of some radius independent of the derivative order and with respect to either an \( l_\infty \) (max) norm or a Hilbert norm.

3 The more precise characterization of the minimax optimal MISE and the optimal degree of smoothness to exploit under \( n \leq (\gamma + 1)^{2\gamma+3} \) is detailed in Section 4.
rich theory based on RKHS for the asymptotic properties of such estimators under the regime where $\gamma$ is finite and $n \to \infty$ (see, e.g., Schölkopf and Smola, 2002; Berlinet and Thomas-Agnan, 2004). These estimators are closely related to smoothing splines methods and Gaussian process regressions (see, Wahba, 1990; Rasmussen and Williams, 2006).

It is worth mentioning the connection between our theoretical results and some numerical findings from the literature. From a practical viewpoint, Marron and Wand (1992) find the exact MISE of kernel density estimators based on Gaussian kernels can increase with the order of kernel being exploited (the assumed degree of smoothness) when the sample size is moderate. Marron (1994) further shows in simulations that the second order kernel produces a smaller MISE than the fourth order kernel when the sample size is between 70 and 10000, and the fourth order kernel is dominantly better than the second order kernel when $n > 10000$. Despite that our focus in this paper is on the minimax optimal rates and our achievability results concern global nonparametric procedures such as KRR (instead of kernel density estimators based on Gaussian kernels), Marron and Wand (1992) and our paper share one general message: the classical rate $\left(\frac{1}{n}\right)^{2\gamma+3}$ is an underestimate of the MISE when $n$ is not large enough. Another message conveyed by our paper is that the optimal degree of smoothness to exploit should depend on the sample size even if one knows the maximum degree of smoothness of the unknown function $f$ in (1) is $\gamma + 1$. When a researcher has zero or little knowledge about the smoothness degree, our results highlight the potential significance of rate adaptive procedures.

A recent paper by Chen et. al (2021) studies sup-norm rate adaptive nonparametric IV estimators when the unknown degree of smoothness is finite and $n \to \infty$, and discusses the potential benefits of such estimators. Interestingly, Chen et. al (2021) find in simulations that the cubic smoothing splines estimator performs the best at estimating a sine function (which is infinitely differentiable). One fruitful direction is to explore whether the smoothness degree used in the data-driven estimators are consistent with our recommendation; that is, use roughly $\left\lceil \frac{\log n}{2} \right\rceil - 2$ degree of smoothness when $n \leq (\gamma + 1)^{2\gamma+3}$ and use $\gamma + 1$ when $n > (\gamma + 1)^{2\gamma+3}$.

We want to emphasize that the implications of our results extend to other applications. Theoretical analysis of a semiparametric procedure often requires establishing an MISE rate or its sample analogue concerning a first-step nonparametric regression. Below are several important examples:

1. When applying a 2SLS-type procedure to estimate a triangular system where the first-stage equations linking the endogenous regressors with instruments take the form of (1), the MSE of the 2SLS estimator for the parameters of interest in the second-stage (main) equation depends on the MISE of the first-stage estimators.

2. When applying the partialling-out type strategy to estimate the parameters of interest in a partially linear model, the first step uses a nonparametric regression to obtain the partial residuals, and the second step uses a least squares procedure or a regularized least squares procedure based on the estimated residuals from the first step. The MSE of the second step estimator depends on the MISE of the first-step estimator.\footnote{Based on several empirical studies with sample sizes ranging from a couple of thousands to at most thirty thousands, Gelman and Imbens (2019) recommend researchers to avoid using high order polynomials but use local linear or local quadratic polynomials to estimate the two conditional mean functions of a pretreatment variable in regression discontinuity designs (RDD) analyses.}

\footnote{For the partially linear models in Item 2, following derivations similar to those in Zhu (2017) would reveal the dependence. For the triangular systems in Item 1, following derivations similar to those in Zhu (2018) would reveal the dependence; in particular, the modifications involve replacing terms like $(Z_{ij} \hat{\pi}_j - Z_{ij} \pi^*_j)^2$ in Zhu (2018) with $(\hat{f}(Z_{ij}) - f(Z_{ij}))^2$, where $j$ is the index of the endogenous variables and $Z_{ij}$ is a instrumental variable for the $j$th
3. The quality of a normal approximation in finite samples for making inference about a parameter of interest in a partially linear model depends on the sample analogue of the MISE of the first-step nonparametric estimator discussed in Item 2. Suppose $\alpha$ is the parameter of interest and $\hat{\alpha}$ is the second step estimator of $\alpha$. One would have $\sqrt{n}(\hat{\alpha} - \alpha) = \text{normal random variable} + \text{remainder}$, where the sample analogue of the MISE (multiplied by $\sqrt{n}$) of the first-step nonparametric estimator enters “remainder”.

4. When applying a (nonparametric) regression adjustment procedure to estimate an average treatment effect, the MSE of the estimator depends on the MISE of the nonparametric regression estimators.

2 Preliminary

2.1 Notation and definitions

**Notation.** Let $[x]$ denote the largest integer smaller than or equal to $x$. For two functions $f(n)$ and $g(n)$, let us write $f(n) \gtrless g(n)$ if $f(n) \geq c g(n)$ for a universal constant $c \in (0, \infty)$; similarly, we write $f(n) \lessgtr g(n)$ if $f(n) \leq c g(n)$ for a universal constant $c' \in (0, \infty)$; and $f(n) \asymp g(n)$ if $f(n) \gtrsim g(n)$ and $f(n) \lessapprox g(n)$. Throughout this paper, we use various $c$ and $C$ letters to denote positive universal constants that are: $\gtrsim 1$ and independent of $n$ and $\gamma$ and the dimension $d$ of the covariates (when $d$—dimensional covariates are of interest); these constants may vary from place to place.

For a $J$—dimensional vector $\theta$, the $l_q$—norm $|\theta|_q := \left(\sum_{j=1}^J |\theta_j|^q\right)^{1/q}$ if $1 \leq q < \infty$ and $|\theta|_q := \max_{j \in \{1, \ldots, J\}}|\theta_j|$ if $q = \infty$. Let $\mathbb{R}_q^J(R) := \\{\theta \in \mathbb{R}_q^J : |\theta|_q \leq R\}$. For functions on $[a, b]$, the unweighted $L^2$—norm $|f - g|_2 := \left(\int_a^b |f(x) - g(x)|^2 dx\right)^{1/2}$, and the weighted $L^2$—norm $|f - g|_{2, P} := \left(\int_a^b |f(x) - g(x)|^2 P(dx)\right)^{1/2}$. For functions on $[a, b]^d$, the supremum norm $|f - g|_\infty := \sup_{x \in [a, b]^d}|f(x) - g(x)|$.

Finally, the $L^2(P_n)$—norm of the vector $f := \{f(x_i)\}_{i=1}^n$, denoted by $|f|_n$, is $\left(\frac{1}{n} \sum_{i=1}^n (f(x_i))^2\right)^{1/2}$.

**Definition** (covering and packing numbers). Given a set $\Lambda$, a set $\{\eta^1, \eta^2, \ldots, \eta^M\} \subset \Lambda$ is a $\delta$—cover of $\Lambda$ in the metric $\rho$ if for each $\eta \in \Lambda$, there exists some $i \in \{1, \ldots, N\}$ such that $\rho(\eta, \eta^i) \leq \delta$.

The $\delta$—covering number of $\Lambda$, denoted by $N_\rho(\delta, \Lambda)$, is the cardinality of the smallest $\delta$—cover. A set $\{\eta^1, \eta^2, \ldots, \eta^M\} \subset \Lambda$ is a $\delta$—packing of $\Lambda$ in the metric $\rho$ if for any distinct $i, j \in \{1, \ldots, M\}$, $\rho(\eta^i, \eta^j) > \delta$. The $\delta$—packing number of $\Lambda$, denoted by $M_\rho(\delta, \Lambda)$, is the cardinality of the largest $\delta$—packing. Throughout this paper, we use $N_\delta(\delta, \mathcal{F})$ and $M_\delta(\delta, \mathcal{F})$ to denote the $\delta$—covering number and the $\delta$—packing number, respectively, of a function class $\mathcal{F}$ with respect to the function norm $|\cdot|_q$ where $q \in \{2, \infty\}$; moreover, $N_{2, P}(\delta, \mathcal{F})$ and $M_{2, P}(\delta, \mathcal{F})$ denote the $\delta$—covering number and the $\delta$—packing number, respectively, of a function class $\mathcal{F}$ with respect to the weighted $L^2(P)$—norm $|\cdot|_{2, P}$.

The following is a standard textbook result that summarizes the relationships between covering and packing numbers:

$$M_\rho(2\delta, \Lambda) \leq N_\rho(\delta, \Lambda) \leq M_\rho(\delta, \Lambda). \tag{2}$$

endogenous variable.
Given this sandwich result, a lower bound on the packing number gives a lower bound on the covering number, and vice versa; similarly, an upper bound on the covering number gives an upper bound on the packing number, and vice versa.

For a non-negative integer $\gamma$, let the generalized Hölder class $U_{\gamma+1} \left((R_k)^{\gamma+1}_{k=0}, [-1, 1]\right)$ be the class of functions such that any function $f \in U_{\gamma+1} \left((R_k)^{\gamma+1}_{k=0}, [-1, 1]\right)$ satisfies: (1) $f$ is continuous on $[-1, 1]$ and all derivatives of $f$ exist; (2) $\left|f^k(x)\right| \leq R_k$ for all $k = 0, ..., \gamma$ and $x \in [-1, 1]$, where $f^0(x) = f(x)$; (3) $\left|f^\gamma(x) - f^\gamma(x')\right| \leq R_{\gamma+1} \left|x - x'\right|$ for all $x, x' \in [-1, 1]$.

Any function $f$ in the Hölder class can be written as

$$f(x) = f(0) + \sum_{k=1}^{\gamma} \frac{x^k}{k!} f^{(k)}(0) + \frac{x^\gamma}{\gamma!} f^{(\gamma)}(0) - \frac{x^\gamma}{\gamma!} f^{(\gamma)}(0)$$

where $z$ is some intermediate value between $x$ and 0. Consequently, we have the following relationships:

$$U_{\gamma+1, 1} \subseteq U_{\gamma+1}, \quad U_{\gamma+1, 2} \subseteq U_{\gamma+1}, \quad U_{\gamma+1} \subseteq U_{\gamma+1, 1} + U_{\gamma+1, 2} := \{f_1 + f_2 : f_1 \in U_{\gamma+1, 1}, f_2 \in U_{\gamma+1, 2}\}$$

where the polynomial subclass

$$U_{\gamma+1, 1} = \left\{f(x) = \sum_{k=0}^{\gamma} \theta_k x^k : (\theta_k)_{k=0}^\gamma \in P_\gamma, x \in [-1, 1]\right\}$$

with the $(\gamma + 1)$-dimensional polyhedron

$$P_\gamma = \left\{(\theta_k)_{k=0}^\gamma \in \mathbb{R}^{\gamma+1} : \theta_k \in \left[-\frac{R_k}{k!}, \frac{R_k}{k!}\right]\right\}$$

and the Hölder subclass $U_{\gamma+1, 2}$ is the class of functions such that any function $f \in U_{\gamma+1, 2}$ satisfies: $f \in U_{\gamma+1}$ such that $f^{(k)}(0) = 0$ for all $k = 0, ..., \gamma$.

Any function $f$ in the Sobolev space on $[0, 1]$ has the expansion

$$f(x) = \sum_{k=0}^{\gamma} f^{(k)}(0) \frac{x^k}{k!} + \int_0^1 f^{(\gamma+1)}(t) \frac{(x-t)^\gamma}{\gamma!} dt,$$

where $(a)_+ = a \vee 0$. As in Wainwright (2019, Chapter 12), one (RK)HS norm associated with a Sobolev space takes the form

$$|f|_{H, \gamma} = \sqrt{\sum_{k=0}^{\gamma} (f^{(k)}(0))^2 + \int_0^1 \left[f^{(\gamma+1)}(t)\right]^2 dt.}$$

Therefore, the Sobolev space can be decomposed into a polynomial subspace and a Sobolev subspace imposed with the restrictions that $f^{(k)}(0) = 0$ for all $k = 0, ..., \gamma$ and $f^{(\gamma+1)}$ belongs to the space $L^2[0, 1]$ (see Wahba, 1990, Chapter 1; Wainwright, 2019, Chapter 12, Examples 12.17 and 12.29). The Sobolev subclass is a special case of the ellipsoid subclass. Based on Wainwright (2019, Chapter 12), we define the generalized ellipsoid subclass of smooth functions as follows:

$$H_{\gamma+1} = \left\{f = \sum_{m=1}^{\infty} \theta_m \phi_m : \text{for } (\theta_m)_{m=1}^\infty \in \ell^2(\mathbb{N}) \text{ such that } \sum_{m=1}^{\infty} \theta_m^2 \mu_m \leq R_{\gamma+1}^2\right\}$$
where $\ell^2(N) := \{(\theta_m)_{m=1}^{\infty} | \sum_{m=1}^{\infty} \theta_m^2 < \infty\}$, $(\mu_m)_{m=1}^{\infty}$ and $(\phi_m)_{m=1}^{\infty}$ are the eigenvalues and eigenfunctions (that forms an orthonormal basis of $\ell^2[0, 1]$, respectively), of an RKHS associated with a continuous and semidefinite kernel function. Assume that $\mu_m = (cm)^{-2(\gamma + 1)}$ for some positive constant $c$. The decay rate of the eigenvalues follows the standard assumption for $(\gamma + 1)-$degree smooth functions in the literature (see, e.g., Steinwart and Christmann, 2008; Wainwright, 2019) and $R_{\gamma+1} \times 1 \in \mathbf{1}$ gives the standard ellipsoid subclass. Moreover, $\mathbf{1}$ is equipped with the inner product $\langle h, g \rangle_H = \sum_{m=1}^{\infty} \frac{\langle h, \phi_m \rangle \langle g, \phi_m \rangle}{\mu_m}$ where $\langle ., . \rangle$ is the inner product in $\ell^2[0, 1]$.

### 2.2 Outline of our theoretical contributions

This paper generalizes the commonly seen smoothness classes in the literature to ones where the absolute values of the derivatives of any member are allowed to depend on the derivative order. The first objective of this paper is to examine the impacts of $\gamma$ and $\{R_k\}_{k=0}^{+1}$ on the size of the generalized smoothness classes via the notion of metric entropy, in particular, covering and packing numbers. We then show how these results can be used to study the minimax optimal MISE rates under two regimes of the sample size $n$.

The existing literature mostly assumes that $R_k$ is a constant independent of the order of derivative, $k$. This assumption may not hold if one considers the class of ordinary differential equation (ODE) solutions. In noisy recovery of solutions to ODEs, researchers often use polynomials and spline bases to approximate the solutions to overcome computational challenges (e.g., Varah, 1982; Ramsay, 1996; Ramsay and Silverman, 2005; Poyton, et. al, 2006; Ramsay, et. al, 2007; Liang and Wu, 2008). As an example from studies of AIDs, Liang and Wu (2008) use local polynomial regressions to estimate the ODE solutions $y$ and their first derivatives $y'$ from noisy measurements of plasma viral load and CD4+ T cell counts; then, the authors regress the estimates $\hat{y}'$ on $f(\hat{y}; \theta)$ to obtain estimates of the parameters $\theta$ in the ODE model. Liang and Wu (2008) mentioned that higher order local polynomials for approximating the solutions can also be used, and doing so would require boundedness on the higher order derivatives of the solutions.

Motivated by these statistical procedures for recovering ODE solutions in the literature, Zhu and Mirzaei (2021) study how the smoothness of ODEs affects the smoothness of the underlying solutions. To illustrate, let us consider the autonomous ODE $y'(x) = f(y(x))$. Like other areas in nonparametric estimation, it can be desirable to only assume smoothness structures on $f$ for hedging against misspecification of the functional form for $f$. Zhu and Mirzaei (2021) show that: (i) If $|f^{(k)}(x)| \leq 1$ for all $x$ on the domain and $k = 0, ..., \gamma + 1$, then $|y^{(k+1)}(x)| \leq k!$; (ii) the factorial bounds are attainable by the solutions to some ODE (e.g., $y' = e^{-y-x}$) and therefore tight. This result motivates the generalized smoothness classes considered in this paper. It is worth pointing out that, owing to the deep links between ODEs and contraction mapping, our generalized smoothness classes may have applications in other problems that involve solving fixed point solutions (which play a critical role in structural estimation of Markov decision processes and games in economics, as well as reinforcement learning in artificial intelligence).

The fundamental contribution of this paper lies in a set of metric entropy bounds. Some of them are original, and some of them improve and/or extend the ones in the literature to allow general (possibly $k-$dependent) $R_k$s. Metric entropy is an important concept in approximation theory and discrete geometry. Therefore, our bounds for the covering and packing numbers are of independent interest even if one does not care about the nonparametric regressions. In mathematical statistics and machine learning theory, metric entropy is a fundamental building block. Combined with the Fano’s inequality from information theory (see, Cover and Thomas, 2005), it allows one to derive the minimax lower bounds for the MISE rates; combined with the notion of “local complexity” in
empirical processes theory, it allows one to derive upper bounds on the MISE rates\footnote{For the \textit{standard} smoothness classes, one may use methods based on “ranks” (for the polynomial subclass) and “eigenvalues” (for the nonparametric subclass) to derive upper bounds on the MISE. However, “ranks” and “eigenvalues” are not very useful for deriving the minimax lower bounds in general. Even for upper bounds in the case of a Hölder class, once we allow \( R_k \) to depend on the order of derivative, \( k \), the “rank”–based argument is hard to generalize as it does not account for the impact of \( R_k \).

\footnote{For a \textit{non-standard} Hölder class, Zhu and Mirzaei (2021) applies the argument in Kolmogorov and Tikhomirov (1959) to derive an upper bound on the covering number. For the lower bound on the covering/packing number, Zhu and Mirzaei (2021) simply takes the classical result \( \delta \frac{1}{\gamma+1} \) from Kolmogorov and Tikhomirov (1959). The consequence is, the lower and upper error bounds have different rates, neither of which is sharp. See Section 5 for the details.}

In contrast to the classical entropy bounds in the literature, our entropy bounds enable us to reveal the minimax optimal MISE rate of roughly \( \log n \) in the regime \( n \leq (\gamma + 1)^{2\gamma + 3} \). When metric entropy results are used to study smoothness classes, virtually every paper including recent textbooks on nonasymptotic statistics (such as Wainwright, 2019) takes \( \log(\delta - \text{covering number}) \times \delta \frac{1}{\gamma+1} \) for \( \delta \)–approximation accuracy. Such a result is dated back to the seminal work by Kolmogorov and Tikhomirov (1959). It would take some diligence for one to recognize that, when \( \delta \) is not small enough, the classical result \( \delta \frac{1}{\gamma+1} \) is not correct. As a consequence, the minimax optimal rate \( \left( \frac{1}{n} \right)^{\frac{2\gamma+2}{2\gamma+3}} \) (which is derived based on \( \delta \frac{1}{\gamma+1} \)) is not correct unless \( n > (\gamma + 1)^{2\gamma + 3} \), in which case, \( \delta \) becomes small enough. We discover that:

1. the derivations of the lower bound \( \delta \frac{1}{\gamma+1} \) on the metric entropy in Kolmogorov and Tikhomirov (1959) as well as the following literature for Hölder and ellipsoid classes ignore the polynomial subclass \( U_{\gamma+1,1} \); see e.g., Wainwright (2019), Example 5.11, which inherits the lower bound derivation in Kolmogorov and Tikhomirov (1959). The lower bound \( \delta \frac{1}{\gamma+1} \) is a lower bound for the standard Hölder subclass \( U_{\gamma+1,2} \) only, and is not sharp even for the \textit{standard} smoothness classes if \( \delta \) is not small enough;

2. the upper bound based on the arguments in Kolmogorov and Tikhomirov (1959) for the polynomial subclass \( U_{\gamma+1,1} \) is far from being tight when \( R_k \) become large enough;

3. the upper bound based on the arguments in Mityagin (1961) and the following literature (Wainwright, 2019, Example 5.12) for the Sobolev subclass (more generally, the ellipsoid subclass) does not give the sharp dependence on \( \gamma \) and \( R_{\gamma+1} \);

4. the existing minimax optimal rate for MISE or its sample analogue associated with the \textit{standard} smoothness classes is \( \left( \frac{1}{n} \right)^{\frac{2\gamma+2}{2\gamma+3}} \), which is not correct when \( n \leq (\gamma + 1)^{2\gamma + 3} \)\footnote{In fact, our metric entropy bounds could be expressed with explicit universal constants that are independent of \( \gamma \) and \( \{ R_k \}_{k=0}^{\gamma+1} \). But when these bounds are applied with other technical lemmas to establish minimax optimal rates for the MISE, the universal constants become complex rather quickly and it is very tedious to track them from lines to lines.}

All these issues are addressed in this paper. Particularly, in deriving the metric entropy bounds for the polynomial subclass \( U_{\gamma+1,1} \), we develop our own arguments; in deriving the metric entropy bounds for the ellipsoid subclass, we base our arguments on the existing literature but use an improved truncation strategy that gives our resulting bounds the sharp dependence on \( \gamma \) and \( R_{\gamma+1} \).

Relative to the existing literature, our results take one step further by revealing more explicit dependence on \( n, \gamma \) and \( \{ R_k \}_{k=0}^{\gamma+1} \). Because of the complexity of our problems, we make no attempt to derive the explicit universal constants that are \textit{independent} of \( n \) and \( \gamma \)\footnote{In fact, our metric entropy bounds could be expressed with explicit universal constants that are independent of \( \gamma \) and \( \{ R_k \}_{k=0}^{\gamma+1} \). But when these bounds are applied with other technical lemmas to establish minimax optimal rates for the MISE, the universal constants become complex rather quickly and it is very tedious to track them from lines to lines.}. Deriving sharp constants for global criteria such as MISE and in the context of global nonparametric procedures is known to
Table 1: Upper and lower bounds on the log(δ – covering number) and log(δ – packing number) of the generalized \( U_{\gamma+1,1}, U_{\gamma+1,2} \) and \( H_{\gamma+1} \) in \( L^q \)-norm

| \( q \) | \( U_{\gamma+1,1} \) \( U_{\gamma+1,2} \) | \( H_{\gamma+1} \) \( q = 2 \) |
|---|---|---|
| \( \gtrsim \) \( \begin{cases} \mathbb{B}_1(\delta) & \text{if } \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4\gamma R_k}{k!\delta} \geq 0 \\ \mathbb{B}_2(\delta) & \text{otherwise} \end{cases} \) | \( R\sqrt[\gamma+1]{\delta \gamma^{\gamma+1}} \) if \( R_{\gamma+1} \gtrsim \gamma + 1 \) \( \delta^{\gamma+1} \) if \( R_{\gamma+1} \gtrsim \gamma + 1 \) |
| \( \gtrsim \) \( \max \{ \mathbb{B}_1(\delta), \mathbb{B}_2(\delta) \} \) | \( \left( R^* R_0 \right) \delta^{\frac{1}{2(\gamma+1)}} \delta^{\frac{1}{2(\gamma+1)}} \) if \( R_0 \gtrsim 1 \) \( \delta^{\frac{1}{2(\gamma+1)}} \) if \( R_0 \gtrsim 1 \) |

where: \( \mathbb{B}_1(\delta) = \sum_{k=0}^{\gamma-1} \log \frac{4\gamma R_k}{k!\delta} \); \( \mathbb{B}_2(\delta) = (\frac{\gamma}{2} + 1) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} \log R_k \); \( \mathbb{B}_1(\delta) = \sum_{k=0}^{\gamma} \log(9^{-\gamma \gamma^{-\gamma}}) + \sum_{k=0}^{\gamma} \log C \sum_{k=0}^{\gamma} \frac{R_k}{R_{\gamma+1}} \) (valid for all \( \delta \) below a threshold detailed in Lemma 3.1); \( R^* = \left( \max_{k \in \{1, \ldots, \gamma+1\}} \frac{R_k}{R_{\gamma+1}} \right)^{\frac{1}{k+1}} \); \( C \) and \( C' \) are positive universal constants that are: \( \gtrsim 1 \), independent of \( \gamma \) and \( \{R_k\}_{k=0}^{\gamma+1} \).

be difficult, which is why the existing literature does not make an attempt in obtaining bounds with explicit constants. The difference in the implicit “constants” between our results and the existing literature is that in the constants in our bounds are truly universal constants that are independent of \( n \) and \( \gamma \), while those in the existing literature could depend on \( \gamma \). In the case \( n \leq (\gamma + 1)^{2\gamma+3} \), to keep the upper bound \( \text{constant} \cdot \left( \frac{1}{\delta} \right)^{\frac{2\gamma+3}{\gamma+1}} \) in the existing literature valid, the “implicit” constant would end up growing with \( n \).

One may wonder if the implications in this paper carry over to the multivariate problem. The analysis for multivariate smooth functions is rather involved because of the additional interplay between the smoothness parameter and the dimension of the covariates. We are only able to provide some partial answers. Nevertheless, we expect similar implications would carry over to the higher dimensional case.

### 3 Covering and packing numbers

In this section, we present bounds on covering and packing numbers associated with \( U_{\gamma+1,1}, U_{\gamma+1,2}, \) and \( H_{\gamma+1} \). Various \( c \) and \( C \) letters in this section denote positive universal constants that are: \( \gtrsim 1 \) and independent of \( \gamma \) and \( \{R_k\}_{k=0}^{\gamma+1} \); these constants may vary from place to place.

Table 1 summarizes the results in this section for easy reference.

#### 3.1 The generalized polynomial subclass, \( U_{\gamma+1,1} \)

**Lemma 3.1.** (i) If \( \delta \) is small enough such that \( \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4\gamma R_k}{k!\delta} \geq 0 \), we have

\[
\log N_{2,P}(\delta, U_{\gamma+1,1}) \leq \log N_{\infty}(\delta, U_{\gamma+1,1}) \leq \sum_{k=0}^{\gamma} \log \frac{4\gamma R_k}{k!\delta};
\]

\[
\mathbb{B}_1(\delta)
\]

if \( \delta \) is large enough such that \( \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4\gamma R_k}{k!\delta} < 0 \), we have

\[
\log N_{2,P}(\delta, U_{\gamma+1,1}) \leq \log N_{\infty}(\delta, U_{\gamma+1,1}) \leq \left( \frac{\gamma}{2} + 1 \right) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} \log R_k.
\]

\[
\mathbb{B}_2(\delta)
\]
(ii) In terms of the lower bounds, we have
\[
\log M_2(\delta, \mathcal{U}_{\gamma+1,1}) \geq B_1(\delta), \\
\log M_{\infty}(\delta, \mathcal{U}_{\gamma+1,1}) \gtrsim B_1(\delta),
\]
where \( B_1(\delta) = \sum_{k=0}^{\gamma} \log (9^{-\gamma} + 2) + \sum_{k=0}^{\gamma} \log C \frac{\gamma^{(\gamma/2)}}{\delta} R_k + \gamma m (\text{with } R_k + 2m > 0 \text{ for } k + 2m > \gamma) \) for some positive universal constant \( C \). Let \( \bar{k} \in \arg \max_{k \in \{0, \ldots, \gamma\}} \frac{R_k}{k^2} \). If
\[
R_k \bar{k}! \delta \left( \frac{\bar{k} + 1}{\bar{k} + 1} \right) \mathcal{R}_k \geq 2^{\gamma + 1}, \tag{10}
\]
we also have
\[
\log M_2(\delta, \mathcal{U}_{\gamma+1,1}) \geq B_2(\delta) = C' (\gamma + 1), \\
\log M_{\infty}(\delta, \mathcal{U}_{\gamma+1,1}) \gtrsim B_2(\delta). \tag{11}
\]

(iii) If the density function \( p(x) \) on \([-1, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then
\[
\log M_{2,p}(\delta, \mathcal{U}_{\gamma+1,1}) \gtrsim B_2(\delta); \tag{12}
\]
under \eqref{eq:10}, we also have
\[
\log M_{2,p}(\delta, \mathcal{U}_{\gamma+1,1}) \gtrsim B_2(\delta). \tag{13}
\]

Remark. When \( R_k = \mathcal{C} \) for \( k = 0, \ldots, \gamma \), \( \bar{k} + 1 \mathcal{R}_k \mathcal{R}_k \gtrsim 2^{\gamma + 1} \); when \( R_0 = \mathcal{C} \) and \( R_k \leq \mathcal{C} (k - 1)! \) for \( k = 1, \ldots, \gamma \), \( (\bar{k} + 1) \mathcal{R}_k \mathcal{R}_k \gtrsim 2 \log (\mathcal{C} + 2) \); when \( R_k = \mathcal{C} \) for all \( k = 0, \ldots, \gamma \), \( (\bar{k} + 1) \mathcal{R}_k \mathcal{R}_k \gtrsim (\mathcal{C}/2^2) \).

The proof for Lemma 3.1 is given in Section A.1

The lower bounds \( B_1(\delta) \) and \( B_2(\delta) \), as well as the upper bound \( \overline{B}_1(\delta) \) are original. The (less original) bound \( \overline{B}_2(\delta) \) generalizes the upper bound associated with the polynomial subclass in Kolmogorov and Tikhomirov (1959), which takes the form \((\gamma + 1) \log \frac{1}{\delta}\). It is worth pointing out that \( \overline{B}_2(\delta) \) holds for all \( \delta \in (0, 1) \) (not just \( \delta \) such that \( \min_{k \in \{0, \ldots, \gamma\}} \log \frac{1}{(\gamma + 1)^2} R_k < 0 \)) but is far from being tight when \( \min_{k \in \{0, \ldots, \gamma\}} \log \frac{1}{(\gamma + 1)^2} R_k \geq 0 \). Obviously \( \overline{B}_1(\delta) \gtrsim \overline{B}_2(\delta) \). When it comes to deriving the upper bounds for the MISE under large enough \( R_k \), \( \overline{B}_1(\delta) \) will be very useful.

For the packing numbers of \( \mathcal{U}_{\gamma+1,1} \), we also present two different lower bounds. In particular, \( \overline{B}_2 \) in \eqref{eq:13} will be useful for deriving the minimax lower bounds for the MISE when \( R_k \) is relatively small, while \( \overline{B}_1(\delta) \) in \eqref{eq:8} will be useful when \( R_k \) is relatively large. When deriving a lower bound for the standard \( \mathcal{U}_{\gamma+1} \) under the assumption that \( R_k = \mathcal{C} \), Kolmogorov and Tikhomirov (1959) constructs a set of functions where the cardinality of this set only gives a lower bound for \( \mathcal{U}_{\gamma+1,2} \). As we will see in Section 3.2, the lower bound in Kolmogorov and Tikhomirov (1959) is not sharp when \( \delta \) is not small enough.

To establish \( \overline{B}_1(\delta), \overline{B}_1(\delta) \) and \( \overline{B}_2 \), we discard the argument in Kolmogorov and Tikhomirov (1959) and develop our own. The derivation of \( \overline{B}_1(\delta) \) is based on a constructive proof. To derive \( \overline{B}_1(\delta) \) and \( \overline{B}_1(\delta) \), we consider two classes (equivalent to \( \mathcal{U}_{\gamma+1,1} \)), each in the form of a \((\gamma + 1)\) -dimensional polyhedron. The lower bound \( \overline{B}_1(\delta) \) is the more delicate part. In particular, for any \( f \in \mathcal{U}_{\gamma+1,1} \), we write \( f(x) = \sum_{k=0}^{\gamma} \theta_k \phi_k(x) \), where \( \phi_k \) are the Legendre polynomials. The key step is to derive sharp lower bounds for the magnitude of \( \left( \theta_k \right)_{k=0}^{\gamma} \) in the worst case.
3.2 The generalized Hölder subclass, $\mathcal{U}_{\gamma+1,2}$

Lemma 3.2. Let $R^s = \left( \max_{k \in \{1, \ldots, \gamma+1\}} \frac{R_k}{(k-1)!} \right) \lor 1$. We have

$$\log N_{2,\mathbb{P}}(\delta, \mathcal{U}_{\gamma+1,2}) \leq \log N_{\infty}(\delta, \mathcal{U}_{\gamma+1,2}) \lesssim R^s \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}}.$$

We also have

$$\log M_{\infty}(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim \log M_2(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim R^s \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}}, \quad \text{if } R_0 \gtrsim 1, \delta \in (0, 1);$$

$$\log M_{\infty}(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim \log M_2(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim (R^s R_0) \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}}, \quad \text{if } R_0 \lesssim 1, \delta \in (0, 1).$$

If the density function $p(x)$ on $[-1, 1]$ is bounded away from zero, i.e., $p(x) \geq c > 0$, then

$$\log M_{2,\mathbb{P}}(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim R^s \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}}, \quad \text{if } R_0 \gtrsim 1, \delta \in (0, 1);$$

$$\log M_{2,\mathbb{P}}(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim (R^s R_0) \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}}, \quad \text{if } R_0 \lesssim 1, \delta \in (0, 1).$$

The proof for Lemma 3.2 is given in Section A.3.

Lemma 3.2 extends Kolmogorov and Tikhomirov (1959) to allow for general $R_k$s. When $R_k \leq \overline{C}k!$ for all $k = 1, \ldots, \gamma + 1$, $R^s \frac{1}{\gamma + 1} \lor 1$. If $R_k \geq \overline{C}k!$ for all $k = 1, \ldots, \gamma + 1$, $R^s \frac{1}{\gamma + 1} \gtrsim 1$; for example, taking $R_k \geq \overline{C}(k!)^2$ for all $k = 1, \ldots, \gamma + 1$ yields $R^s \frac{1}{\gamma + 1} \gtrsim \gamma$.

Given Lemmas 3.1-3.2, (3) and (5), we have

$$\log N_{2,\mathbb{P}}(2\delta, \mathcal{U}_{\gamma+1}) \leq \log N_{\infty}(2\delta, \mathcal{U}_{\gamma+1})$$

$$\leq \begin{cases} B_1(\delta) + R^s \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}} & \text{if } \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k^2} \geq 0 \\ B_2(\delta) + R^s \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}} & \text{if } \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k^2} < 0 \end{cases} \quad (14)$$

and

$$\log M_{\infty}(\delta, \mathcal{U}_{\gamma+1}) \gtrsim \log M_2(\delta, \mathcal{U}_{\gamma+1}) \gtrsim \max \left\{ B_1(\delta), B_2, R^s \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}} \right\} \quad \text{if } R_0 \gtrsim 1$$

$$\gtrsim \max \left\{ B_1(\delta), B_2, (R^s R_0) \frac{1}{\gamma + 1} \frac{1}{\delta^{\gamma + 1}} \right\} \quad \text{if } R_0 \lesssim 1.$$

Our lower bounds above sharpen the classical result in Kolmogorov and Tikhomirov (1959). In particular, the lower bound for $\mathcal{U}_{\gamma+1}$ in Kolmogorov and Tikhomirov (1959) (derived under the assumption that $R_k = \overline{C}$) takes the form $\delta^{\gamma + 1}$. This result and its proof are inherited later in papers and textbooks including the more recent textbook on nonasymptotic statistics by Wainwright (2019, Example 5.11), where in the derivation of the lower bound, a set of functions are constructed in the way such that their $k$th order derivatives evaluated at zero are zero for all $k = 0, \ldots, \gamma$. In other words, $\mathcal{U}_{\gamma+1,1}$ is a singleton in this construction and the cardinality of this set only gives a lower bound for $\mathcal{U}_{\gamma+1,2}$. In particular, the lower bound $\delta^{\gamma + 1}$ is not sharp when $\delta$ is not small enough.

3.3 The ellipsoid subclass, $\mathcal{H}_{\gamma+1}$

Lemma 3.3. If $R_{\gamma+1} \gtrsim \gamma + 1$, we have

$$\log N_2(\delta, \mathcal{H}_{\gamma+1}) \asymp (R_{\gamma+1} \delta^{-1}) \frac{1}{\gamma + 1}.$$
If \( R_{\gamma+1} \preceq \gamma + 1 \), we have

\[
\log N_2 (\delta, \mathcal{H}_{\gamma+1}) \preceq \delta^{\frac{\gamma+1}{\gamma+1}},
\]

(15)

\[
\log N_2 (\delta, \mathcal{H}_{\gamma+1}) \succeq (R_{\gamma+1}\delta^{-1})^{\frac{1}{\gamma+1}}.
\]

(16)

If the density function \( p(x) \) on \([0, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then the bounds above also hold for \( \log N_{2,p} (\delta, \mathcal{H}_{\gamma+1}) \).

The proof for Lemma 3.3 is given in Section [A.3].

When \( R_{\gamma+1} = 1 \), Lemma 3.3 sharpens the upper bound for \( \log N_2 (\delta, \mathcal{H}_{\gamma+1}) \) in Wainwright (2019) from \( (\gamma \vee 1) \delta^{\frac{\gamma}{\gamma+1}} \) to \( \delta^{\frac{\gamma+1}{\gamma+1}} \); in particular, the upper and lower bounds in Wainwright (2019) (the last two inequalities on p.131) scale as \( (\gamma \vee 1) \delta^{\frac{\gamma}{\gamma+1}} \) and \( \delta^{\frac{\gamma+1}{\gamma+1}} \), respectively, while our upper and lower bounds in Lemma 3.3 have the same scaling \( \delta^{\frac{\gamma+1}{\gamma+1}} \). We discover the cause of the gap lies in that the “pivotal” eigenvalue (that balances the “estimation error” and the “approximation error” from truncating for a given resolution \( \delta \)) in Wainwright (2019) is not optimal. The truncation in Wainwright (2019) is commonly used in the existing literature and seems to originate from Theorem 3 in Mityagin (1961). We close the gap by finding the optimal “pivotal” eigenvalue.

More generally, for the case of \( R_{\gamma+1} \preceq \gamma + 1 \), we consider two different truncations, one giving the upper bound \( \delta^{\frac{\gamma+1}{\gamma+1}} \) and the other giving the lower bound \( (R_{\gamma+1}\delta^{-1})^{\frac{1}{\gamma+1}} \). Note that \( (R_{\gamma+1}\delta^{-1})^{\frac{1}{\gamma+1}} \asymp \delta^{\frac{\gamma+1}{\gamma+1}} \) when \( R_{\gamma+1} \asymp 1 \). For the case of \( R_{\gamma+1} \succeq \gamma + 1 \), we use only one truncation to show that both the upper bound and the lower bound scale as \( (R_{\gamma+1}\delta^{-1})^{\frac{1}{\gamma+1}} \).

4 Minimax optimal rates in commonly seen cases

In this section, we revisit the minimax optimal MISE rates associated with some commonly seen smoothness classes in the literature.

Definition (standard smoothness classes). Let \( \overline{C} \) be a universal constant independent of \( n \) and \( \gamma \). The standard Hölder class corresponds to \( \mathcal{U}_{\gamma+1} \) with \( R_k = \overline{C} \) for all \( k = 0, \ldots, \gamma + 1 \). We define the standard Sobolev class as follows:

\[
\mathcal{S}_{\gamma+1} := \{ f : [0, 1] \to \mathbb{R} | f \text{ is } \gamma + 1 \text{ times differentiable a.e.,} \ f^{(k)} \text{ is absolutely continuous and,} \ |f|_{H,k} \leq \overline{C}, \text{ for all } k = 0, \ldots, \gamma \}
\]

where

\[
|f|_{H,k} = \sqrt{\sum_{j=0}^{k} (f^{(j)}(0))^2 + \int_0^1 [f^{(k+1)}(t)]^2 \, dt}.
\]

(17)

Note that we have defined \( \mathcal{S}_{\gamma+1} \) in the way that is consistent with how we define the standard Hölder class. These definitions ensure \( \mathcal{U}_{k+1} \subseteq \mathcal{U}_{k'+1} \) and \( \mathcal{S}_{k+1} \subseteq \mathcal{S}_{k'+1} \) for any \( k \geq k' \). When we write \( \mathcal{U}_{\gamma+1} \) or \( \mathcal{S}_{\gamma+1} \) in this section, \( \mathcal{U}_{\gamma+1} \) refers to the standard Hölder class and \( \mathcal{S}_{\gamma+1} \) refers to the standard Sobolev class. The regression model (11) is subject to the following assumption.

Assumption 1. \( \{\varepsilon_i\}_{i=1}^n \) are independent \( \mathcal{N}(0, \sigma^2) \) where \( \sigma \asymp 1 \); \( \{\varepsilon_i\}_{i=1}^n \) are independent of
\{X_i\}_{i=1}^n; \{\epsilon_i\}_{i=1}^n\} are independent draws from a distribution on the domain associated with \(\mathcal{U}_{\gamma+1}\) (respectively, \(\mathcal{S}_{\gamma+1}\)) and with density \(p(x)\) bounded away from zero; that is, \(p(x) \geq c > 0\).

**Remark.** In the literature on minimax lower bounds, when both \(\{X_i\}_{i=1}^n\) and \(\{\epsilon_i\}_{i=1}^n\) are stochastic, the normality assumption on \(\{\epsilon_i\}_{i=1}^n\) and the assumption of \(\{\epsilon_i\}_{i=1}^n\) being independent of \(\{X_i\}_{i=1}^n\) are the most common for technical reasons; see, e.g., Yang and Barron (1999) and Raskutti, et. al (2011). To relax the normality of \(\{\epsilon_i\}_{i=1}^n\), one possibility is to assume \(X_i\) is deterministic and \(X_i = \frac{1}{n}\) for \(i = 1, \ldots, n\); see, e.g., Assumption B and Corollary 2.3 in Tsybakov (2009). Typically, one either makes fewer assumptions about the covariates but imposes a distributional form on the noise, or makes fewer assumptions about the noise but imposes a form on the covariates. Until very recently, Zhao and Yang (2022) provide bounds on the Kullback-Leibler divergence of distributions in the location-scale family subjective to some technical conditions. The bounds in Zhao and Yang (2022) can be used to relax the normality assumption on \(\{\epsilon_i\}_{i=1}^n\) here without changing the essence of our paper. However, to focus on the key points, we stick to the standard normality assumption as in, for example, Yang and Barron (1999) and Raskutti, et. al (2011).

The assumption \(\sigma \approx 1\) is not critical and can be relaxed, but allows us to simplify the presentations of our results and focus on the key points.

**Remark.** For the upper bounds, the normality of \(\{\epsilon_i\}_{i=1}^n\) can be replaced with a sub-Gaussian assumption, which is rather standard in the literature on empirical process theory (e.g., van de Geer, 2000). This relaxation does not impose any additional restrictions on \(\{X_i\}_{i=1}^n\) beyond what has been assumed in Assumption 1. The supporting lemmas we use in this paper for the derivation of the upper bounds extend easily to models with sub-Gaussian noise and our results would still hold; however, to establish minimax optimality, it is more sensible to consider a model with the same set of assumptions on \(\{\epsilon_i\}_{i=1}^n\) and \(\{X_i\}_{i=1}^n\) for the minimax lower and upper bounds.

The proofs for the minimax optimality results in this section as well as Section 5 are based on our Section 3 as well as techniques from empirical processes, machine learning theory, and information theory. Even for the commonly seen smoothness classes, the existing minimax optimal rate \(\left(\frac{\sigma^2}{n}\right)^{\frac{2\gamma+2}{2\gamma+3}}\) is not correct when \(n \leq (\gamma + 1)^{2\gamma+3}\), because the classical metric entropy result \(\asymp \delta^{-\frac{1}{2\gamma+3}}\) applied into these techniques ignores the polynomial subclass. The key to show the correct rate in the regime of \(n \leq (\gamma + 1)^{2\gamma+3}\) lies in the metric entropy bounds established in Section 3.

### 4.1 Mean integrated squared error

**Theorem 4.1** (lower bounds). Suppose Assumption 1 holds.

(i) If

\[
\frac{n}{\sigma^2} > (\gamma + 1)^{2\gamma+3},
\]

then we have

\[
\inf_{f} \sup_{f \in \mathcal{S}_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2,\mathcal{P}}^2 \right) \geq \mathcal{L}_0 \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{3(\gamma+1)+1}},
\]

\[
\inf_{f} \sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2,\mathcal{P}}^2 \right) \geq \mathcal{L}_0 \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{3(\gamma+1)+1}},
\]

---

9In the cases of Sobolev classes, we consider the interval \([0, 1]\) (instead of \([-1, 1]\)). This is purely for simplifying notations and also consistent with the literature.
for some universal constant \( c_0 \in (0, 1] \) independent of \( n \) and \( \gamma \). Note that \( \frac{\sigma^2(\gamma+1)}{n} < \left( \frac{\sigma^2}{n} \right)^{2(\gamma+1)} \) in this case.

(ii) If \( \frac{n}{\sigma^2} \leq (\gamma + 1)^{2\gamma+3} \), we let \( \gamma^* \in \{0, \ldots, \gamma\} \) be the smallest integer such that \( \frac{n}{\sigma^2} \leq (\gamma^* + 1)^{2\gamma^*+3} \); in addition, if

\[
\frac{n}{\sigma^2} \geq c_0 4\gamma^* (\gamma^* + 1)
\]

for some universal constant \( c_0 \in (0, 1] \) independent of \( n \) and \( \gamma \), then we have

\[
\inf_f \sup_{f \in S_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_F^2 \right) \geq c \frac{\sigma^2 (\gamma^* + 1)}{n},
\]

\[
\inf_f \sup_{f \in U_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_F^2 \right) \geq c \frac{\sigma^2 (\gamma^* + 1)}{n},
\]

for some universal constant \( c \in (0, 1] \) independent of \( n \) and \( \gamma \) such that \( c \leq \frac{\sigma^2}{\sigma^2} \). Note that \( \frac{\sigma^2(\gamma+1)}{n} \geq \left( \frac{\sigma^2}{n} \right)^{2(\gamma+1)} \) in this case.

The proof for Theorem 4.1 is given in Section B.1, which relies on the constructions behind the bound \( B_2 \) in Lemma 3.1, as well as Lemma 3.2.

The following two theorems show the achievability of the rates in Theorem 4.1. In particular, we show that estimators constrained to exploit the optimal degree of smoothness in each regime achieve the respective rate in Theorem 4.1. We consider the constrained nonparametric least squares estimator (CNLS)

\[
\hat{f} \in \arg\min_{f \in F} \frac{1}{2n} \sum_{i=1}^{n} (y_i - \hat{f}(x_i))^2.
\]

The CNLS is commonly seen in the minimax optimality literature (e.g., Raskutti, et. al 2011) and the Kernel Ridge Regression (KRR) literature. Let \( k = \gamma \) in the large sample regime and \( k = \gamma^* \) in the small sample regime. We consider either \( F = U_{\gamma+1} \) or

\[ F = S_{\gamma+1} \]

\[ := \{ f : [0, 1] \rightarrow \mathbb{R} \mid f \text{ is } k + 1 \text{ times differentiable a.e.,} \]

\[ f^{(k)} \text{ is absolutely continuous and } |f|_{\mathcal{H},k} \leq C \}

where \( |\cdot|_{\mathcal{H},k} \) is the norm defined in (17). Both cases can be of interest but the latter is more widely implemented in practice, as we explain below.

**Kernel Ridge Regression (KRR) in machine learning**

Constraining the estimators to be in \( S_{\gamma+1} \) allows one to implement (20) via kernel functions. Let the matrix \( K_{\gamma+1} \in \mathbb{R}^{n \times n} \) consist of entries \( \frac{1}{n} K_{\gamma+1}(x_i, x_{i'}) \), taking the form

\[
K_{\gamma+1}(x_i, x_{i'}) = 1 + (x_i \wedge x_{i'}) \quad \text{for } k = 0,
\]

\[
K_{\gamma+1}(x_i, x_{i'}) = \sum_{j=0}^{k} \frac{x_i^j x_{i'}^j}{j!} + \int_0^1 (x_i - t)^{k+1} (x_{i'} - t)^{k+1} \frac{k!}{k!} dt \quad \text{for } k > 0,
\]

where \( (a)_+ = a \vee 0 \). The kernel function \( K_{\gamma+1}(w, z) = \sum_{j=0}^{k} \frac{w^j z^j}{j!} \) generates the \( k \)th degree polynomial subspace and the kernel function \( K_{\gamma+1}(w, z) = \int_0^1 \frac{(w-t)^k}{k!} \frac{(z-t)^k}{k!} dt \) for \( k > 0 \) \( (w \wedge z \text{ for } \)}
$k = 0$) generates the $(k+1)$th order Sobolev subspace imposed with the restrictions that $f^{(j)}(0) = 0$ for all $j = 0, \ldots, k$ and $f^{(k+1)}$ belongs to the space $L^2[0, 1]$.

When $F = S_{k+1}$ in (20), $\hat{f}$ can be written as

$$\hat{f}(\cdot) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \hat{\pi}_i K_{k+1} (\cdot, x_i')$$  \hspace{1cm} (23)

where

$$\hat{\pi} := \{ \hat{\pi}_i \}_{i=1}^{n} = \arg \min_{\pi \in \mathbb{R}^n} \frac{1}{2n} \sum_{i=1}^{n} \left( y_i - \frac{1}{\sqrt{n}} \sum_{i'=1}^{n} \pi_{i'} K_{k+1}(x_i, x_i') \right)^2$$ \hspace{1cm} (24)

s.t. $\pi^T \mathbb{K}_{k+1} \pi \leq C^2$.

In particular, (25) comes from the representation $|\hat{f}|_{H,k}^2 = \pi^T \mathbb{K}_{k+1} \pi$ when $F = S_{k+1}$ in (20) and $\hat{f}$ takes the form $\hat{f}(\cdot) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \pi_i K_{k+1} (\cdot, x_i')$.

By the Lagrangian duality, solving (24) is equivalent to solving

$$\hat{\pi} = \arg \min_{\pi \in \mathbb{R}^n} \frac{1}{2n} \sum_{i=1}^{n} \left( y_i - \frac{1}{\sqrt{n}} \sum_{i'=1}^{n} \pi_{i'} K_{k+1}(x_i, x_i') \right)^2 + \lambda \pi^T \mathbb{K}_{k+1} \pi$$ \hspace{1cm} (26)

for a properly chosen regularization parameter $\lambda > 0$. Consequently, the optimal weight vector $\hat{\pi}$ takes the form

$$\hat{\pi} = (\mathbb{K}_{k+1} + \lambda I_n)^{-1} \frac{Y}{\sqrt{n}}$$ \hspace{1cm} (27)

where $Y = \{ y_i \}_{i=1}^{n}$. The KRR estimators associated with $S_{k+1}$ are related to the smoothing splines methods and Gaussian process regressions in machine learning. We refer interested readers to Wahba (1990), Schölkopf and Smola (2002), as well as Rasmussen and Williams (2006) for more details.

**Theorem 4.2** (upper bounds for standard Sobolev). Suppose Assumption 1 holds.

(i) If

$$\frac{n}{\sigma^2} > (\gamma + 1)^{2\gamma+3},$$ \hspace{1cm} (28)

let $\hat{f}(\cdot) = \frac{1}{\sqrt{n}} \sum_{i'=1}^{n} \hat{\pi}_{i'} K_{\gamma+1} (\cdot, x_i')$ where $\{ \hat{\pi}_{i'} \}_{i'=1}^{n} = (\mathbb{K}_{\gamma+1} + \lambda I_n)^{-1} \frac{Y}{\sqrt{n}}$ and $\lambda \asymp (\frac{1}{n})^{2(\gamma+1)}/2(\gamma+1)+1$. Then we have

$$\sup_{f \in S_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2,p}^2 \right) \leq \bar{c} \left[ r_1^2 + \exp \{ -cnr_1^2 \} \right],$$

for some universal constant $\bar{c} \in (1, \infty)$, where $r_1^2 = \left( \frac{\sigma^2}{n} \right)^{(2(\gamma+1)+1)/(\gamma+1)}$.

(ii) If

$$\frac{n}{\sigma^2} \leq (\gamma + 1)^{2\gamma+3},$$ \hspace{1cm} (29)

let $\hat{f} = \frac{1}{\sqrt{n}} \sum_{i'=1}^{n} \hat{\pi}_{i'} K_{\gamma+1} (\cdot, x_i')$ where $\{ \hat{\pi}_{i'} \}_{i'=1}^{n} = (\mathbb{K}_{\gamma+1} + \lambda I_n)^{-1} \frac{Y}{\sqrt{n}}$ with $\gamma^*$ defined in Theorem 4.1, and $\lambda \asymp \frac{\gamma^*+1}{n}$. If $\frac{n}{\sigma^2} \geq \gamma^* + 1$, then we have

$$\sup_{f \in S_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2,p}^2 \right) \leq \bar{c} \left[ r_2^2 + \exp \{ -cnr_2^2 \} \right]$$
Theorem 4.3 (upper bounds for standard Hölder). Suppose Assumption 1 holds.

(i) If 
\[ \frac{n}{\sigma^2} > (\gamma + 1)^{2\gamma + 3}, \]
then we have 
\[ \sup_{f \in \mathcal{U}_{\gamma + 1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2, \mathbb{P}}^2 \right) \leq \tau [r_1^2 + \exp \{-cnr_1^2\}], \]
for some universal constant \( \tau \in (1, \infty) \), where 
\[ r_1^2 = \left( \frac{\sigma^2}{n} \right)^{2(\gamma + 1)^{2\gamma + 1}}. \]

(ii) If 
\[ \frac{n}{\sigma^2} \leq (\gamma + 1)^{2\gamma + 3}, \]
let \( \hat{f} \) be \([20] \) with \( \mathcal{F} = \mathcal{U}_{\gamma + 1} \) with \( \gamma^* \) defined in Theorem 4.1. Then we have 
\[ \sup_{f \in \mathcal{U}_{\gamma + 1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2, \mathbb{P}}^2 \right) \leq \tau [r_2^2 + \exp \{-cnr_2^2\}] \]
for some universal constant \( \tau \in (1, \infty) \), where 
\[ r_2^2 = \frac{\sigma^2(\gamma^* + 1)}{n}. \]

Table 2 summarizes the results in this subsection for easy reference.

4.2 The sample mean squared error

When deriving the upper bounds in Theorems 4.2-4.3, we obtain the following bounds on the sample mean squared error (SMSE) as intermediate results.

Corollary 4.1. Suppose the conditions in Theorem 4.2 hold. Under \([28] \), we have 
\[ \left| \hat{f} - f \right|_{n}^2 \lesssim r_1^2 \quad \text{for any } f \in \mathcal{S}_{\gamma + 1}, \]
for some universal constant \( \tau \in (1, \infty) \).
with probability at least $1 - c_0 \exp \{-cnr_1^2\}$. Under (29), we have
\[ |\hat{f} - f|_2^2 \lesssim r_2^2 \quad \text{for any } f \in \mathcal{S}_{\gamma+1}, \]
with probability at least $1 - c_0 \exp \{-cnr_2^2\}$.

**Corollary 4.2.** Suppose the conditions in Theorem 4.3 hold. Under (30), we have
\[ |\hat{f} - f|_2^2 \lesssim r_1^2 \quad \text{for any } f \in \mathcal{U}_{\gamma+1}, \]
with probability at least $1 - c_0 \exp \{-cnr_1^2\}$. Under (31), we have
\[ |\hat{f} - f|_2^2 \lesssim r_2^2 \quad \text{for any } f \in \mathcal{U}_{\gamma+1}, \]
with probability at least $1 - c_0 \exp \{-cnr_2^2\}$.

## 5 Minimax optimal rates in non-standard cases

In this section, we explore the minimax optimal MISE rates associated with several non-standard smoothness classes motivated in Section 2. The results in this section rely on the bounds $B_1(\delta)$, $\hat{B}_1(\delta)$ and $B_2$ in Lemma 3.1, as well as the bounds in Lemmas 3.2-3.3.

**Theorem 5.1.** Suppose Assumption 1 holds.

(i) Let $\hat{f}$ be (23) based on the kernel function $K(\cdot, \cdot)$ associated with $\mathcal{H}_{\gamma+1}$ in (7), where $\hat{\pi}$ is given by (27) with $\lambda \approx R - \frac{4(\gamma+1)}{2(\gamma+1)+1} \sigma_n^2 \frac{2(\gamma+1)+1}{2(\gamma+1)^3}$. Suppose $K$ is continuous, positive semidefinite, and satisfies $K(x, x') \lesssim 1$ for all $x, x' \in [0, 1]$. If $R_{\gamma+1} \gtrsim 1$, we have
\[ \inf_{\tilde{f}} \sup_{f \in \mathcal{H}_{\gamma+1}} \mathbb{E} \left( |\hat{f} - f|_2^2 \right) \gtrsim r_1^2, \]
\[ \sup_{f \in \mathcal{H}_{\gamma+1}} \mathbb{E} \left( |\hat{f} - f|_2^2 \right) \lesssim r_2^2 + \exp \{-cnr_2^2\}, \]
where $r_2^2 = R_{\gamma+1} \sigma_n^2 \frac{2(\gamma+1)+1}{2(\gamma+1)^3}$. If $R_{\gamma+1} \gtrsim 1$, we have
\[ \inf_{\tilde{f}} \sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( |\hat{f} - f|_2^2 \right) \gtrsim r_2^2, \]
\[ \sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( |\hat{f} - f|_2^2 \right) \lesssim r_2^2 + \exp \{-cnr_2^2\}, \]
where $r_2^2 = (R^n \sigma_n^2 \frac{2(\gamma+1)+1}{2(\gamma+1)^3}) \gtrsim 1$.

The proof for Theorem 5.1 is given in Section B.5.
Theorems 4.1-4.3 suggest that the blessing of exploiting higher degree of smoothness arises when \( n \geq (\gamma + 1)^{2\gamma + 3} \), which clearly includes the degenerate case of \( \gamma \) being finite and \( n \) tending to \( \infty \). In these cases, the minimax optimal rate for the MISE is \( \left( \frac{\sigma^2}{n} \right)^{2+\gamma + 3} \), which decreases in \( \gamma \). Theorem 5.1 suggests that the blessing of exploiting higher degree of smoothness may also arise when a smoothness class is imposed with the restrictions that \( f^{(k)}(0) = 0 \) for all \( k = 0, \ldots, \gamma \). Note that if \( R_{\gamma+1}^{2} \approx 1 \) in the case of \( \mathcal{H}_{\gamma+1} \) and \( (R^{*})^{2+\gamma + 3} \approx 1 \) in the case of \( \mathcal{U}_{\gamma+1,2} \), the minimax optimal rate for the MISE is \( \left( \frac{\sigma^2}{n} \right)^{2+\gamma + 3} \).

A somewhat counter-intuitive finding from Theorem 5.1 is that the parameters \( R_{\gamma+1} \) and \( R^{*} \) only scale the standard minimax optimal MISE rate \( \left( \frac{\sigma^2}{n} \right)^{2+\gamma + 3} \) by \( R_{\gamma+1}^{2} \) instead of \( R \) (where \( R = R_{\gamma+1} \) in the case of \( \mathcal{H}_{\gamma+1} \), and \( R = R^{*} \) in the case of \( \mathcal{U}_{\gamma+1,2} \)). Because of the different forms \( R_{\gamma+1} \) and \( R^{*} \) take, the optimal rates can differ between \( \mathcal{H}_{\gamma+1} \) and \( \mathcal{U}_{\gamma+1,2} \). For example, when \( R_{k} = (k - 1)! \) for all \( k = 0, \ldots, \gamma + 1, \) \( R^{*} = 1 \) and \( r^{2} = \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \) in Theorem 5.1(ii). Meanwhile, when \( R_{\gamma+1} = \gamma! \), \( r^{2} \approx \gamma \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \) in Theorem 5.1(i). Note that this difference cannot be revealed by minimax optimal rates derived based on the classical metric entropy bounds (which would simply yield \( \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \)).

The next two theorems explore the minimax optimal MISE rates for cases motivated in Section 2. There are many interesting results that can be explored using the bounds in Section 3. We focus on the Hölder classes which reveal an interesting contrast coming from the polynomial subclass when \( R_{k} \) is increased from \( \mathcal{O}(k - 1)! \) to \( \mathcal{O}k! \).

**Theorem 5.2.** Suppose Assumption 1 holds, \( R_{0} = \mathcal{O} \) and \( R_{k} \) can be any value in \([\mathcal{O}, \mathcal{O}(k - 1)!]\) for \( k = 1, \ldots, \gamma + 1 \). Let \( R_{1}^{\mathcal{U}} := 1 \vee \sum_{k=0}^{\gamma} \frac{R_{k}}{k!} \).

(i) If

\[
\frac{n}{\sigma^{2}} > (\gamma + 1)^{2\gamma + 3},
\]

then we have

\[
\inf_{f} \sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( \| \hat{f} - f \|_{2,p}^{2} \right) \geq c_{0} r_{1}^{2},
\]

\[
\sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( \| \hat{f} - f \|_{2,p}^{2} \right) \leq \sigma \left( r_{1}^{2} + \exp \{ -cnr_{1}^{2} \} \right),
\]

for some universal constants \( c_{0} \in (0, 1] \) and \( \sigma \in (1, \infty) \) independent of \( n \) and \( \gamma \), where \( r_{1}^{2} = \left( \frac{\sigma^{2}}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \).

(ii) If \( \frac{n}{\sigma^{2}} \leq (\gamma + 1)^{2\gamma + 3} \), we let \( \gamma^{*} \in \{0, \ldots, \gamma\} \) be the smallest integer such that \( \frac{n}{\sigma^{2}} \leq (\gamma^{*} + 1)^{2\gamma^{*} + 3} \); in addition, if

\[
\frac{n}{\sigma^{2}} \geq c_{0} 4\gamma^{*} (\gamma^{*} + 1) R^{12}
\]

for some universal constant \( c_{0} \in (0, 1] \) independent of \( n \) and \( \gamma \), then we have

\[
\inf_{f} \sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( \| \hat{f} - f \|_{2,p}^{2} \right) \geq \frac{\sigma^{2} (\gamma^{*} + 1)}{n}
\]
for some universal constant \( \zeta \in (0, 1] \) independent of \( n \) and \( \gamma \) such that \( \zeta \leq \frac{\zeta}{2} \).

(iii) If

\[
\frac{n}{\sigma^2} \leq (\gamma + 1)^{2\gamma + 3},
\]

let \( \hat{f} \) be (24) with \( \mathcal{F} = \mathcal{U}_{k+1} \). Then we have

\[
\sup_{f \in \mathcal{U}_{k+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2,\mathbb{P}}^2 \right) \leq \mathcal{C} \left[ r_2^2 + \exp \left\{ -cnr_2^2 \right\} \right]
\]

where \( r_2^2 = \frac{\sigma^2(\gamma + 1)^{2\gamma + 3}}{n} \).

**Remark.** When \( R_0, R_1 = \overline{C} \) and \( R_k \leq \overline{C} (k - 2)! \) for all \( k = 2, ..., \gamma + 1 \), the part \( \frac{n}{\sigma^2} \geq c_0 4^\gamma (\gamma + 1) R^{12n} \) in (33) says \( \frac{n}{\sigma^2} \geq 4^\gamma \gamma^{\gamma + 1} + 1 \) when \( R_0 = \overline{C} \) and \( R_k = \overline{C} (k - 1)! \) for all \( k = 1, ..., \gamma + 1 \), (33) says \( \frac{n}{\sigma^2} \geq 4^\gamma (\gamma + 1) (\log (\gamma + 2))^2 \). We can improve this condition to \( \frac{n}{\sigma^2} \geq 4^\gamma (\gamma + 1) + 1 \) using the bound \( \mathcal{B}_1(\delta) \) in Lemma 3.1. But to allow the generality that \( R_k \) can be any value in \( \{ \overline{C}, \overline{C} (k - 1)! \} \) in Theorem 5.2, we use the bound \( \mathcal{B}_2 \) in Lemma 3.1, which gives (33).

The proof for Theorem 5.2 is given in Section 3.6.

Theorem 5.2 is another example (besides Theorems 4.1–4.3) that illustrates the importance of Lemma 3.1. In particular, Zhu and Mirzaei (2021) applies the counting argument in Kolmogorov and Tikhomirov (1959) to derive an upper bound for the covering number of the polynomial subclass under \( R_k = (k - 1)! \). If this result is used to derive an upper bound for the MISE, we would have obtained (35) with \( r_2^2 = \frac{\sigma^2(\gamma + 1)^{2\gamma + 3}}{n} \). With the new bound \( \mathcal{B}_1(\delta) \) developed in our Lemma 3.1, the upper bound for the MISE shown in Theorem 5.2 improves \( \frac{n}{\sigma^2} \geq c_0 4^\gamma (\gamma + 1) (\log (\gamma + 2))^2 \) by a factor of \( (\gamma + 1) \log (\gamma + 2) \). For the lower bound on the covering number of the Hölder class under \( R_k = (k - 1)! \), Zhu and Mirzaei (2021) simply takes the classical lower bound \( \delta \frac{\log(\gamma + 2)}{n} \). As discussed in Section 3, this result ignores the polynomial subclass and is not sharp unless \( \delta \) is small enough.

**Theorem 5.3.** Suppose Assumption 1 holds and \( R_k = \overline{C} k! \) for \( k = 0, ..., \gamma + 1 \).

(i) If

\[
\frac{n}{\sigma^2} \geq \left( (\gamma + 1) \log (\gamma + 2) \right)^{2\gamma + 3},
\]

then we have

\[
\inf_{\hat{f}} \sup_{f \in \mathcal{U}_{k+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2,\mathbb{P}}^2 \right) \geq \mathcal{C} r_1^2,
\]

\[
\sup_{f \in \mathcal{U}_{k+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2,\mathbb{P}}^2 \right) \leq \mathcal{C} \left[ r_1^2 + \exp \left\{ -cnr_2^2 \right\} \right],
\]

for some universal constants \( \mathcal{C} \in (0, 1] \) and \( \mathcal{C} \in (1, \infty) \) independent of \( n \) and \( \gamma \), where \( r_1^2 = \frac{\sigma^2(\gamma + 1)^{2\gamma + 3}}{n} \).

(ii) If \( \frac{n}{\sigma^2} \leq \left( (\gamma + 1) \log (\gamma + 2) \right)^{2\gamma + 3} \), we let \( \gamma^* \in \{ 0, ..., \gamma \} \) be the smallest integer such that \( \frac{n}{\sigma^2} \leq \left( (\gamma^* + 1) \log (\gamma^* + 2) \right)^{2\gamma^* + 3} \); in addition, if

\[
\frac{n}{\sigma^2} \geq c_0 4^\gamma (\gamma + 1) \log (\gamma + 2)
\]

(37)
6 Some insights about multivariate smooth functions

The extension of our analysis to $d$--variate smooth functions is a lot more complex, because of an additional interplay between the smoothness parameter $\gamma$ and the dimension $d$. We provide below
Table 4: Minimax optimal MISE bounds of non-standard $U_{\gamma+1}$

| $R_0 = \overline{c}$, $R_k \in \overline{c}(k-1)!$ | $\forall k = 1, \ldots, \gamma + 1$ |
|-------------------------------------------------|----------------------------------|
| MISE $a_1 \leq \frac{\sigma^2 \gamma}{n} \leq \frac{(\gamma + 1)2^{\gamma+3}}{n}$ | $\in \left[\frac{n}{2} \left(\frac{\gamma^2 (\gamma + 1)}{n} \right), \frac{n}{2} \left(\frac{\gamma^2 (\gamma + 1)}{n} \right)\right]$ |
| $\frac{\sigma^2 \gamma}{n} \leq (\gamma + 1)2^{\gamma+3}$ | $\in \left[\frac{n}{2} \left(\frac{\gamma^2 (\gamma + 1)}{n} \right), \frac{n}{2} \left(\frac{\gamma^2 (\gamma + 1)}{n} \right)\right]$ |

where $\mathbf{a}_1 := c_0 4^{\gamma} (\gamma + 1) R_1^2, R_1^2 := 1 \vee \sum_{k=0}^{\gamma} \frac{2k}{\gamma}$, and $\mathbf{a}_2 := c_0 4^{\gamma} (\gamma + 1) \log (\gamma + 2)$; $c_0, c_0, \mathbf{a}_0 \in (0, 1]$ and $\mathbf{a} \in (1, \infty)$ are universal constants independent of $n$ and $\gamma$; these constants can vary from the first class to the second class; $\mathbf{c} \leq \frac{\sigma^2}{n}$ in the first class and $\mathbf{c} \leq \frac{\sigma^2}{n}$ in the second class; $\gamma^*$ is the smallest integer in $\{0, \ldots, \gamma\}$ such that $\frac{\sigma^2}{n} \leq (\gamma + 1)2^{\gamma+3}$ in the first class (respectively, $\mathbf{c} \leq (\gamma + 1)2^{\gamma+3}$ in the second class).

some partial results about the higher dimensional generalized Hölder class.

Let $p = (p_j)_{j=1}^{d}$ and $P = \sum_{j=1}^{d} p_j$ where $p_j$ is non-negative integers; $x = (x_j)_{j=1}^{d}$ and $x^P = \prod_{j=1}^{d} x_j^{p_j}$. Write $D^p f (x) = \partial^p f / \partial x_1^{p_1} \cdots \partial x_d^{p_d}$.

For a non-negative integer $\gamma$, let the generalized Hölder class $U_{\gamma+1} (\gamma (R_k)_{k=0}^{\gamma+1}, [-1, 1]^d)$ be the class of functions such that any function $f \in U_{\gamma+1} (\gamma (R_k)_{k=0}^{\gamma+1}, [-1, 1]^d)$ satisfies: (1) $f$ is continuous on $[-1, 1]^d$; and all partial derivatives of $f$ exist for all $p$ with $P := \sum_{k=1}^{d} p_k \leq \gamma$; (2) $|D^p f (x)| \leq R_k$ for all $p$ with $P = k$ ($k = 0, \ldots, \gamma$) and $x \in [-1, 1]^d$, where $D^0 f (x) = f (x)$; (3) $|D^p f (x) - D^p f (x')| \leq R_{\gamma+1} \left| x - x' \right|_\infty$ for all $p$ with $P = \gamma$ and $x, x' \in [-1, 1]^d$.

Given any function $f$ in the $d$-variate Hölder class, we have

$$f(x) = \sum_{k=0}^{\gamma} \sum_{p:P=k} \left[ x^P D^p f (0) \right] \frac{k!}{k!} + \sum_{p:P=\gamma} \left[ x^P D^p f (z) \right] \frac{\gamma!}{\gamma!} - \sum_{p:P=\gamma} \left[ x^P D^p f (0) \right] \frac{\gamma!}{\gamma!}$$

for some intermediate value $z$. Similar to Section 2, we have the following relationships:

$$U_{\gamma+1}^d \subseteq U_{\gamma+1}^d \subseteq U_{\gamma+1}^d, \quad U_{\gamma+1,2}^d \subseteq U_{\gamma+1}^d$$

$$U_{\gamma+1,1}^d \subseteq U_{\gamma+1,1}^d + U_{\gamma+1,2}^d := \{ f_1 + f_2 : f_1 \in U_{\gamma+1,1}^d, f_2 \in U_{\gamma+1,2}^d \}$$

where

$$U_{\gamma+1,1}^d = \left\{ f = \sum_{k=0}^{\gamma} \sum_{p:P=k} x^p \theta_{(p,k)} : \left\{ \theta_{(p,k)} \right\}_{(p,k)} \in P_{\Gamma}, x \in [-1, 1]^d \right\}$$

with the $\Gamma := \sum_{k=0}^{\gamma} \left( \begin{array}{c} d+k-1 \\ d-1 \end{array} \right)$-dimensional polyhedron

$$P_{\Gamma} = \left\{ \left\{ \theta_{(p,k)} \right\}_{(p,k)} \in \mathbb{R}^\Gamma : \text{for any given } k = 0, \ldots, \gamma, \theta_{(p,k)} \in \left[ -\frac{R_k}{k!}, \frac{R_k}{k!} \right] \text{ for all } p \text{ with } P \leq k \right\}$$

where $\theta = \left\{ \left\{ \theta_{(p,k)} \right\}_{(p,k)} \right\}$ denotes the collection of $\theta_{(p,k)}$ over all $(p,k)$ configurations. The Hölder subclass $U_{\gamma+1,2}^d$ is the class of functions such that any function $f \in U_{\gamma+1,2}^d$ satisfies: $f \in U_{\gamma+1}^d$ such that $D^p f (0) = 0$ for all $p$ with $P \leq k$, $k = 0, \ldots, \gamma$.  

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Lemma 6.1. Let $R^* = \left( \max_{k \in \{1, \ldots, \gamma + 1\}} \frac{D_k^* R_k}{(k-1)!} \right) \vee 1$. We have

$$\log N_2, p \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \leq \log N_\infty \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \approx d^d R^* \delta^{-\frac{d}{d-1}},$$

(39)

$$\log M_\infty \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \approx \log M_2 \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \approx d^d R^* \delta^{-\frac{d}{d-1}}.$$  (40)

Remark. With Lemma 6.1, we can easily establish the minimax optimal MSE rate for $\mathcal{U}^d_{\gamma+1,1}$, using arguments almost identical to those for Theorem 5.1.

The proof for Lemma 6.1 is given in Section D.4.

Lemma 6.2. If $\delta$ is small enough such that $\min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1) D_k^* R_k}{\delta k!} \geq 0$, we have

$$\log N_2, p \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \leq \log N_\infty \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \leq \sum_{k=0}^\gamma D_k^* \log \frac{4(\gamma+1) D_k^* R_k}{\delta k!}$$

where $D_k^* = \left( \begin{array}{c} d + k - 1 \\ d - 1 \end{array} \right)$; if $\delta$ is large enough such that $\min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1) D_k^* R_k}{\delta k!} < 0$, we have

$$\log N_2, p \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \leq \log N_\infty \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right) \approx \left( \sum_{k=0}^\gamma D_k^* \right) \log \frac{1}{\delta} + \sum_{k=0}^\gamma D_k^* \log R_k.$$  (41)

Remark. The bound (41) holds for all $\delta \in (0, 1)$ (not just $\delta$ such that $\min_k \log \frac{4(\gamma+1) D_k^* R_k}{\delta k!} < 0$) but is too loose when $\delta$ is small enough.

Remark. A simple upper bound on $\sum_{k=0}^\gamma D_k^*$ is $\sum_{k=1}^\gamma d^k \approx d^d$. Let us show a lower bound on $\sum_{k=0}^\gamma D_k^*$ for the case of $\gamma \geq 2d^2$ to illustrate how large $\frac{4^2}{n} \sum_{k=0}^\gamma D_k^*$ can be. We can write $D_k^* = \frac{(k+d-1)!}{(d-1)!k!} = \prod_{j=1}^{d-1} \frac{k+j}{j}$. Because $\gamma \geq 2d^2$, we have

$$\sum_{k=0}^\gamma D_k^* = \left( \sum_{k=0}^\gamma \prod_{j=1}^{d-1} \frac{k+j}{j} \right) \geq \left( \sum_{k=d}^{d} \prod_{j=1}^{d-1} \frac{k+j}{j} \right) \geq \left( d^2 \left( \frac{d^2}{d} + 1 \right)^{d-1} \right) \geq d^{d+1}.$$  (42)

The proof for Lemma 6.2 is given in Section D.2. In theory, our arguments for $B_1(\delta)$ in Lemma 3.1 can be extended for analyzing the lower bound for $\log M_2 \left( \delta, \mathcal{U}^d_{\gamma+1,1} \right)$. However, this extension is very intensive. Arguments similar to those for $B_3$ in Lemma 3.1 will not lead to a useful bound for $\mathcal{U}^d_{\gamma+1,1}$. Despite the lack of lower bounds, we can still gain some insights from Lemma 6.2, as it implies

$$\mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,F} \right) \lesssim r^2 + \exp \left\{ -cnr^2 \right\}$$

where $r^2 = \frac{2^2}{n} \sum_{k=0}^\gamma D_k^*$ and $\hat{f}$ is the estimator in (20) with $F = \mathcal{U}^d_{\gamma+1,1}$. The quantity $\sum_{k=0}^\gamma D_k^*$ is the higher dimensional analogue of $\gamma + 1$ and arises from the fact that a function in $\mathcal{U}^d_{\gamma+1,1}$ has $D_k^*$ distinct $k$th partial derivatives.
Suppose $R_k = 1$ for all $k = 0, ..., \gamma + 1$. If $d$ is small relative to $\gamma$ and $n$, Lemma 6.1 implies that the minimax optimal rate concerning $U^d_{\gamma+1, 2}$ is roughly \( \left( \frac{\sigma^2}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \), the classical rate for $U^d_{\gamma+1}$ derived under the regime where $\gamma$ and $d$ are finite but $n \to \infty$. Observe that

\[
\frac{\sigma^2}{n} \sum_k \gamma \sum_{k=0}^{\gamma} D^* k \approx \left( \frac{\sigma^2}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \text{ whenever } \frac{\sigma^2}{n} \sum_k \gamma \sum_{k=0}^{\gamma} D^* k \approx \left( \frac{\sigma^2}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \text{ whenever } \frac{\sigma^2}{n} \sum_k \gamma \sum_{k=0}^{\gamma} D^* k \approx \left( \frac{\sigma^2}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} .
\]

Therefore, the classical asymptotic minimax rate \( \left( \frac{\sigma^2}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \) could be an underestimate of the MISE when $n$ is not large enough and the optimal degree of smoothness to exploit may not be the maximum smoothness degree $\gamma + 1$, but rather depend on both $n$ and $d$.

### 7 Conclusion and future directions

When the unknown regression function of a single variable is known to have derivatives up to the $(\gamma + 1)$th order bounded in absolute values by a common constant everywhere or a.e., the classical minimax optimal rate of the mean integrated squared error (MISE) \( \left( \frac{1}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \) leads one to conclude that, as $\gamma$ gets larger, the rate gets closer to \( \frac{1}{n} \). This paper shows that: (i) if $n \leq (\gamma + 1)^{2\gamma+3}$, the minimax optimal MISE rate is roughly \( \frac{\log n}{n} \) and the optimal degree of smoothness to exploit is roughly \( \left[ \frac{\log n}{2} \right] - 2 \); (ii) if $n > (\gamma + 1)^{2\gamma+3}$, the minimax optimal MISE rate is \( \left( \frac{1}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \) and the optimal degree of smoothness to exploit is $\gamma + 1$.

The building blocks of our minimax optimality results are a set of metric entropy bounds we develop in this paper for smooth function classes. Some of our bounds are original, and some of them improve and/or generalize the ones in the literature to allow the magnitude of derivatives to depend on their orders. We use our metric entropy bounds to explore the minimax optimal MISE rates associated with some commonly seen smoothness classes and also several non-standard smoothness classes. Our metric entropy bounds can also be of independent interest even if one does not care about the nonparametric regressions.

Discussions of related literature in Section 1 indicate that the classical rate \( \left( \frac{1}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \) is an underestimate of the MISE for local smoothing methods such as kernel density estimators and local polynomials when $n$ is not large enough. For this problem, we could consider (1) where $X_i = \frac{i}{n}$ for $i = 1, ..., n$ and \( \{ \epsilon_i \}_{i=1}^n \) satisfies the assumptions in Corollary 2.3 of Tsybakov (2009). This setup is different from the one in this paper which relaxes the assumption on \( \{ X_i \}_{i=1}^n \) but imposes the normality assumption on \( \{ \epsilon_i \}_{i=1}^n \) (see the remark following Assumption 1 in Section 4). Like how we establish the results in this paper, we would first show the minimax lower bound under the small sample regime, and then show that the MISE of a local smoothing method has an upper bound that matches the lower bound up to some universal constant independent of $n$ and $\gamma$. The proofs would be fairly different from the ones in this paper. There is some theoretical evidence (although not a proof) suggesting that it would require a large $n$ for higher order local polynomials to become beneficial; for example, Tsybakov (2009) requires the smallest eigenvalue associated with the local polynomials to be bounded away from zero (Assumption LP1) to establish the upper bound \( \left( \frac{1}{n} \right)^{2\gamma+2 + \frac{2}{2\gamma+3}} \). This eigenvalue condition in Tsybakov (2009) requires a large enough $n$ and a sufficient condition given in Tsybakov (2009) is that $n \to \infty$. 


A Proofs for Section 3

A.1 Proof for Lemma 3.1

The upper bound. Recall the definition of $U_{\gamma+1,1}$:

$$U_{\gamma+1,1} = \left\{ f = \sum_{k=0}^{\gamma} \theta_k x^k : (\theta_k)_{k=0}^{\gamma} \in \mathcal{P}_\gamma, x \in [-1, 1] \right\}$$

with the $(\gamma + 1)$-dimensional polyhedron

$$\mathcal{P}_\gamma = \left\{ (\theta_k)_{k=0}^{\gamma} \in \mathbb{R}^{\gamma+1} : \theta_k \in \left[ \frac{-R_k}{k!}, \frac{R_k}{k!} \right] \right\}$$

where $R_k$ is allowed to depend on $k \in \{0, ..., \gamma\}$ only. We first derive an upper bound for $N_{\infty}(\delta, U_{\gamma+1,1})$. Because the weighted $L^2(\mathbb{P})$-norm is no greater than the sup norm and a smallest $\delta$-cover of $U_{\gamma+1,1}$ with respect to the $||\cdot||_\infty$ norm also covers $U_{\gamma+1,1}$ with respect to the $||\cdot||_2(\mathbb{P})$ norm, we have

$$N_{2,\mathbb{P}}(\delta, U_{\gamma+1,1}) \leq N_{\infty}(\delta, U_{\gamma+1,1}).$$

To bound $\log N_{\infty}(\delta, U_{\gamma+1,1})$ from above, note that for $f, f' \in U_{\gamma+1,1}$, we have

$$\left| f - f' \right|_\infty \leq \sum_{k=0}^{\gamma} \left| \theta_k - \theta'_k \right|$$

where $f' = \sum_{k=0}^{\gamma} \theta'_k x^k$ such that $\theta' \in \mathcal{P}_\gamma$. Therefore, the problem is reduced to bounding $N_1(\delta, \mathcal{P}_\gamma)$.

Consider $(a_k)_{k=0}^{\gamma}$ such that $a_k > 0$ for every $k = 0, ..., \gamma$ and $\sum_{k=0}^{\gamma} a_k = 1$. To cover $\mathcal{P}_\gamma$ within $\delta$-precision, we find a smallest $a_k \delta$-cover of $\left[ \frac{-R_k}{k!}, \frac{R_k}{k!} \right]$ for each $k = 0, ..., \gamma$, $\left\{ \theta_1^k, ..., \theta_{N_k}^k \right\}$, such that for any $\theta \in \mathcal{P}_\gamma$, there exists some $i_k \in \{1, ..., N_k\}$ with

$$\sum_{k=0}^{\gamma} \left| \theta_k - \theta_{i_k}^k \right| \leq \delta.$$

As a consequence, we have

$$\log N_1(\delta, \mathcal{P}_\gamma) \leq \sum_{k=0}^{\gamma} \log \frac{4R_k}{a_k k! \delta} = - \sum_{k=0}^{\gamma} \log a_k + \sum_{k=0}^{\gamma} \log \frac{4R_k}{k! \delta}. \quad (42)$$

For $(a_k)_{k=0}^{\gamma}$ such that $\sum_{k=0}^{\gamma} a_k = 1$, the function

$$h(a_0, ..., a_\gamma) := - \sum_{k=0}^{\gamma} \log a_k = - \log \left( \prod_{k=0}^{\gamma} a_k \right)$$

is minimized at $a_k = \frac{1}{\gamma+1}$. Consequently, the minimum of $\sum_{k=0}^{\gamma} \log \frac{4R_k}{a_k k! \delta}$ equals $\sum_{k=0}^{\gamma} \log \frac{4(\gamma+1)R_k}{k! \delta}$ and we have

$$\log N_1(\delta, \mathcal{P}_\gamma) \leq \sum_{k=0}^{\gamma} \log \frac{4(\gamma+1)R_k}{k! \delta}.$$
Therefore,
\[
\log N_{2,P} (\delta, U_{\gamma+1,1}) \leq \log N_\infty (\delta, U_{\gamma+1,1}) \leq \sum_{k=0}^{\gamma} \log \frac{4(\gamma + 1)R_k}{k! \delta}.
\]
(43)

If \(\delta\) is large enough such that \(\min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma + 1)R_k}{k! \delta} < 0\), we can evoke the counting argument in Kolmogorov and Tikhomirov (1959) to obtain
\[
\log N_{2,P} (\delta, U_{\gamma+1,1}) \leq \log N_\infty (\delta, U_{\gamma+1,1}) \leq \left(\frac{\gamma}{2} + 1\right) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} \log R_k.
\]
(44)

**The lower bound.** We first derive a lower bound for \(M_2 (\delta, U_{\gamma+1,1})\). Let \(\phi_{k=0}^{\gamma}\) be the Legendre polynomials on \([-1, 1]\). For any function \(f \in U_{\gamma+1,1}\), we can write
\[
f (x) = \sum_{k=0}^{\gamma} \tilde{\theta}_k \phi_k (x)
\]
(45)
such that
\[
\tilde{\theta}_k = \left(\frac{2k + 1}{2}\right) \int_{-1}^{1} f(x) \phi_k(x) dx.
\]
(46)

In Lemma A.1 of Section A.2, we show that
\[
\tilde{\theta}_k = \left(k + \frac{1}{2}\right) \sum_{m=0}^{[\gamma/2]} \frac{f^{(k+2m)}(0)}{2k+2m m! \left(\frac{1}{2}\right)_{k+m+1}}
\]
where \((a)_k = a(a + 1) \cdots (a + k - 1)\) is known as the Pochhammer symbol. Recall \(|f^{(k)}(0)| \leq R_k\) for \(k = 0, \ldots, \gamma\) and \(f^{(k)}(0) = 0\) for \(k > \gamma\). We can rewrite
\[
U_{\gamma+1,1} = \left\{ f = \sum_{k=0}^{\gamma} \tilde{\theta}_k \phi_k (x) : \left(\tilde{\theta}_k\right)_{k=0}^{\gamma} \in \mathcal{P}_L^{\gamma}, x \in [-1, 1] \right\}
\]
with the \((\gamma + 1)\)-dimensional polyhedron
\[
\mathcal{P}_L^{\gamma} = \left\{ \left(\tilde{\theta}_k\right)_{k=0}^{\gamma} \in \mathbb{R}^{\gamma+1} : \tilde{\theta}_k \in \left[ -\overline{R}_k, \overline{R}_k\right] \right\}
\]
where \(\overline{R}_k := \sum_{m=0}^{[\gamma/2]} b_k,m R_{k+2m}\) and \(b_{k,m} = \frac{(k+\frac{1}{2})}{2k+2m m! \left(\frac{1}{2}\right)_{k+m+1}}\). If we can bound \(\overline{R}_k\) from below by \(\underline{R}_k\), then we have
\[
\mathcal{P}_L^{\gamma} \supseteq \mathcal{P}_L^{\gamma} = \left\{ \left(\tilde{\theta}_k\right)_{k=0}^{\gamma} \in \mathbb{R}^{\gamma+1} : \tilde{\theta}_k \in \left[ -\underline{R}_k, \underline{R}_k\right] \right\}.
\]
(47)

Let us derive \(\underline{R}_k\). Because \(f^{(l)}(0) = 0\) for \(l > \gamma\),
\[
\frac{f^{(k+2m)}(0)}{2k+2m m! \left(\frac{1}{2}\right)_{k+m+1}} = 0 \quad \text{if} \quad k + 2m > \gamma.
\]

There are at most \(\gamma + 1\) terms that are multiplied in the product \(m! \left(\frac{1}{2}\right)_{k+m+1}\). Note that \(m \leq \frac{\gamma}{2} \leq \frac{3\gamma}{2} + 1\) and
\[
\left( \frac{1}{2} \right)_{k+m+1} = \frac{1}{2} \frac{1+2}{2} \cdots \frac{1+2(k+m)}{2} \\
\leq \frac{1}{2} \frac{2+2}{2} \cdots \frac{2+2(k+m)}{2} \\
= (k+m+1)!
\]

where \( k + m + 1 \leq \frac{3\gamma}{2} + 1 \). Hence, we have
\[
m! \left( \frac{1}{2} \right)_{k+m+1} \leq m! (k + m + 1)! \leq 1 \cdot \left( \frac{3\gamma}{2} + 1 \right) \leq (3\gamma)^2.
\]

As a result, we have
\[
R_k = \left\lfloor \frac{\gamma}{2} \right\rfloor \sum_{m=0}^{\gamma/2} b_{k,m} R_{k+2m} = \left\lfloor \frac{\gamma}{2} \right\rfloor \sum_{m=0}^{\gamma/2} \frac{(k+1/2) R_{k+2m}}{2^{k+2m} m! \left( \frac{1}{2} \right)_{k+m+1}} \\
\geq \left( k + \frac{1}{2} \right) 2^{-\gamma} 3^{-\gamma} \gamma^{-\gamma} \sum_{m=0}^{\gamma/2} R_{k+2m} \\
\geq \frac{9^{-\gamma} \gamma^{-\gamma}}{2} \sum_{m=0}^{\gamma/2} R_{k+2m} =: R_k.
\]

Note that for any \( f, g \in \mathcal{U}_{\gamma+1,1} \) with \( f(x) = \sum_{k=0}^{\gamma} \tilde{\theta}_k \phi_k(x) \) and \( g(x) = \sum_{k=0}^{\gamma} \tilde{\theta}'_k \phi_k(x) \), we have
\[
|f - g|^2 = \sum_{k=0}^{\gamma} \left[ \sqrt{\frac{2}{2k+1}} \left( \tilde{\theta}_k - \tilde{\theta}'_k \right) \right]^2.
\]

In view of (47) and (49), to construct a packing set of \( \mathcal{U}_{\gamma+1,1} \) with \( \delta \)-separation, we find a largest \( \sqrt{\frac{2k+1}{2}} \sqrt{\gamma+1} \)-packing of \([ -R_k, R_k ]\) for each \( k = 0, \ldots, \gamma \), \( \{ \tilde{\theta}_k^1, \ldots, \tilde{\theta}_k^M \} \), such that for any distinct \( \tilde{\theta}_k^i \) and \( \tilde{\theta}_k^j \) in the packing sets,
\[
\sum_{k=0}^{\gamma} \left[ \sqrt{\frac{2}{2k+1}} \left( \tilde{\theta}_k^i - \tilde{\theta}_k^j \right) \right]^2 > \delta^2.
\]

Therefore\(^\text{10}\)
\[
\log M_2 (\delta, \mathcal{U}_{\gamma+1,1}) \geq \sum_{k=0}^{\gamma} \log \sqrt{\frac{2}{2k+1}} \frac{R_k}{\sqrt{2k+1} \delta}.
\]

Bounds (51) and (48) together give
\[
\log M_2 (\delta, \mathcal{U}_{\gamma+1,1}) \geq \sum_{k=0}^{\gamma} \log (9^{-\gamma} \gamma^{-\gamma}) + \sum_{k=0}^{\gamma} \log C \sum_{m=0}^{\gamma/2} \frac{R_{k+2m}}{\delta} =: B_1 (\delta)
\]

for some positive universal constant \( C \).

The following argument gives another useful bound for \( \log M_2 (\delta, \mathcal{U}_{\gamma+1,1}) \).

\(^{10}\)In fact, we can make the same statement about an exactly \( \delta \)-separated set, i.e., \( = \delta^2 \) rather than \( > \delta^2 \) in (50).
Let $\tilde{k} \in \arg \max_{k \in \{0, ... \gamma \}} \frac{R_k}{k!}$. We consider a $3\delta \left[\frac{\tilde{k} + 1}{\gamma} \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!}\right]$-grid of points on $\left[\frac{-R_k}{k!}, \frac{R_k}{k!}\right]$ and denote the collection of these points by $\left( \theta^{x_i}_{k} \right)_{k=1}^{\ell}$, where $M_0 = \left[\frac{2R_k}{3k!\delta \left(\frac{\tilde{k} + 1}{\gamma} \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!}\right)}\right] + 1$.

We choose $\delta$ such that $M_0 \geq 2^{\gamma + 1}$ and $3\delta \left[\frac{\tilde{k} + 1}{\gamma} \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!}\right] \leq \frac{2R_k}{k!}$. Let us fix $\theta^*_k \in \left[0, \frac{R_k\delta}{bk!(k+1)}\right]$ for $k \in \{0, ..., \gamma \} \setminus \tilde{k}$ and define

$$f^*_\lambda(x) = \theta^*_k x^{\tilde{k}} + \sum_{k \in \{0, ..., \gamma \} \setminus \tilde{k}} \lambda_{i,k} \theta^*_k x^k, \quad x \in [-1, 1] \quad (53)$$

where $(\lambda_{i,k})_{k \in \{0, ..., \gamma \} \setminus \tilde{k}} = \lambda_i \in \{0, 1\}^\gamma$ for all $i = 1, ..., M_0$. For any $\lambda_{i,k}$, $\lambda_{j,k} \in \{0, 1\}^\gamma$ such that $i \neq j$, we have

$$\left| f^*_\lambda - f^*_\lambda \right|_2 = \left[ \int_{-1}^{1} \left( \theta^*_k - \theta^*_j \right) x^{\tilde{k}} + \sum_{k \in \{0, ..., \gamma \} \setminus \tilde{k}} \left( 1 \{ \lambda_{i,k} \neq \lambda_{j,k} \} \theta^*_k x^k \right) \right]^2 dx \right]^{\frac{1}{2}}$$

$$\geq \left[ \int_{0}^{1} \left( \theta^*_k - \theta^*_j \right) x^{\tilde{k}} + \sum_{k \in \{0, ..., \gamma \} \setminus \tilde{k}} \left( 1 \{ \lambda_{i,k} \neq \lambda_{j,k} \} \theta^*_k x^k \right) \right]^2 dx \right]^{\frac{1}{2}}$$

$$\geq \left[ \left( \frac{2\delta}{k + 1} \sum_{k=0}^{\gamma} R_k \right) \vee (2\delta) \right]$$

where the third line follows from the Jensen’s inequality and the concavity of $\sqrt{\cdot}$ on $[0, 1]$, and the fourth line follows from the triangle inequality. Hence, we have constructed a $\delta-$packing set. The cardinality of this packing set is at least $2^{\gamma + 1}$. That is,

$$\log M_2 (\delta, \mathcal{U}_{\gamma+1,1}) \geq \gamma + 1 =: B_2.$$}

Note that the lower bound $\log M_2 (\delta, \mathcal{U}_{\gamma+1,1}) \geq \gamma + 1$ holds for all $\delta$ such that

$$1 \geq 2^{\gamma + 1} \text{ and } 3\delta \left[\frac{\tilde{k} + 1}{\gamma} \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!}\right] \leq \frac{2R_k}{k!}.$$ 

Because $|\cdot|_\infty \geq \frac{1}{2} |\cdot|_2$, we clearly have

$$\log M_\infty (\delta, \mathcal{U}_{\gamma+1,1}) \geq \gamma + 1$$

for all $\delta$ such that

$$\left[\frac{2R_k}{3k!\delta (\tilde{k} + 1) \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!}}\right] + 1 \geq 2^{\gamma + 1} \text{ and } 3\delta \left[\frac{\tilde{k} + 1}{\gamma} \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!}\right] \leq \frac{2R_k}{k!}\tag{12}$$

and also

$$\log M_\infty (\delta, \mathcal{U}_{\gamma+1,1}) \leq B_1 (\delta).$$

\textsuperscript{11} The parameter $b \in [1, \infty)$ is chosen according to need later when we derive the minimax lower bounds. For Lemma 3.1, we can simply set $b = 1$.

\textsuperscript{12} Note that these two conditions can be reduced to

$$\left[\frac{2R_k}{3k!\delta (\tilde{k} + 1) \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!}}\right] + 1 \geq 2^{\gamma + 1}.$$
Finally, if the density function \( p(x) \) on \([-1, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then
\[
\log M_{2,p}(\delta, U_{\gamma+1,1}) \asymp \log M_2(\delta, U_{\gamma+1,1})
\]
and therefore we have claim (iii).

### A.2 Lemma A.1 and its proof

**Lemma A.1.** Let \( \{\phi_k\}_{k=1}^\infty \) be the Legendre polynomials on \([-1, 1]\). For any \( f \in U_{\gamma+1,1} [-1, 1] \), we have 
\[
f(x) = \sum_{k=0}^\gamma \theta_k \phi_k(x)
\]
such that
\[
\tilde{\theta}_k = \left( k + \frac{1}{2} \right) \frac{|\gamma/2|}{2^k} \sum_{m=0}^{k/2} \frac{f(k+2m)(0)}{2^{k+2m} m! \left( \frac{1}{2} \right)_{k+m+1}}
\]
where \((a)_k = a(a+1) \cdots (a+k-1)\) is known as the Pochhammer symbol.

**Proof.** To obtain the correct formula for finite sums, we carefully modify the derivations in Cantero and Iserles (2012) which concerns infinite sums. The Legendre expansion of \( x^k \) yields
\[
x^k \frac{1}{k!} = \frac{1}{2^k} \sum_{m=0}^{\lfloor k/2 \rfloor} \frac{k - 2m + \frac{1}{2}}{m! \left( \frac{1}{2} \right)_{k-m+1}} \phi_{k-2m}(x), \tag{54}
\]
First, let us consider the case where \( \gamma \) is odd. Applying (54) gives
\[
f(x) = \sum_{k=0}^\gamma \frac{f(k)(0)}{2^k} \sum_{m=0}^{\lfloor k/2 \rfloor} \frac{k - 2m + \frac{1}{2}}{m! \left( \frac{1}{2} \right)_{k-m+1}} \phi_{k-2m}(x)
\]
\[
\quad = \sum_{k=0}^{\lfloor \gamma/2 \rfloor} \frac{f(2k)(0)}{2^{2k}} \sum_{m=0}^{k} \frac{2k - 2m + \frac{1}{2}}{m! \left( \frac{1}{2} \right)_{2k-m+1}} \phi_{2k-2m}(x) \quad \text{(even } k\text{)} \tag{55}
\]
\[
\quad + \sum_{k=0}^{\lfloor \gamma/2 \rfloor} \frac{f(2k+1)(0)}{2^{2k+1}} \sum_{m=0}^{k} \frac{2k - 2m + \frac{3}{2}}{m! \left( \frac{3}{2} \right)_{2k-m+2}} \phi_{2k-2m+1}(x) \quad \text{(odd } k\text{)}
\]
\[
\quad = \sum_{m=0}^{\lfloor \gamma/2 \rfloor} \sum_{k=m}^\gamma \frac{2k - 2m + \frac{1}{2}}{m! \left( \frac{1}{2} \right)_{2k-m+1}} \frac{f(2k)(0)}{2^{2k}} \phi_{2k-2m}(x) \quad \text{(interchanging sums)}
\]
\[
\quad + \sum_{m=0}^{\lfloor \gamma/2 \rfloor} \sum_{k=m}^\gamma \frac{2k - 2m + \frac{3}{2}}{m! \left( \frac{3}{2} \right)_{2k-m+2}} \frac{f(2k+1)(0)}{2^{2k+1}} \phi_{2k-2m+1}(x)
\]
\[
\quad = \sum_{m=0}^{\lfloor \gamma/2 \rfloor} \sum_{l=0}^{\lfloor \gamma/2 \rfloor} \frac{2l + \frac{1}{2}}{m! \left( \frac{1}{2} \right)_{2l+m+1}} \frac{f(2l+2m)(0)}{2^{2l+2m}} \phi_{2l}(x) \quad \text{(letting } l = k - m\text{)}
\]
\[
\quad + \sum_{m=0}^{\lfloor \gamma/2 \rfloor} \sum_{l=0}^{\lfloor \gamma/2 \rfloor} \frac{2l + \frac{3}{2}}{m! \left( \frac{3}{2} \right)_{2l+m+2}} \frac{f(2l+2m+1)(0)}{2^{2l+2m+1}} \phi_{2l+1}(x)
\]
\[
\quad = \sum_{l=0}^{\lfloor \gamma/2 \rfloor} \sum_{m=0}^{\lfloor \gamma/2 \rfloor} \frac{2l + \frac{1}{2}}{m! \left( \frac{1}{2} \right)_{2l+m+1}} \frac{f(2l+2m)(0)}{2^{2l+2m}} \phi_{2l}(x) \quad \text{(interchanging sums)}
\]
\[
\quad + \sum_{l=0}^{\lfloor \gamma/2 \rfloor} \sum_{m=0}^{\lfloor \gamma/2 \rfloor} \frac{2l + \frac{3}{2}}{m! \left( \frac{3}{2} \right)_{2l+m+2}} \frac{f(2l+2m+1)(0)}{2^{2l+2m+1}} \phi_{2l+1}(x)
\]
which gives the claim in Lemma A.1.

For the case of even $\gamma$, note that the term in (55) takes the form

$$
\sum_{k=0}^{[\gamma/2]} \frac{f^{(2k+1)}(0)}{2^{2k+1}} \sum_{m=0}^{k} \frac{2k - 2m + \frac{3}{2}}{m! \left(\frac{1}{2}\right)^{2k-m+2}} \phi_{2k-2m+1}(x)
\]

and hence the previous derivations go through.

### A.3 Proof for Lemma 3.2

**The upper bound.** The following derivations generalize Kolmogorov and Tikhomirov (1959). Any function $f \in U_{\gamma+1,2}$ can be written as

$$
f(x + \Delta) = f(x) + \Delta f'(x) + \frac{\Delta^2}{2!} f''(x) + \cdots + \frac{\Delta^{\gamma-1}}{(\gamma-1)!} f^{(\gamma-1)}(x) + \frac{\Delta^\gamma}{\gamma!} f^{(\gamma)}(z)
\]

where $x, x + \Delta \in (-1, 1)$ and $z$ is some intermediate value. Let $REM_0(x + \Delta) := f(x + \Delta) - F_{\gamma - 1}(x) - \frac{\Delta^\gamma}{\gamma!} f^{(\gamma)}(x)$ and note that

$$
|REM_0(x + \Delta)| = \left| \frac{\Delta^\gamma}{\gamma!} \right| |f^{(\gamma)}(z) - f^{(\gamma)}(x)|
\]

$$
\leq \frac{|\Delta|^{\gamma+1}}{\gamma!} R_{\gamma + 1}.
\]

In other words,

$$
f(x + \Delta) = \sum_{k=0}^{\gamma} \frac{\Delta^k}{k!} f^{(k)}(x) + REM_0(x + \Delta)
\]

where $|REM_0(x + \Delta)| \leq \frac{|\Delta|^{\gamma+1}}{\gamma!} R_{\gamma + 1}$. Similarly, any $f^{(i)} \in U_{\gamma+1-i,2}$ for $1 \leq i \leq \gamma$ can be written as

$$
f^{(i)}(x + \Delta) = \sum_{k=0}^{\gamma - i} \frac{\Delta^k}{k!} f^{(i+k)}(x) + REM_i(x + \Delta)
\]

where $|REM_i(x + \Delta)| \leq \frac{|\Delta|^{\gamma+1-i}}{(\gamma-i)!} R_{\gamma + 1-i}$.

For some $\delta_0, \ldots, \delta_\gamma > 0$, suppose that $|f^{(k)}(x) - g^{(k)}(x)| \leq \delta_k$ for $k = 0, \ldots, \gamma$, where $f, g \in U_{\gamma+1,2}$. Then we have

$$
|f(x + \Delta) - g(x - \Delta)| \leq \sum_{k=0}^{\gamma} \frac{|\Delta^k\delta_k}{k!} + 2\frac{|\Delta|^{\gamma+1}}{\gamma!} R_{\gamma + 1}.
\]
Let \( \left( \max_{k \in \{1, \ldots, \gamma + 1\}} \frac{R_k}{(k-1)!} \right) \vee 1 =: R^* \). Consider \( |\Delta| \leq (R^{s-1} \delta)^{-\frac{1}{\gamma+1}} \) and \( \delta_k = R^{s-1} \frac{\delta}{\gamma+1} \) for \( k = 0, \ldots, \gamma \). Then,

\[
|f(x + \Delta) - g(x - \Delta)| \leq \delta \sum_{k=0}^{\gamma} \left( R^{s-1} \frac{\delta}{\gamma+1} \frac{1}{k!} \right) + 2R^* |\Delta|^{\gamma+1}
\]

\[
\leq \delta \sum_{k=0}^{\gamma} \frac{1}{k!} + 2\delta \leq 5\delta.
\]

(58)

Let us consider the following \( (R^{s-1} \delta)^{-\frac{1}{\gamma+1}} \)-grid of points in \([-1, 1] \):

\[
x_{-s} < x_{-s+1} < \cdots < x_{-1} < x_0 < x_1 < \cdots < x_{s-1} < x_s,
\]

with \( x_0 = 0 \) and \( s \gtrsim (R^{s-1} \delta)^{-\frac{1}{\gamma+1}} \).

It suffices to cover the \( k \)th derivative functions in \( U_{\gamma+1, 2} \) within \( \delta_k \)-precision at each grid point. Then by (58), we obtain a \( 5\delta \)-cover of \( U_{\gamma+1, 2} \). Following the arguments in Kolmogorov and Tikhomirov (1959), bounding \( N_\infty(\delta, U_{\gamma+1, 2}) \) can be reduced to bounding the cardinality of

\[
\Lambda = \left\{ \left[ \left\lfloor \frac{f^{(k)}(x_i)}{\delta_k} \right\rfloor \right], \; -s \leq i \leq s, \; 0 \leq k \leq \gamma \right\} : f \in U_{\gamma+1, 2} \right\}
\]

with \( \lfloor x \rfloor \) denoting the largest integer smaller than or equal to \( x \). Starting with \( x_0 = 0 \), the number of possible values of the vector \( \left[ \left\lfloor \frac{f^{(k)}(x_0)}{\delta_k} \right\rfloor \right]_{k=0}^{\gamma} \) when \( f \) ranges over \( U_{\gamma+1, 2} \) is 1. For \( i = 1, \ldots, s \), given the value of \( \left[ \left\lfloor \frac{f^{(k)}(x_{i-1})}{\delta_k} \right\rfloor \right]_{k=0}^{\gamma} \), we count the number of possible values of \( \left[ \left\lfloor \frac{f^{(k)}(x_i)}{\delta_k} \right\rfloor \right]_{k=0}^{\gamma} \). The counting for \( \left[ \left\lfloor \frac{f^{(k)}(x_i)}{\delta_k} \right\rfloor \right]_{k=0}^{\gamma} \) is similar. For each \( 0 \leq k \leq \gamma \), let \( B_{k,i-1} := \left[ \frac{f^{(k)}(x_{i-1})}{\delta_k} \right] \). Observe that \( B_{k,i-1} \delta_k \leq f^{(k)}(x_0) < (B_{k,i-1} + \frac{1}{2} \delta_k) \).

Taking (57) with \( x = x_{i-1} \) and \( \Delta = x_i - x_{i-1} \) gives

\[
\left| f^{(i)}(x_i) - \sum_{k=0}^{\gamma-i} \frac{\Delta_k}{k!} f^{(i+k)}(x_{i-1}) \right| \leq \frac{|\Delta|^{\gamma+1-i}}{(\gamma-i)!} R_{\gamma+1-i}.
\]

As a result,

\[
\left| f^{(i)}(x_i) - \sum_{k=0}^{\gamma-i} \frac{\Delta_k}{k!} B_{i+k,i-1} \right|
\leq \left| f^{(i)}(x_i) - \sum_{k=0}^{\gamma-i} \frac{\Delta_k}{k!} f^{(i+k)}(x_{i-1}) \right| + \sum_{k=0}^{\gamma-i} \frac{\Delta_k}{k!} \left( f^{(i+k)}(x_{i-1}) - B_{i+k,i-1} \right)
\leq \frac{|\Delta|^{\gamma+1-i}}{(\gamma-i)!} R_{\gamma+1-i} + \sum_{k=0}^{\gamma-i} \frac{|\Delta|k}{k!} \delta_{i+k}
\leq (R^{s-1} \delta)^{-\frac{1}{\gamma+1}} R_{\gamma+1-i} \sum_{k=0}^{\gamma-i} \left[ \frac{1}{k!} \right] (R^{s-1} \delta)^{-\frac{1}{\gamma+1}} R^{s-1} \delta^{\frac{1}{\gamma+1}}
\leq R^{s} \delta^{\frac{1}{\gamma+1}} \delta^{\frac{1}{\gamma+1}} + R^{s} \delta^{\frac{1}{\gamma+1}} \delta^{\frac{1}{\gamma+1}} \sum_{k=0}^{\gamma-i} \frac{1}{k!} \leq 4\delta_i.
\]

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Hence, the number of possible values of \(\left(\frac{f^{(k)}(x_i)}{\delta_k}\right)\) is at most 4 given the value of \(\left(\frac{f^{(k)}(x_{i+1})}{\delta_{k+1}}\right)\). Consequently, we have
\[
\text{card } (\Lambda) \lesssim 4^2s \lesssim 16(R^{*1}\delta)^{\frac{1}{\gamma+1}}
\]
which implies
\[
\log N_2(\delta, \mathcal{U}_{\gamma+1,2}) \leq \log N_\infty(\delta, \mathcal{U}_{\gamma+1,2}) \lesssim R^{*\frac{1}{\gamma+1}}\delta^{\frac{1}{\gamma+1}}. \tag{59}
\]

**The lower bound.** In the derivation of the lower bound, Kolmogorov and Tikhomirov (1959) considers a \(\delta^{\frac{1}{\gamma+1}}\)-grid of points
\[
\cdots < a_1 < \overline{a}_1 < a_2 < \overline{a}_2 < \cdots < a_{2s} < \overline{a}_{2s}
\]
where \(\overline{a}_i - a_i = \delta^{\frac{1}{\gamma+1}}\) and \(s \gtrsim \delta^{-\frac{1}{\gamma+1}}\). Recall that we have previously considered a \((R^{*1}\delta)^{\frac{1}{\gamma+1}}\)-grid of points in \([-1, 1]\) in the derivation of the upper bound for \(\log N_\infty(\delta, \mathcal{U}_{\gamma+1,2})\). To obtain a lower bound for \(\log M_\infty(\delta, \mathcal{U}_{\gamma+1,2})\) with the same scaling as our upper bound, the key modification we need is to replace the \(\overline{a}_i - a_i = \delta^{\frac{1}{\gamma+1}}\) with \(\overline{a}_i - a_i = (R^{*1}\delta)^{\frac{1}{\gamma+1}}\) and \(s \gtrsim \delta^{-\frac{1}{\gamma+1}}\) with \(s \gtrsim (R^{*1}\delta)^{\frac{1}{\gamma+1}}\). The rest of the arguments are similar to those in Kolmogorov and Tikhomirov (1959). In particular, let us consider
\[
f_\lambda(x) = R^* \sum_{i=1}^{2s} \lambda_i (\overline{a}_i - a_i)^{-1\gamma+1} h_0 \left(\frac{x - a_i}{\overline{a}_i - a_i}\right)
\]
where \(\lambda_i \in \{0, 1\}\) and \(\lambda \in \{0, 1\}^{2s}\), and \(h_0\) is a function on \(\mathbb{R}\) satisfying: (1) \(h_0\) restricted to \([-1, 1]\) belongs to \(\mathcal{U}_{\gamma+1,2}\); (2) \(h_0(x) = 0\) for \(x \notin [0, 1]\) and \(h_0(x) > 0\) for \(x \in [0, 1]\); (3) \(h_0 \left(\frac{1}{2}\right) = \max_{x \in [0, 1]} h_0(x) = R_0\). As an example, we can take \(h_0(x) = \begin{cases} 0 & x \notin [0, 1] \\ b2^{(\gamma+1)}x^{\gamma+1}(1-x)^{\gamma+1} & x \in [0, 1] \end{cases}\) for some properly chosen constant \(b\) that can only depend on \(R_0\). Note that the functions \(h(x) := R^* (\overline{a}_i - a_i)^{-1\gamma+1} h_0 \left(\frac{x - a_i}{\overline{a}_i - a_i}\right)\) and also \(f_\lambda(x)\) belong to \(\mathcal{U}_{\gamma+1,2}\) if \(\delta \in (0, 1)\). For any distinct \(\lambda, \lambda' \in \{0, 1\}^{2s}\), we have
\[
|f_\lambda - f_{\lambda'}|_\infty = R^* (\overline{a}_i - a_i)^{-1\gamma+1} h_0 \left(\frac{1}{2}\right) = R_0\delta.
\]
If \(R_0 \gtrsim 1\), then \(R_0\delta \gtrsim \delta\) and
\[
\log M_\infty(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim R^*^{\frac{1}{\gamma+1}}\delta^{\frac{1}{\gamma+1}}.
\]
If \(R_0 \lesssim 1\), then we obtain
\[
\log M_\infty(R_0\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim R^{*\frac{1}{\gamma+1}}\delta^{\frac{1}{\gamma+1}}
\]
which implies that
\[
\log M_\infty(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim R^{*\frac{1}{\gamma+1}} \left(\frac{\delta}{R_0}\right)^{\frac{1}{\gamma+1}}.
\]
Standard argument in the literature based on the Vasharmov-Gilbert Lemma further gives
\[
\log M_2(\delta, \mathcal{U}_{\gamma+1,2}) \gtrsim \begin{cases} R^{*\frac{1}{\gamma+1}}\delta^{\frac{1}{\gamma+1}} & \text{if } R_0 \gtrsim 1 \\ (R^* R_0)^{\frac{1}{\gamma+1}}\delta^{\frac{1}{\gamma+1}} & \text{if } R_0 \lesssim 1 \end{cases}. \tag{60}
\]
To show the last two bounds in Lemma 3.2, we apply the same arguments for showing claim (iii) in Lemma 3.1.
Remark A. Sections A.1 and A.3 derive bounds for $U_{1,1}$ and $U_{1,2}$ on $[−1, 1]$. These derivations can be easily extended for $U_{\gamma,1,1}$ and $U_{\gamma,1,2}$ on a general bounded interval $[c_1, c_2]$, where $c_1$ and $c_2$ are universal constants that are independent of $\gamma$ and $\{R_k\}_{k=0}^{\gamma+1}$. In particular, the resulting bounds have the same scaling (in terms of $\delta$, $\gamma$, and $\{R_k\}_{k=0}^{\gamma+1}$) as those in Sections A.1 and A.3.

A.4 Proof for Lemma 3.3

In the special case of $R_{\gamma+1} = 1$, the argument below sharpens the upper bound for $\log N_2 (\delta, \mathcal{H}_{\gamma+1})$ in Wainwright (2019) from $(\gamma+1)\delta^{-\frac{1}{\gamma+1}}$ to $\delta^{-\frac{1}{\gamma+1}}$. We find the cause of the gap lies in that the “pivotal” eigenvalue (that balances the “estimation error” and the “approximation error” from truncating for a given resolution $\delta$) in Wainwright (2019) is not optimal. We close the gap by finding the optimal “pivotal” eigenvalue.

More generally, for the case of $R_{\gamma+1} \gtrsim \gamma+1$, we consider two different truncations, one giving the upper bound $\delta^{-\frac{1}{\gamma+1}}$ and the other giving the lower bound $\left( R_{\gamma+1} \delta^{-1} \right)^{\frac{1}{\gamma+1}}$. Note that $\left( R_{\gamma+1} \delta^{-1} \right)^{\frac{1}{\gamma+1}} \propto \delta^{\frac{1}{\gamma+1}}$ when $R_{\gamma+1} \asymp 1$. For the case of $R_{\gamma+1} \gtrsim \gamma+1$, we use only one truncation to show that both the upper bound and the lower bound scale as $\left( R_{\gamma+1} \delta^{-1} \right)^{\frac{1}{\gamma+1}}$.

In view of (7), given $\left( \phi_m \right)_{m=1}^{\infty}$ and $\left( \mu_m \right)_{m=1}^{\infty}$, to compute $N_2 (\delta, \mathcal{H}_{\gamma+1})$, it suffices to compute $N_2 (\delta, \mathcal{E}_{\gamma+1})$ where

$$\mathcal{E}_{\gamma+1} = \left\{ \left( \theta_m \right)_{m=1}^{\infty} : \sum_{m=1}^{\infty} \frac{\theta_m^2}{\mu_m} \leq R_{\gamma+1}^2, \mu_m = (cm)^{-2(\gamma+1)} \right\}.$$

Let us introduce the $M$-dimensional ellipsoid

$$\overline{\mathcal{E}}_{\gamma+1} = \left\{ \left( \theta_m \right)_{m=1}^{M} \text{ coincide with the first } M \text{ elements of } \left( \theta_m \right)_{m=1}^{\infty} \text{ in } \mathcal{E}_{\gamma+1} \right\}$$

where $M = M (\gamma+1, \delta)$ is the smallest integer such that, for a given resolution $\delta > 0$ and weight $w_{\gamma+1}, w_{\gamma+1}^2 \delta^2 \geq \mu_M$. In other words, $\mu_m \geq w_{\gamma+1}^2 \delta^2$ for all indices $m \leq M$. Consequently, we have:

1. $\forall M \geq 1$ \begin{equation}
\mathbb{B}_2^M (w_{\gamma+1} R_{\gamma+1} \delta) \subseteq \overline{\mathcal{E}}_{\gamma+1};
\end{equation}

2. $\mu_{M-1} = (c (M-1))^{-2(\gamma+1)} > w_{\gamma+1}^2 \delta^2$ and $\mu_{M-1} = (c (M+1))^{-2(\gamma+1)} < w_{\gamma+1}^2 \delta^2$, which yield

$$M \asymp (w_{\gamma+1} \delta)^{-\frac{1}{\gamma+1}}.$$ 

Note that (61), (62), and the fact $\mathcal{E}_{\gamma+1} \supseteq \overline{\mathcal{E}}_{\gamma+1}$ give

$$\log N_2 (\delta, \mathcal{E}_{\gamma+1}) \geq \log N_2 (\delta, \overline{\mathcal{E}}_{\gamma+1}) \gtrsim M \log (w_{\gamma+1} R_{\gamma+1}) \asymp (w_{\gamma+1} \delta)^{-\frac{1}{\gamma+1}} \log (w_{\gamma+1} R_{\gamma+1}).$$

In the following, let $A_1 + A_2 := \{ a_1 + a_2 : a_1 \in A_1, a_2 \in A_2 \}$ for sets $A_1$ and $A_2$. For the upper
bound, we have

\[
N_2(\delta, \mathcal{E}_{\gamma+1}) \leq \frac{\text{vol} \left( \frac{2}{\delta} \mathcal{E}_{\gamma+1} + B_2^M(1) \right)}{\text{vol} (B_2^M(1))}
\]

\[
\leq \left( \frac{2}{\delta} \right)^M \frac{\text{vol} (\mathcal{E}_{\gamma+1} + B_2^M(\delta))}{\text{vol} (B_2^M(1))}
\]

\[
\leq \left( \frac{2}{\delta} \right)^M \max \left\{ \frac{\text{vol} (2\mathcal{E}_{\gamma+1})}{\text{vol} (B_2^M(1))}, \frac{\text{vol} (2B_2^M(\delta))}{\text{vol} (B_2^M(1))} \right\}
\]

\[
\leq \max \left\{ \left( \frac{4R_{\gamma+1}}{\delta} \right)^M \prod_{m=1}^M \sqrt{\mu_m}, 2^M \right\}
\]  

(64)

where the first inequality follows from the standard volumetric argument, and the last inequality follows from the standard result for the volume of ellipsoids. The fact \( \mu_m = (cm)^{-2(\gamma+1)} \) and the elementary inequality \( \sum_{m=1}^M \log m \geq M \log M - M \) give

\[
\log \left[ \left( \frac{4R_{\gamma+1}}{\delta} \right)^M \prod_{m=1}^M \sqrt{\mu_m} \right] \leq M (\log (4R_{\gamma+1}) + \gamma + 1) +
\]

\[
M \left( \log \frac{1}{\delta} - (\gamma + 1) \log (cM) \right)
\]

\[
= M (\log (4R_{\gamma+1}) + \gamma + 1) +
\]

\[
M \left( \log \frac{1}{\delta} - (\gamma + 1) \log (cM) + \log \frac{1}{w_{\gamma+1}} - \log \frac{1}{w_{\gamma+1}} \right)
\]

\[
\leq M (\log 4R_{\gamma+1} + \gamma + 1) + M \log w_{\gamma+1}
\]

\[
\leq M \log (w_{\gamma+1} ((\gamma + 1) \vee R_{\gamma+1}))
\]  

(65)

where we have used the fact \( \mu_M = (cm)^{-2(\gamma+1)} \leq w_{\gamma+1}^2 \delta^2 \) in the second inequality. Inequalities (62), (64) and (65) together yield

\[
\log N_2(\delta, \mathcal{E}_{\gamma+1}) \preceq \left( w_{\gamma+1}\delta \right)^{-\frac{1}{\gamma+1}} \max \{ \log (w_{\gamma+1} ((\gamma + 1) \vee R_{\gamma+1})), \log 2 \}.
\]

For any \( \theta \in \mathcal{E}_{\gamma+1} \), note that for a given \( \delta \), we have

\[
\sum_{m=M+1}^{\infty} \theta_{m}^2 \leq \mu_M \sum_{m=M+1}^{\infty} \frac{\theta_{m}^2}{\mu_m} \leq w_{\gamma+1}^2 R_{\gamma+1}^2 \delta^2.
\]  

(66)

To cover \( \mathcal{E}_{\gamma+1} \) within \( (1 + w_{\gamma+1}^2 R_{\gamma+1}^2)^\frac{\gamma}{2} \delta \) precision, we find a smallest \( \delta \)-cover of \( \mathcal{E}_{\gamma+1} \), \{ \theta^1, ..., \theta^N \}, such that for any \( \theta \in \mathcal{E}_{\gamma+1} \), there exists some \( i \) from the covering set with

\[
|\theta - \theta^i|^2 \leq \sum_{m=1}^{M} (\theta_m - \theta^i_m)^2 + w_{\gamma+1}^2 R_{\gamma+1}^2 \delta^2 \leq (1 + w_{\gamma+1}^2 R_{\gamma+1}^2) \delta^2
\]

where we have used (66). Consequently, we have

\[
\log N_2(\delta, \mathcal{E}_{\gamma+1}) \preceq \log N_2 \left( \left( 1 + w_{\gamma+1}^2 R_{\gamma+1}^2 \right)^{-\frac{1}{2}}, \mathcal{E}_{\gamma+1} \right)
\]

\[
\preceq \left( w_{\gamma+1} \delta \left( 1 + w_{\gamma+1}^2 R_{\gamma+1}^2 \right)^{-\frac{1}{2}} \right)^{-\frac{1}{2(\gamma+1)}} \max \{ \log (w_{\gamma+1} ((\gamma + 1) \vee R_{\gamma+1})), \log 2 \}.
\]  

(67)
Case 1: \( R_{\gamma+1} \preceq \gamma + 1 \). Setting \( w_{\gamma+1} \asymp R_{\gamma+1}^{-1} \) in (63) and (67) solves

\[
(w_{\gamma+1}^2 \delta \left( 1 + w_{\gamma+1}^2 R_{\gamma+1}^2 \right)^{-\frac{1}{\gamma+1}})^{-\frac{1}{\gamma+1}} \max \{ \log (w_{\gamma+1} ((\gamma + 1) \lor R_{\gamma+1})), \log 2 \} \]

\[
\asymp (w_{\gamma+1}^2 \delta)^{-\frac{1}{\gamma+1}} \log (w_{\gamma+1} R_{\gamma+1}) 
\]

and gives

\[
\log N_2 (\delta, \mathcal{E}_{\gamma+1}) \asymp (R_{\gamma+1}^{-1} \delta^{-1})^{\frac{1}{\gamma+1}}. 
\]

Case 2: \( R_{\gamma+1} \preceq \gamma + 1 \). Setting \( w_{\gamma+1} \asymp (\gamma + 1)^{-1} \) in (67) gives

\[
\log N_2 (\delta, \mathcal{E}_{\gamma+1}) \preceq \delta^{\frac{1}{\gamma+1}}.
\]

Note that the lower bound obtained by setting \( w_{\gamma+1} \asymp (\gamma + 1)^{-1} \) in (63) is not particularly useful. Instead, we consider a different truncation with \( w_{\gamma+1} \asymp R_{\gamma+1}^{-1} \). Then (63) with \( w_{\gamma+1} \asymp R_{\gamma+1}^{-1} \) gives

\[
\log N_2 (\delta, \mathcal{E}_{\gamma+1}) \asymp R_{\gamma+1}^{-1} \delta^{\frac{1}{\gamma+1}}. 
\]

To show the last claim in Lemma 3.3, we apply the same arguments for showing claim (iii) in Lemma 3.1.

### B Proofs for Sections 4–5

#### B.1 Proof for Theorem 4.1

The lower bound \( \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \) in part (i) of Theorem 4.1 is the standard one in the literature. In particular, note that \( \mathcal{U}_{\gamma+2} \) with \( R_k = C \) for all \( k = 0, \ldots, \gamma + 1 \) is a subset of \( \mathcal{S}_{\gamma+1} \). One simply applies Lemma C.1(ii) in Section C and the standard metric entropy bound \( \left( \frac{1}{\delta} \right)^{\frac{1}{\gamma+1}} \) (that is, Lemma 3.2 with \( R_k = C \) for all \( k = 0, \ldots, \gamma + 1 \)). Therefore, we only show part (ii) of Theorem 4.1 below.

**Standard Sobolev \( \mathcal{S}_{\gamma+1} \).** We apply Lemma C.1(i) in Section C and the construction in Section B.2 To construct the packing subset in Lemma C.1(i), we construct \( \mathcal{M} \), a set in the \((\gamma^*+1)\)th order polynomial subclass. By (83) in Section C for a set

\[
\{ f^1, f^2, \ldots, f^M \} = \mathcal{M} \subseteq \mathcal{U}_{\gamma^*+1,1} 
\]

(where \( \mathcal{U}_{\gamma^*+1,1} \) is defined the same way as (70)), we have

\[
D_{KL} (\mathbb{P}^j \times \mathbb{P}^X \parallel \mathbb{P}^l \times \mathbb{P}^X) = \frac{n}{2\sigma^2} \left| f^j - f^l \right|_{2,\mathbb{P}}^2 .
\]

Let us consider the packing set consisting of \( M_0 \) elements in the form (83) for \( \mathcal{U}_{\gamma^*+1,1} \).
Following the notation in Section A.1 (the derivations for $\mathcal{B}_2$), we have

$$\left| f^j - f^l \right|_{2,p}^2 = \left| f_{\lambda^j} - f_{\lambda^l} \right|_{2,p}^2$$

$$= \int_0^1 \left( \left( \theta_k^{\gamma_j} - \theta_k^{\gamma_l} \right) x^k + \sum_{k \in \{0, \ldots, \gamma^*\} \setminus k} \left( 1 \{ \lambda_j, k \neq \lambda_l, k \} \theta_k^j x^k \right) \right)^2 p(x) \, dx$$

$$\lesssim \left( \theta_k^{\gamma_j} - \theta_k^{\gamma_l} \right)^2 + \left( \sum_{k \in \{0, \ldots, \gamma^*\} \setminus k} \theta_k^j \right)^2$$

$$\lesssim \delta^2 \left( \tilde{k} + 1 \right)^2 \sum_{k = 0}^{\gamma^*} \frac{R_k}{k!}$$

$$\lesssim \delta^2$$

for any $j, l \in \mathcal{M}, j \neq l$

where the last line follows from that $R_0 = \sqrt{\frac{2}{\pi}}$ and $R_k = \sqrt{\frac{c}{3\gamma}}$ for $k = 1, \ldots, \gamma^*$, in which case we have $\tilde{k} = 0$ and $\sum_{k = 0}^{\gamma^*} \frac{R_k}{k!} \asymp 1$. Recall that the lower bound $\log M_0 \gtrsim \gamma^* + 1$ in Section A.1 holds for all $\delta$ such that

$$\frac{R_k}{k! \left( \tilde{k} + 1 \right)^\gamma \gamma^*} \geq c \gamma^* + 1$$

and

$$\delta \left( \tilde{k} + 1 \right)^\gamma \gamma^* \lesssim \frac{2 R_k}{k!}$$

where $\tilde{k} = 0$, $\sum_{k = 0}^{\gamma^*} \frac{R_k}{k!} \asymp 1$ and $c \in (1, \infty)$ is a universal constant. Let us take $\delta^2 = \frac{c' 2^{2(\gamma^*+1)}}{n}$ for a sufficiently small universal constant $c' \in (0, 1)$ such that

$$\left( c c_0^{-1} \left( \tilde{k} + 1 \right)^\gamma \gamma^* \right)^2 = \tilde{c}_0 \in (0, 1]$$

$$\delta^2 \left( 1 - \frac{2 R_k}{k! \left( \tilde{k} + 1 \right)^\gamma \gamma^*} \right) \leq \tilde{c}_0 \frac{c' \left( \tilde{k} + 1 \right)^\gamma \gamma^*}{n}$$

where the positive universal constants satisfy $\tilde{c}_0 \lesssim \frac{1}{2} \tilde{c}_0$. Therefore,

$$\delta^2 \left( 1 - \frac{2 + \frac{1}{M^2} \sum_{j, l \in \{1, \ldots, M\}} D_{\mathcal{KL}} \left( \mathbb{P}_j \times \mathbb{P}_X \mid \mathbb{P}_l \times \mathbb{P}_X \right)}{\log M} \right) \geq \frac{\sigma^2 (\gamma^* + 1)}{n}$$

for some universal constant $\tilde{c} \in (0, 1]$. Note that we can choose $c'$ in $\delta$ above to be small enough such that $\tilde{c} \leq \frac{1}{2} \tilde{c}_0$ as stated in Theorem 4.1(ii).

**Standard Hölder $U_{\gamma+1}$**. The proof for the standard $U_{\gamma+1}$ is identical to the proof for $\mathcal{S}_{\gamma+1}$ shown previously. We consider the $\delta-$packing set consisting of $M_0$ elements in the form (53) for $U^*_{\gamma+1, 1}$.

**B.2 Lemma B.1 and its proof**

**Lemma B.1.** We have

$$\log M_2 \left( \delta, \mathcal{S}_{\gamma+1} \right) \gtrsim \gamma + 1, \forall \frac{1}{\delta} \gtrsim 2^{\gamma+1}.$$
If the density function \( p(x) \) on \([0, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then
\[
\log M_{2, p}(\delta, \overline{\mathbb{S}}_{\gamma+1}) \preceq \gamma + 1, \forall \frac{1}{\delta} \preceq 2^{\gamma+1}.
\] (69)

**Proof.** To prove Lemma B.1, we use the bound \( B_2 \) in Lemma 3.1 (and Remark A at the end of Section A.3). Let us consider
\[
\mathcal{U}_{\gamma+1, 1}^* = \left\{ f = \sum_{k=0}^{\gamma} \theta_k x^k : (\theta_k)_{k=0}^{\gamma} \in \mathcal{P}_\gamma^*, x \in [0, 1] \right\}
\] (70)
with the \((\gamma + 1)\)-dimensional polyhedron
\[
\mathcal{P}_\gamma^* = \left\{ (\theta_k)_{k=0}^{\gamma} : \theta_0 \in \left[-\sqrt{\frac{C}{3}}, \sqrt{\frac{C}{3}}\right], \theta_k \in \left[-\sqrt{\frac{C}{3^k k!}}, \sqrt{\frac{C}{3^k k!}}\right], k = 1, ..., \gamma \right\}.
\]
Note that \( \mathcal{U}_{\gamma+1, 1}^* \subset \overline{\mathbb{S}}_{\gamma+1} \).

As a result, we can apply (11) in Lemma 3.1 to show
\[
\log M_{2, \mathcal{U}_{\gamma+1, 1}^*}(\delta, \delta) \preceq \gamma + 1, \forall \frac{1}{\delta} \preceq 2^{\gamma+1}.
\]

If the density function \( p(x) \) on \([0, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then
\[
\log M_{2, p}(\delta, \overline{\mathbb{S}}_{\gamma+1}) \preceq \log M_{2, \mathcal{U}_{\gamma+1, 1}^*}(\delta, \overline{\mathbb{S}}_{\gamma+1}).
\]
Therefore we have (69).

### B.3 Proof for Theorem 4.2

**Step 1.** We apply Lemma C.8 (in Section C) where \( W \) corresponds to the Sobolev space containing \( \mathcal{S}_{k+1} \) (\( k = \gamma \) in part (i) and \( k = \gamma^* \) in part (ii)) and the kernel functions correspond to (21) and (22). Then solving (101) is reduced to solving
\[
\left( r \sqrt{\frac{(k+1) \wedge n}{n}} \right) \vee \left( \frac{1}{\sqrt{n}} \left( \frac{2k+1}{2k+2} \right)^{\frac{k+1}{2}} \right) \preceq \frac{C \sigma^2}{\sigma}.
\]

Under the condition \( n \geq k + 1, r = \tilde{\delta}_1 = c_1 \left[ \sqrt{\frac{\sigma^2(k+1)}{n}} \vee \left( \frac{2k+1}{2k+2} \right)^{\frac{k+1}{2}} \right] \) solves the above. In a similar fashion, \( r = \tilde{\delta}_2 = c_2 \left[ \sqrt{\frac{k+1}{n}} \vee \left( \frac{1}{n} \right)^{\frac{k+1}{2k+3}} \right] \) solves (102). Note that both \( \tilde{\delta}_1 \) and \( \tilde{\delta}_2 \) are non-random and do not depend on the values of \( \{x_i\}_{i=1}^n \).

**Step 2.** Given \( \sigma \asymp 1 \) (in Assumption 1) and \( \tilde{\delta}_1 \), we apply Lemma C.6 to show that
\[
\left| \hat{f} - f \right|_n^2 \preceq \tilde{t}_1^2 \text{ for any } t_1 \geq \tilde{\delta}_1
\] (72)
with probability at least \( 1 - c' \exp \left( -c'' \frac{nt_2^2}{\sigma^2} \right) \), whenever \( \lambda \asymp t_1^2 \).

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Step 3. Given $\delta_2$, we now connect $|\hat{f} - f|^2_n$ with $|\hat{f} - f|^2_{2,\mathcal{F}}$. We divide the argument into two cases depending on whether $\delta_2 \geq r^*$, the smallest positive solution to (88) with $c = C$.

Case 1 (when $\delta_2 \leq r^*$). Note that $\delta_2$ is an upper bound for $\tilde{r}^*$, the smallest positive solution to (90) with $c_0 = C^{-1}$. For case 1, we can apply Lemma C.4 together with (72) to show that

$$|\hat{f} - f|^2_{2,\mathcal{F}} \lesssim t_1^2 + t_2^2$$

for any $t_1 \geq \delta_1, t_2 \in [\delta_2, r^*]$ with probability at least

$$1 - c \exp \left(-c'' 2\delta_2^2\right) - C \exp \left(-c_0'' n \delta_2^2\right),$$

which is greater than

$$1 - c \exp \left(-c'' n \delta_2^2\right).$$

Case 2 (when $\delta_2 > r^*$). In this case, we can apply Lemma C.2 (where we take $\tilde{r} = r^*$) together with (72) to show that

$$|\hat{f} - f|^2_{2,\mathcal{F}} \lesssim t_1^2 + t_2^2$$

for any $t_1 \geq \delta_1, t_2 \geq \delta_2$ with probability at least (73).

Applying Lemmas C.2 and C.4 requires the shifted class $\mathcal{F}$ associated with $\mathcal{F} = \mathcal{S}_{k+1}$ to be a bounded class such that for all $g \in \mathcal{F}$, $|g|_\infty \lesssim 1$. This condition holds easily given the kernel functions (21) and (22) and Lemma C.9.

Step 4. Integrating the tail probability in the form of (73) gives

$$E \left(|\hat{f} - f|^2_{2,\mathcal{F}}\right) \lesssim \tilde{r}^2 + \exp \{-cn\tilde{r}^2\},$$

where $\tilde{r}^2 = \sigma^2(k+1) n \sqrt{\left(\frac{\epsilon_n^2}{n}\right)^{\frac{2(k+1)}{2(k+1)+1}}} \times (\epsilon_n^2) \left(\frac{k+1}{n}\right)^{\frac{2(k+1)}{2(k+1)+1}}$ since $\sigma \asymp 1$. Finally, we take sup and obtain

$$\sup_{f \in \mathcal{S}_{k+1}} E \left(|\hat{f} - f|^2_{2,\mathcal{F}}\right) \lesssim \tilde{r}^2 + \exp \{-cn\tilde{r}^2\}.$$

For part (i), we have

$$\sup_{f \in \mathcal{S}_{k+1}} E \left(|\hat{f} - f|^2_{2,\mathcal{F}}\right) \leq \overline{C} \left[r_1^2 + \exp \{-cnr_1^2\}\right]$$

for some universal constant $\overline{C} \in (1, \infty)$, where $r_1^2 = \left(\frac{\sigma^2}{n}\right)^{\frac{2(k+1)}{2(k+1)+1}}$.

For part (ii), we have

$$\sup_{f \in \mathcal{S}_{k+1}} E \left(|\hat{f} - f|^2_{2,\mathcal{F}}\right) \leq \overline{C} \left[r_2^2 + \exp \{-cnr_2^2\}\right]$$

for some universal constant $\overline{C} \in (1, \infty)$, where $r_2^2 = \frac{\sigma^2(\gamma+1)}{n}$.
B.4 Proof for Theorem 4.3

**Step 1.** We apply Lemma C.7 (in Section C) where \( F \) corresponds to the standard \( U_{k+1} (k = \gamma \text{ in part (i)} \) and \( k = \gamma^* \text{ in part (ii)} \). Taking \( R_j = C \) for \( j = 0, \ldots, k + 1 \) in (14) (the second bound) yields

\[
\log N_{\infty} (\delta, U_{k+1}) \lesssim (k + 1) \log \left( \frac{1}{\delta} \right) + \left( \frac{1}{\delta} \right)^{1+1},
\]

where we have used the fact that \( R^* \approx 1 \). Note that

\[
\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega(r; F))} d\delta
\]

\[
\leq \frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_{\infty}(\delta, F)} d\delta
\]

\[
\lesssim r \sqrt{\frac{k + 1}{n} + \frac{1}{\sqrt{n}}} \left( \frac{2k + 2}{2k + 3} \right)^{T(r)}
\]

where the last line follows from (74). Setting \( \sigma T(r) \approx r^2 \) yields \( r = \bar{\delta}_1 = c_1 \left[ \sqrt{\frac{\sigma^2 (k+1)}{n}} \vee \left( \frac{\sigma}{n} \right)^{\frac{k+1}{2k+3}} \right] \), which solves (99). In a similar fashion, \( r = \bar{\delta}_2 = c_2 \left[ \sqrt{\frac{k + 1}{n}} \vee \left( \frac{1}{n} \right)^{\frac{k+1}{2k+3}} \right] \) solves (100). Note that both \( \bar{\delta}_1 \) and \( \bar{\delta}_2 \) are non-random and do not depend on the values of \( \{x_i\}_{i=1}^n \).

**Step 2.** Given \( \sigma \approx 1 \) (in Assumption 1) and \( \bar{\delta}_1 \), we apply Lemma C.5 to show that

\[
\left| \hat{f} - f \right| \lesssim t_1^2 \text{ for any } t_1 \geq \bar{\delta}_1
\]

with probability at least \( 1 - c' \exp \left( -c'' \frac{nt_1}{\sigma} \right) \).

**Steps 3 and 4.** The arguments are identical to those in Step 3 and Step 4 of the proof for Theorem 4.2 in Section B.3. The verification that \( |g|_{\infty} \lesssim 1 \) for all \( g \in \mathcal{F} \) associated with the standard \( U_{k+1} \) is obvious given its definition.

B.5 Proof for Theorem 5.1

To show the lower bounds in Theorem 5.1, we can apply either Lemma C.1(i) or Lemma C.1(ii) in Section C but the latter gives more insight about where the rates in Theorem 5.1 are coming from. The arguments for the upper bound in Claim (i) of Theorem 5.1 are similar to those in Section B.3. The arguments for the upper bound in Claim (ii) are similar to those in Section B.4.

**The lower bound (Sobolev).** We apply Lemma C.1(ii) in Section C with \( \mathcal{F} = \mathcal{H}_{\gamma+1} \) and the results in Lemma 3.3. By (84) and Lemma 3.3, we have

\[
\log N_{KL}(\epsilon, Q) = \log N_{2,p} \left( \sqrt{\frac{2}{n} \sigma \epsilon, U_{\gamma+1,2}} \right) \lesssim \left( \frac{R_{\gamma+1} \sqrt{n}}{\sigma \epsilon} \right)^{\frac{1}{\gamma+1}}.
\]
Setting \((\frac{R_{\gamma+1} \sqrt{n}}{\sigma})^{\frac{1}{\gamma+1}} \times \epsilon^2\) yields \( \epsilon^2 \propto \left( \frac{nR_{\gamma+1}^2}{\sigma^2} \right)^{\frac{2(\gamma+1)+1}{2(\gamma+1)+1}} =: \epsilon^*\). Observe that setting

\[
\delta \approx R_{\gamma+1} \left( \frac{1}{\gamma+1} \right)^{\frac{1}{\gamma+1}} \left( \frac{\sigma^2}{n} \right)^{\frac{2}{2(\gamma+1)+1}}
\]

ensures

\[
(R_{\gamma+1} \delta^{-1})^{\frac{1}{\gamma+1}} \times R_{\gamma+1}^2 \left( \frac{n}{\sigma^2} \right)^{\frac{1}{2(\gamma+1)+1}} \approx \epsilon^*.
\]

Consequently, we have

\[
1 - \log 2 + \log N_{KL}(\epsilon^*, \mathcal{Q}) + \epsilon^2 \geq \frac{1}{2}
\]

and

\[
\inf_{f} \sup_{f \in \mathcal{H}_{\gamma+1}} \mathbb{E} \left( |\hat{f} - f|_{2,p}^2 \right) \approx R_{\gamma+1}^2 \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)+1}{2(\gamma+1)+1}}.
\]

The upper bound (Sobolev). Step 1. We apply Lemma C.8 where \(W\) corresponds to the RKHS associated with the kernel function \(K\), which is continuous, positive semidefinite, and satisfies \(K(x, x') \leq 1\) for all \(x, x' \in [0, 1]\). Moreover, \(W\) contains \(\mathcal{H}_{\gamma+1}\). Then solving (101) is reduced to

\[
\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega(r, F))} d\delta
\]

Note that \(r = \delta_1 = c_1 R_{\gamma+1}^{-2(\gamma+1)+1} \left( \frac{\sigma^2}{n} \right)^{\frac{2}{2(\gamma+1)+1}}\) solves the above. In a similar fashion, \(r = \delta_2 = c_2 R_{\gamma+1}^{-2(\gamma+1)+1} \left( \frac{2}{n} \right)^{\frac{2}{2(\gamma+1)+1}}\) solves (102). Note that both \(\delta_1\) and \(\delta_2\) are non-random and do not depend on the values of \(\{x_i\}_{i=1}^n\).

Steps 2-4. The arguments are identical to those in Steps 2-4 in Section B.3.

The lower bound (Hölder). We apply Lemma C.1(ii) with \(F = \mathcal{U}_{\gamma+1,2}\) and the results in Lemma 3.2. By (84) and Lemma 3.2, we have

\[
\log N_{KL}(\epsilon, \mathcal{Q}) = \log N_{2,p} \left( \sqrt{\frac{2}{n}} \sigma \epsilon, \mathcal{U}_{\gamma+1,2} \right) \approx \left( \frac{R^* \sqrt{n}}{\sigma \epsilon} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}.
\]

The rest of the arguments are identical to those for the lower bound concerning \(\mathcal{H}_{\gamma+1}\) by simply replacing \(R_{\gamma+1}\) with \(R^*\).

The upper bound (Hölder). Step 1. We apply Lemma C.7 where \(F\) corresponds to \(\mathcal{U}_{\gamma+1,2}\). Note that

\[
\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega(r, F))} d\delta
\]

\[
\leq \frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_{\infty}(\delta, \mathcal{F})} d\delta
\]

\[
\leq \frac{1}{\sqrt{n}} \left( R^* \right)^{\frac{1}{2(\gamma+2)}} \left( \frac{\sigma^2}{\gamma+1} \right) \frac{1}{T(r)}
\]

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where the last line follows from Lemma 3.2.

Setting \( \sigma T(r) \propto r^2 \) yields \( r = \delta_1 = c_1 (R^*)^{\frac{1}{2(\gamma + 1)} + 1} \left( \frac{q^2}{n} \right)^{\frac{1}{2(\gamma + 1)} + 1} \), which solves \( (99) \). In a similar fashion, \( r = \delta_2 = c_2 (R^*)^{\frac{1}{2(\gamma + 1)} + 1} \left( \frac{1}{n} \right)^{\frac{1}{2(\gamma + 1)} + 1} \) solves \( (100) \). Note that both \( \delta_1 \) and \( \delta_2 \) are non-random and do not depend on the values of \( \{x_i\}_{i=1}^n \).

Steps 2-4. The arguments are identical to those in Steps 2-4 in Section B.4.

B.6 Proof for Theorem 5.2

The arguments for the lower bounds are almost identical to those in Section B.1. The arguments for the upper bounds are almost identical to those in Section B.4. In proving Theorem 5.2, we use the bounds \( B_1(\delta) \) and \( B_2(\delta) \) in Lemma 3.1, as well as the bounds in Lemma 3.2.

The lower bound. We apply Lemma C.1(i) in Section C. Let us consider the packing set consisting of \( M_0 \) elements in the form \( (53) \) for \( \gamma_k + 1 \), \( R_0 = C \) and \( R_k \) taking a value in \( [C, C(k-1)!] \) for all \( k = 1, \ldots, \gamma^* \). Let us choose \( b = \gamma \lor 1 \) in \( \theta^k \)s of \( (53) \) for this construction. Recall that the lower bound \( \log M_0 \gtrsim \gamma^* + 1 \) in Section A.1 holds for all \( \delta \) such that

\[
\frac{R_0}{\delta \left( 1 \lor \sum_{k=0}^{\gamma^*} \frac{R_k}{k!} \right)} \geq c2^{\gamma^*+1}
\]

and

\[
\delta \left( k + 1 \right) \lor \sum_{k=0}^{\gamma^*} \frac{R_k}{k!} \leq \frac{2R_k}{3\delta}
\]

where \( k = 0 \) and \( c \in (1, \infty) \) is a universal constant. These conditions are reduced to

\[
\delta \left( 1 \lor \sum_{k=0}^{\gamma^*} \frac{R_k}{k!} \right) \geq c2^{\gamma^*+1},
\]

(76)

\[
\delta \left( 1 \lor \sum_{k=0}^{\gamma^*} \frac{R_k}{k!} \right) \leq \frac{2}{3} R_0.
\]

The rest of the arguments are identical to those in Section B.1.

The upper bound. Taking \( R_0 = C \) and \( R_j = C(j-1)! \) for \( j = 1, \ldots, k+1 \) in \( (14) \) (the first bound) yields

\[
\log N_\infty(\delta, U_{k+1}) \lesssim (k + 1) \log \frac{1}{\delta} + \left( \frac{1}{\delta} \right)^{\frac{1}{\gamma + 1}},
\]

(77)

where we have used the fact that \( R^* \approx 1 \). The rest of the arguments are identical to those in Section B.4.

B.7 Proof for Theorem 5.3

In proving Theorem 5.3, we use the bounds \( B_1(\delta) \) and \( B_2(\delta) \) in Lemma 3.1 for \( U_{k+1,1} \), as well as the bounds in Lemma 3.2 for \( U_{k+1,2} \). When \( R_j = Cj! \) for all \( j = 0, \ldots, k+1 \), \( R^* \approx 1 \) and

\[
\log M_{2,\infty}(\delta, U_{k+1,2}) \gtrsim \left( \frac{1}{\delta} \right)^{\frac{1}{\gamma + 1}}.
\]

Moreover,

\[
\log N_\infty(\delta, U_{k+1}) \lesssim (k + 1) \log \frac{k + 1}{\delta} + \left( \frac{1}{\delta} \right)^{\frac{1}{\gamma + 1}};
\]

(78)

for \( k > 1 \), we have
\[
\log M_{2,p}(\delta, U_{k+1,1}) \geq c' \left[ (k + 1) \log \frac{1}{\delta} - k^2 \right] \\
\quad - (k + 1) \log k + (k + 1) \log (k - 1)!
\approx k \log \frac{1}{\delta} - k^2; \tag{79}
\]
for \( k \in \{0, 1\} \), we simply have
\[
\log M_{2,p}(\delta, U_{k+1,1}) \geq (k + 1) \log \frac{1}{\delta} - 1. \tag{80}
\]

**The lower bound.** The arguments for the lower bounds are similar to those in Section B.1. Let us spell out the differences below.

To show part (ii), we can construct a packing set \( M \) of \( U_{\gamma^* + 1, 1} \) such that each element in this subset is \( \delta \)-apart and by setting \( \delta \leq 2^{-(\gamma^* + 1)} \) in (79) and (80), we have
\[
\log |M| \geq (\gamma^* + 1)^2. \tag{81}
\]
Let us take \( \delta^2 = c_2^2 (\gamma^* + 1)^2 \frac{\log (\gamma^* + 2)}{n} \) for a sufficiently small universal constant \( c \in (0, 1] \). We need the condition \( c_4 (\gamma^* + 1) \frac{\log (\gamma^* + 2)}{n} \leq \frac{n}{\delta^2} \) to ensure \( \delta = \sqrt{c_2^2 (\gamma^* + 1)^2 \frac{\log (\gamma^* + 2)}{n}} \leq 2^{-(\gamma^* + 1)} \) so we can apply \( \log |M_1| \geq (\gamma^* + 1)^2 \geq (\gamma^* + 1) \log (\gamma^* + 2) \) below. When \( c \in (0, 1] \) is chosen to be sufficiently small, we are guaranteed to have
\[
\frac{1}{M^2} \sum_{j,d \in \{1,\ldots,M\}} D_{KL}(P_j \times \mathbb{P}_X | P_i \times \mathbb{P}_X) \leq C_0 (\gamma^* + 1) \log (\gamma^* + 2),
\]
\[
\log M = \log |M_1| + \log |M_2| \geq C_0 (\gamma^* + 1) \log (\gamma^* + 2),
\]
where the positive universal constants satisfy \( C_0 \leq \frac{1}{2} C_0 \). Therefore,
\[
\delta^2 \left( 1 - \frac{\log 2 + \frac{1}{M^2} \sum_{j,d \in \{1,\ldots,M\}} D_{KL}(P_j \times \mathbb{P}_X | P_i \times \mathbb{P}_X)}{\log M} \right) \geq \frac{\sigma^2 (\gamma^* + 1) \log (\gamma^* + 2)}{n}
\]
for some universal constant \( c \in (0, 1] \). Note that we can choose \( c \) in \( \delta^2 \) above to be small enough such that \( c \leq \frac{1}{4} \sigma_0 \) as stated in Theorem 5.3(ii).

**The upper bound.** In this case, solving (99) yields \( r = \tilde{\delta}_1 = c_1 \left[ \sqrt{\frac{\sigma^2 (k+1) \log (k\sqrt{2})}{n}} \vee \left( \frac{\sigma^2}{n} \right)^{\frac{k+1}{2k+3}} \right] \).

In a similar fashion, solving (100) yields \( r = \tilde{\delta}_2 = c_2 \left[ \sqrt{\frac{(k+1) \log (k\sqrt{2})}{n}} \vee \left( \frac{1}{n} \right)^{\frac{k+1}{2k+3}} \right] \). Note that both \( \tilde{\delta}_1 \) and \( \tilde{\delta}_2 \) are non-random and do not depend on the values of \( \{x_i\}_{i=1}^n \). The rest of the arguments are similar to those in Section B.4.

### C Supporting lemmas for Appendix E

The set of lemmas in this section support our proofs in Appendix E and are based on Dudley (1967), Ledoux and Talagrand (1991), Yang and Barron (1999), van de Geer (2000), Bartlett and
Lemma C.1 below provides two versions of Fano’s inequality. In some of our derivations of the minimax lower bounds, we apply the first version as it is more useful for showing the minimax optimal MISE rates in the small sample regime. In other cases, we apply the second version as it gives more insight where the rates are from.

**Lemma C.1.** (i) Let \( \{f^1, f^2, ..., f^M\} \) be a \( c\delta \)-separated set in the \( L^2(\mathbb{P}) \) norm. Then

\[
\inf_{\hat{f}} \sup_{f \in \mathcal{F}} \mathbb{E} \left( \left| \hat{f} - f \right|^2 \right) \geq \delta^2 \left( 1 - \frac{\log 2 + \frac{1}{M^2} \sum_{j,l \in \{1, ..., M\}} D_{KL}(\mathbb{P}_j \times \mathbb{P}_X \parallel \mathbb{P}_l \times \mathbb{P}_X)}{\log M} \right)
\]

where \( D_{KL}(\mathbb{P}_j \times \mathbb{P}_X \parallel \mathbb{P}_l \times \mathbb{P}_X) \) denotes the KL–divergence of \( (Y, \{X_i\}_{i=1}^n) \) under \( f^j \) and \( f^l \), \( \mathbb{P}_X \) denotes the product distribution of \( \{X_i\}_{i=1}^n \), and \( \mathbb{P}_j \) denotes the the distribution of \( Y \) given \( \{x_i\}_{i=1}^n \) when the truth is \( f^j \).

(ii) Let \( N_{KL}(\epsilon, \mathcal{Q}) \) denote the \( \epsilon \)-covering number of \( \mathcal{F} \) with respect to the square root of the KL–divergence, and \( M_{2,\mathbb{P}}(\delta, \mathcal{F}) \) denote the \( \delta \)-packing number of \( \mathcal{F} \) with respect to \( \| \cdot \|_{2,\mathbb{P}} \). Then the Yang and Barron version of Fano’s inequality gives

\[
\inf_{\hat{f}} \sup_{f \in \mathcal{F}} \mathbb{E} \left( \left| \hat{f} - f \right|^2 \right) \geq \sup_{\delta, \epsilon} \delta^2 \left( 1 - \frac{\log 2 + \log N_{KL}(\epsilon, \mathcal{Q}) + \epsilon^2}{\log M_{2,\mathbb{P}}(\delta, \mathcal{F})} \right).
\]

**Remark.** Under our model assumptions, observe that

\[
D_{KL}(\mathbb{P}_j \times \mathbb{P}_X \parallel \mathbb{P}_l \times \mathbb{P}_X) = \mathbb{E}_X \left[ D_{KL}(\mathbb{P}_j \parallel \mathbb{P}_l) \right] = \frac{n}{2\sigma^2} \|f^j - f^l\|_{2,\mathbb{P}}^2
\]

and

\[
\log N_{KL}(\epsilon, \mathcal{Q}) = \log N_{2,\mathbb{P}} \left( \sqrt{\frac{2}{n\sigma^2}} \epsilon, \mathcal{F} \right).
\]

**Definition** (local complexity). Let \( \Omega_n(r; \mathcal{F}) = \{g \in \mathcal{F} : |g|_n \leq r\} \) with

\[
\bar{\mathcal{F}} := \{g = g_1 - g_2 : g_1, g_2 \in \mathcal{F}\}.
\]

Conditional on \( \{x_i\}_{i=1}^n \), the *empirical local Gaussian complexity* is defined as

\[
\mathcal{G}_n(r; \bar{\mathcal{F}}) := \mathbb{E}_{\tilde{\varepsilon}} \left[ \sup_{g \in \Omega_n(r; \bar{\mathcal{F}})} \left| \frac{1}{n} \sum_{i=1}^n \tilde{\varepsilon}_i g(x_i) \right| \right],
\]

where \( \tilde{\varepsilon} = \{\tilde{\varepsilon}_i\}_{i=1}^n \) are i.i.d. standard normal random variables, independent of \( \{X_i\}_{i=1}^n \). The *empirical local Rademacher complexity* \( \mathcal{R}_n(r; \bar{\mathcal{F}}) \) is defined in a similar fashion where \( \tilde{\varepsilon} = \{\tilde{\varepsilon}_i\}_{i=1}^n \) are i.i.d. Rademacher variables taking the values of either \(-1\) or \(1\) equiprobably, and independent of \( \{X_i\}_{i=1}^n \).

Let \( \Omega(r; \bar{\mathcal{F}}) = \{g \in \mathcal{F} : |g|_{2,\mathbb{P}} \leq r\} \). The *population local Rademacher complexity* is defined as

\[
\mathcal{R}(r; \bar{\mathcal{F}}) := \mathbb{E}_{\tilde{\varepsilon}, X} \left[ \sup_{g \in \Omega(r; \bar{\mathcal{F}})} \left| \frac{1}{n} \sum_{i=1}^n \tilde{\varepsilon}_i g(X_i) \right| \right],
\]
where $\tilde{\varepsilon} = \{\tilde{\varepsilon}_i\}_{i=1}^n$ are i.i.d. Rademacher variables taking the values of either $-1$ or $1$ equiprobably, and independent of $\{X_i\}_{i=1}^n$.

**Definition** (star-shaped function class). The class $\bar{F}$ is a star-shaped function class if for any $g \in \bar{F}$ and $\alpha \in [0, 1]$, $\alpha g \in \bar{F}$.

**Remark.** The smoothness classes considered in this paper are star-shaped.

**Lemma C.2.** Suppose the class $\bar{F}$ is star-shaped, and for all $g \in \bar{F}$, $|g|_{\infty} \leq c$ for some universal constant $c$. Let $\bar{r}$ be any positive solution to the critical inequality

$$R(r; \bar{F}) \leq \frac{r^2}{c}.$$  

Then for any $\delta \geq \bar{r}$ and all $g \in \bar{F}$, we have

$$\frac{1}{2} |g|_{2,p}^2 \leq |g|_n^2 + \frac{\delta^2}{2}$$

with probability at least $1 - c_1 \exp(-c_2 n \delta^2)$.

**Lemma C.3.** For any star-shaped $\bar{F}$, the function $r \mapsto \frac{R_n(r; \bar{F})}{r}$ is non-increasing on $(0, \infty)$. As a result, the critical inequality

$$R_n(r; \bar{F}) \leq c_0 r^2$$

has a smallest positive solution for any constant $c_0 > 0$. Similarly, the function $r \mapsto \frac{R(r; \bar{F})}{r}$ is non-increasing on $(0, \infty)$. As a result, the critical inequality

$$R(r; \bar{F}) \leq c_0 r^2$$

has a smallest positive solution for any constant $c_0 > 0$.

**Lemma C.4.** Suppose the class $\bar{F}$ is star-shaped, and for all $g \in \bar{F}$, $|g|_{\infty} \leq c$ for some universal constant $c$. Let $\bar{r}^*$ be the smallest positive solution to (90) with $c_0 = c^{-1}$ and $r^*$ be the smallest positive solution to (91) with $c_0 = c^{-1}$. We have

$$|g|_{2,p}^2 \gtrsim |g|_n^2 + \bar{r}^* n$$

with probability at least

$$1 - c_1 \exp(-c_2 n \bar{r}^*).$$

In the least squares problem (20), if we can bound $|\hat{f} - f|_n^2$ with high probability, then we can apply Lemmas C.2 or C.4 to bound $|\hat{f} - f|_{2,F}^2$ with high probability. The following lemmas provide bounds for $|\hat{f} - f|_n^2$.

**Lemma C.5.** Suppose the class $\bar{F}$ is star-shaped. Let $\delta$ be any positive solution to the critical inequality

$$G_n(r; \bar{F}) \leq \frac{r^2}{2 \sigma}.$$  

$$1 - c_1 \exp(-c_2 n \bar{r}^*).$$
Then for any $\delta \geq \bar{\delta}$, we have
\[ |\hat{f} - f|^2_n \preceq \delta \bar{\delta} \]  
(95)
with probability at least $1 - c_1 \exp\left(-c_2 \frac{n \delta^2}{\sigma^2}\right)$.

The following lemma concerns the regularized least squares in the form
\[ \hat{f} \in \arg \min_{\tilde{f} \in \mathcal{W}} \frac{1}{2n} \sum_{i=1}^{n} (y_i - \tilde{f}(x_i))^2 + \lambda |\tilde{f}|^2_{\mathcal{H}} \]  
(96)
where $\mathcal{W}$ is a space of real-valued functions with an associated semi-norm and contains $\mathcal{F}$. When $\mathcal{W}$ is an RKHS with its RKHS norm $|\cdot|_{\mathcal{H}}$, (96) is referred to as the Kernel Ridge Regression (KRR) estimators. In particular, as we discuss in Section 4, when $\mathcal{F} = S_{k+1}$ in (20), we can transform (20) into the form (96), which is equivalent to solving (26) by exploiting the (reproducing) kernel function associated with the Sobolev space. To state the following lemma, let us introduce the empirical local Gaussian complexity specifically for RKHS:
\[ G_n(r; \bar{\mathcal{W}}) := \mathbb{E}_{\tilde{\varepsilon}} \left[ \sup_{g \in \Omega_n(r; \bar{\mathcal{W}})} \left| \frac{1}{n} \sum_{i=1}^{n} \tilde{\varepsilon}_i g(x_i) \right| \right], \]
where
\[ \Omega_n(r; \bar{\mathcal{W}}) = \{ g \in \bar{\mathcal{W}} : |g|_n \leq r, |g|_{\mathcal{H}} \leq 3 \} \]
and
\[ \bar{\mathcal{W}} := \{ g = g_1 - g_2 : g_1, g_2 \in \mathcal{W} \}. \]

Lemma C.6. Suppose the class $\mathcal{W}(\supseteq \mathcal{F})$ is convex. Let $\bar{\delta}$ be any positive solution to the critical inequality
\[ G_n(r; \bar{\mathcal{W}}) \leq \frac{R^2}{2\sigma} \]  
(97)
where $R$ is a user defined radius. Then for any $\delta \geq \bar{\delta}$, if (96) is solved with $\lambda \geq 2\delta^2$, we have
\[ |\hat{f} - f|^2_n \preceq R^2 \delta^2 + R^2 \lambda \]  
(98)
with probability at least $1 - c_1 \exp\left(-c_2 \frac{n R^2 \delta^2}{\sigma^2}\right)$.

Remark. Concerning the problem in Section 4, $\mathcal{W}$ corresponds to the Sobolev space, which is convex and contains $\mathcal{F}$. Moreover, when $\mathcal{F} = S_{k+1}$ in (20), we can take $R = \overline{\mathcal{C}}$.

In order to make use of Lemmas C.5 and C.6 to establish sharp bounds on $|\hat{f} - f|^2_n$, we need good candidates for $\bar{\delta}$ that solves (94) and (97), respectively. To make use of Lemmas C.2 and C.4 to connect $|\hat{f} - f|^2_n$ with $|\hat{f} - f|^2_{2,\mathcal{P}}$, we need a good candidate that solves (90). The following lemmas serve this purpose.

Lemma C.7. Suppose the class $\bar{\mathcal{F}}$ is star-shaped. Let $N_n(\delta, \Omega_n(r; \bar{\mathcal{F}}))$ be the $\delta$–covering number of the set $\Omega_n(r; \bar{\mathcal{F}})$ in the $|\cdot|_n$ norm.
Any $\delta \in (0, \sigma]$ that solves
\[
\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega_n(r; \mathcal{F}))} d\delta \asymp \frac{r^2}{\sigma}
\]
solves (94).

(ii) Suppose $|g|_\infty \leq c$ for all $g \in \mathcal{F}$. Then any $\delta > 0$ that solves
\[
\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega_n(r; \mathcal{F}))} d\delta \asymp r^2
\]
solves (90).

The following lemma concerns the KRR estimator (96) when $\mathcal{W}$ in Lemma C.6 is an RKHS.

Lemma C.8. Suppose $\mathcal{W}$ is a convex RKHS and the KRR estimator (96) is of interest. Let $\tilde{\mu}_1 \geq \tilde{\mu}_2 \geq ... \geq \tilde{\mu}_n \geq 0$ be the eigenvalues of the kernel matrix $K \in \mathbb{R}^{n \times n}$ consisting of entries $\frac{1}{n} K(x_i, x_j)$, where $K$ is the kernel function associated with $\mathcal{W}$. Suppose $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a positive semidefinite kernel function such that $K(x, x') \preceq 1$ for all $x, x' \in \mathcal{X}$.

(i) Any $\delta > 0$ that solves
\[
\sqrt{\frac{1}{n} \sum_{i=1}^n \min \{r^2, \tilde{\mu}_i\} \times \frac{R \sigma}{r}} \asymp \frac{R \sigma}{r}
\]
solves (97).

(ii) Any $\delta > 0$ that solves
\[
\sqrt{\frac{1}{n} \sum_{i=1}^n \min \{r^2, \tilde{\mu}_i\} \times r^2}
\]
solves (90) where $c_0 \asymp 1$.

The following lemma is useful when applying Lemmas C.2 and C.4 in the case of RKHS and KRR.

Lemma C.9. Let $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a positive semidefinite kernel function such that $K(x, x') \preceq 1$ for all $x, x' \in \mathcal{X}$. Then, $|f|_\infty \preceq 1$ for any function $f$ in the ball of the associated RKHS where the ball has a constant radius (with respect to the RKHS norm).
D Proofs for Section 6

D.1 Proof for Lemma 6.1

Like in Section A.3, the proper choice of the grid of points on each dimension of \([-1, 1]^d\) is the key in this case. Any function \(f \in U_{\gamma+1,2}^d\) can be written as

\[
f(x + \Delta) = \sum_{k=0}^\gamma \sum_{p: P = k} \frac{\Delta^p D^p f(x)}{k!} + \sum_{p: P = \gamma} \left[ \frac{\Delta^p D^p f(z)}{\gamma!} - \frac{\Delta^p D^p f(x)}{\gamma!} \right] := REM_0(x + \Delta)
\]

where \(x, x + \Delta \in (-1, 1)^d\) and \(z\) is some intermediate value. For a given \(k \in \{0, \ldots, \gamma\}\), recall \(\text{card}(\{p: P = k\}) = D_k^*\). Therefore, we have

\[
|REM_0(x + \Delta)| \leq \frac{D_k^* R_{\gamma+1} |\Delta|_{\infty}^{\gamma+1}}{\gamma!}.
\]  (103)

In a similar way, writing

\[
D_{\tilde{p}} f(x + \Delta) = \sum_{k=0}^{\gamma - \tilde{p}} \sum_{p: P = k} \frac{\Delta^p D^p + \tilde{p} f(x)}{k!} + \sum_{p: P = \gamma - \tilde{p}} \left[ \frac{\Delta^p D^p + \tilde{p} f(z)}{\gamma - \tilde{p} \choose \gamma - \tilde{p}} - \frac{\Delta^p D^p + \tilde{p} f(x)}{\gamma - \tilde{p} \choose \gamma - \tilde{p}} \right] := REM_{\tilde{p}}(x + \Delta)
\]

for \(1 \leq \tilde{p} := \sum_{j=1}^d \tilde{p}_j \leq \gamma\) and \(\tilde{p} = (\tilde{p}_j)_{j=1}^d\), we have

\[
|REM_{\tilde{p}}(x + \Delta)| \leq \frac{D_{\gamma - \tilde{p}}^* R_{\gamma - \tilde{p} + 1} |\Delta|_{\infty}^{\gamma+1 - \tilde{p}}}{(\gamma - \tilde{p} \choose \gamma - \tilde{p})!}.
\]  (104)

For some \(\delta_0, \ldots, \delta_\gamma > 0\), suppose that \(|D^p f(w) - D^p g(w)| \leq \delta_k\) for all \(p\) with \(P = k \in \{0, \ldots, \gamma\}\), where \(f, g \in U_{\gamma+1,2}^d\). Then we have

\[
|f(x + \Delta) - g(x + \Delta)| \\
\leq \sum_{k=0}^\gamma \sum_{p: P = k} \frac{\Delta^p}{k!} (D^p f(x) - D^p g(x)) + 2 \frac{D_k^* R_{\gamma+1} |\Delta|_{\infty}^{\gamma+1}}{\gamma!} \\
\leq \sum_{k=0}^\gamma \frac{D_k^* |\Delta|_{\infty}^k \delta_k}{k!} + 2 \frac{D_k^* R_{\gamma+1} |\Delta|_{\infty}^{\gamma+1}}{\gamma!}.
\]
Let \( \max_{k \in \{1, \ldots, \gamma +1\}} D_{k-1}^* R_k \) for \( k = 0, \ldots, \gamma \). Then, for \( \theta \) and \( \theta' \) such that for any \( \theta \in \mathcal{P}_\Gamma \), there exists some \( i_{(p,k)} \in \{1, \ldots, N_k\} \) with

\[
\sum_{k=0}^{\gamma} \sum_{p:P=k} \left| \theta_{(p,k)} - \theta'_{i(p,k)} \right| \leq \delta.
\]

As a consequence, we have

\[
\log N_1 (\delta, \mathcal{P}_\Gamma) \leq \sum_{k=0}^{\gamma} D_k^* \log \frac{4 (\gamma + 1) D_k^* R_k}{\delta k!}
\]
and
\[
\log N_{2,P} \left( \delta, \mathcal{U}_{\gamma+1,1}^d \right) \leq \log N_{\infty} \left( \delta, \mathcal{U}_{\gamma+1,1}^d \right) \leq \sum_{k=0}^\gamma D_k^* \log \frac{4(\gamma + 1) D_k^* R_k}{\delta k!}.
\]

If \( \delta \) is large enough such that \( \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma + 1) D_k^* R_k}{\delta k!} < 0 \), we use the counting argument in Kolmogorov and Tikhomirov (1959) to obtain
\[
\log N_{2,P} \left( \delta, \mathcal{U}_{\gamma+1,1}^d \right) \leq \log N_{\infty} \left( \delta, \mathcal{U}_{\gamma+1,1}^d \right) \lesssim \left( \sum_{k=0}^\gamma D_k^* \right) \log \frac{1}{\delta} + \sum_{k=0}^\gamma D_k^* \log R_k.
\]

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