Phase transitions in nonparametric regressions: a curse of exploiting higher degree smoothness assumptions in finite samples

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Abstract

When the regression function belongs to a smooth class consisting of univariate functions with derivatives up to the \((\gamma + 1)\)th order bounded in absolute values for a finite \(\gamma\), it is generally viewed that exploiting higher degree smoothness assumptions helps reduce the estimation error. This paper shows that the minimax optimal mean integrated squared error (MISE) \(\) increases in \(\gamma\) when the sample size \(n\) is small relative to the order of \((\gamma + 1)^{2\gamma + 3}\), and decreases in \(\gamma\) when \(n\) is large relative to the order of \((\gamma + 1)^{2\gamma + 3}\). In particular, this phase transition property is shown to be achieved by common nonparametric procedures. Consider \(\gamma_1\) and \(\gamma_2\) such that \(\gamma_1 < \gamma_2\), where the \((\gamma_2 + 1)\)th degree smoothness class is a subset of the \((\gamma_1 + 1)\)th degree class. What is surprising about our results is that they imply, if \(n\) is small relative to the order of \((\gamma_1 + 1)^{2\gamma_1 + 3}\), the optimal rate achieved by the estimator constrained to be in the smoother class (to exploit the \((\gamma_2 + 1)\)th degree smoothness) is slower. In data sets with fewer than hundreds-of-thousands observations, our results suggest that one should not exploit beyond the third or fourth degree of smoothness. To some extent, our results provide a theoretical basis for the widely adopted practical recommendations given by Gelman and Imbens (2019).

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 the most commonly seen smoothness classes and also several non-standard smoothness classes in the nonasymptotic setting where \(n\) is not taken to infinity.

1 Introduction

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

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

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 $f$ is that it belongs to a smoothness class consisting of univariate functions with derivatives up to a given (finite) $(\gamma + 1)$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 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 Ullah, 1999).

When $\gamma$ is finite and the sample size $n \to \infty$, classical results show that the minimax optimal MISE rate decreases as $\gamma$ increases. The classical results give rise to the so called “blessing of smoothness” folklore (i.e., the more smoothness, the better). Empirical researchers are often 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). In this paper, we study the minimax optimal MISE rates under the regime where neither $n$ nor $\gamma$ are taken to infinity, and show that exploiting higher degree smoothness assumptions could result in a larger MISE if $n$ is not enormously large.

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 any estimators (by taking the infimum 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 constants independent of $n$ (and in our interest, also independent of $\gamma$); 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 class, we show the following phase transition phenomenon: (i) if $n$ is small relative to the order of $(\gamma + 1)^{2\gamma + 3}$, the minimax optimal MISE rate is $\frac{2^{2\gamma + 3}}{n}$, which is slower than the classical asymptotic optimal rate $\left(\frac{1}{n}\right)^{\frac{2^{2\gamma + 3}}{2\gamma + 3}}$ obtained by assuming $\gamma$ is finite and $n \to \infty$ (ii) if $n$ is large relative to the order of $(\gamma + 1)^{2\gamma + 3}$ (which clearly includes the degenerate case of $\gamma$ being finite and $n$ tending to infinity), the minimax optimal MISE rate is $\left(\frac{1}{n}\right)^{\frac{2^{2\gamma + 3}}{2\gamma + 3}}$, which is slower than $\frac{2^{2\gamma + 3}}{n}$. To our knowledge, this paper is the first in the literature to show the phase transition in the minimax optimal rate and the growth rate of the sample size $n$ (i.e., $(\gamma + 1)^{2\gamma + 3}$) at which the minimax optimal rate transitions from $\frac{2^{2\gamma + 3}}{n}$ to $\left(\frac{1}{n}\right)^{\frac{2^{2\gamma + 3}}{2\gamma + 3}}$.

Particularly, we show in this paper that, if $f$ belongs to a $(\gamma + 1)$th degree smoothness class, estimators which minimize the sum of squared residuals and are constrained to be in the same class to exploit the $(\gamma + 1)$th degree smoothness achieve the minimax optimal MISE rates. These estimators will be referred to as the constrained nonparametric least squares estimator (CNLS) in

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1 In this paper, a standard $(\gamma + 1)$th degree smoothness class refers to one that consists of functions with derivatives belonging to a ball of constant radius with respect to either an $L_\infty$ (max) norm or a Hilbert norm.

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

Consider $\gamma_1$ and $\gamma_2$ such that $\gamma_1 < \gamma_2$, where the $(\gamma_2 + 1)$th degree smoothness class is a subset of the $(\gamma_1 + 1)$th degree class. What is striking about our results is that they imply, if $n$ is small relative to the order of $(\gamma_1 + 1)^{2\gamma_1 + 3}$, the optimal rate achieved by the CNLS estimators is faster when the class is less smooth. This phenomenon is opposite to the common wisdom based on classical asymptotic rates. The explanation for our result comes from the Taylor series expansion of smooth functions, which allows one to decompose a smoothness class into two orthogonal subspaces: a polynomial subspace and an infinite-dimensional nonparametric subspace. In other words, any function $f$ in a smoothness class can be written as $f = f_1 + f_2$, where $f_1$ belongs to the polynomial subspace and $f_2$ belongs to the nonparametric subspace. What may not be obvious to applied researchers is that exploiting more smoothness is in fact fitting higher order polynomials, a practice that is not recommended in recent years. In finite sample settings, there is a trade-off between the approximation of $f_1$ and the approximation of $f_2$. Exploiting a higher degree of smoothness increases the error in estimating $f_1$ and decreases the error in estimating $f_2$, and vice versa. If $n$ is not large enough, a “smarter” estimator that leads to lower MISE would resort to a lower order Taylor’s approximation, which uses lower order polynomials to approximate $f_1$ but a less smooth function to approximate the infinite-dimensional $f_2$. As $n \to \infty$ while $\gamma$ stays finite, the trade-off disappears as the benefit of using the $(\gamma + 1)$th degree smoothness approximation for $f_2$ dominates the cost of fitting $\gamma$th order polynomials.

1.1 Practical implications of our results

As a simple example, suppose $f$ ranges over the class of sixth order polynomials. Any function in this class can be expressed in the form of exactly sixth order polynomials and therefore, the nonparametric subspace for this class is the singleton $\{0\}$. Notably, the class of sixth order polynomials is a subset of any $(\gamma + 1)$th degree smoothness classes with $\gamma \leq 6$. The common wisdom might say, fitting exactly sixth order polynomials is a finite-dimensional parametric estimation problem and better than using a nonparametric approximation method. On the other hand, our results imply that approximating $f$ with a function from a lower than seventh degree smoothness class (decomposed into a lower than sixth degree polynomial subspace and a lower than seventh degree smoothness nonparametric subspace) may lead to a smaller MISE when $n$ is not enormously large.

As we have brought up the trade-off between a polynomial subspace and an infinite-dimensional nonparametric subspace, it is worth mentioning the connection between our theoretical results and the empirical findings from the highly influential paper by Gelman and Imbens (2019), which implements high order polynomials in regression discontinuity designs (RDD) analyses. In particular, when applying RDD to perform causal inference, two conditional mean functions of a pretreatment variable are estimated from (1). There are several empirical issues of using high order polynomials raised in Gelman and Imbens (2019). Our results in this paper are most related to their paper on the issue of mean squared errors (MSE) in finite samples.

As discussed in Gelman and Imbens (2019, p. 456), researchers frequently use high order (such as fifth or sixth order) polynomials for three reasons: (i) any smooth function on a compact set can be
approximated by high order polynomials arbitrarily well; (ii) the fit from high order polynomials is expected to be smooth when the relation between the pretreatment variable and outcome is strong; (iii) many textbooks recommend including relevant predictors in causal inference to reduce bias and when the sample size is large, it is expected that the reduction in bias by including high order polynomials is larger than the increase in variance. Through various empirical studies, Gelman and Imbens (2019) discover that fitting high order polynomials in RDD analyses results in noisy estimates and poor coverage of confidence intervals. The authors conjecture that fitting high order polynomials of the pretreatment variable can incur bias and high variance (overall a high MSE), hence damaging coverage, even in large samples.

Our focus in this paper is on the global criterion MISE while the concern of Gelman and Imbens (2019) is about the MSE of the high order polynomial implementation at a point. From the perspective of the minimax optimal MISE rate without taking \( n \) to infinity, our results reinforce the empirical evidence and the conjecture in Gelman and Imbens (2019) by suggesting that, fitting higher order polynomials could also induce higher MSE globally even in large (but finite) samples.


\[ n = \left(\frac{\gamma^* + 1}{n}\right)^{\frac{2\gamma^*+3}{\gamma^*+2}} \]

and choose the \((\gamma^* + 1)\)th or the \((\gamma^* + 2)\)th degree smoothness approximation. A further rule for choosing between the \((\gamma^* + 1)\)th degree and the \((\gamma^* + 2)\)th degree is detailed in Section 4.3, which says: if

\[ n = \left(\frac{\gamma^* + 1}{n}\right)^{\frac{2\gamma^*+3}{\gamma^*+2}} \]

choose the \((\gamma^* + 1)\)th degree; if

\[ n = \left(\frac{\gamma^* + 2}{n}\right)^{\frac{2\gamma^*+3}{\gamma^*+2}} \]

choose the \((\gamma^* + 2)\)th degree. Our recommended smoothness selection rule above applies naturally to the global nonparametric estimators such as KRR and smoothing splines. Note that when \( \gamma^* = 2, 3, 4 \) in (2), \((\gamma^* + 1)^{\frac{2\gamma^*+3}{\gamma^*+2}} = 2187, 262144, 48828125\), respectively. In data sets with fewer than hundreds-of-thousands observations, higher than fifth order smoothing splines methods should be avoided.

Regarding the following data sets studied in Gelman and Imbens (2019), the Jacob-Lefgren data (Jacob and Lefgren, 2004), Lee data (Lee, 2008), Matsudaira data (Matsudaira, 2008), the LaLonde data (LaLonde, 1986), and the census data in 1974, 1975 and 1978, the sample sizes used in the implementation of Gelman and Imbens (2019) range from a couple of thousands to at most thirties of thousands, which are all far below \((3 + 1)^{\frac{2\gamma^*+3}{\gamma^*+2}} = 262144\). Based on their empirical evidence from studying these data sets, Gelman and Imbens (2019) recommend researchers to avoid using high

\[ n = \left(\frac{\gamma^* + 1}{n}\right)^{\frac{2\gamma^*+3}{\gamma^*+2}} \]

and the proof for the pointwise problem is typically simpler). Nevertheless, it is well known that the minimax optimal MISE rate coincides with the minimax optimal pointwise MSE rate in the regime where \( \gamma \) is finite and \( n \to \infty \) (see Tsybakov, 2009). We do not expect that the minimax optimal rates would differ between MISE and pointwise MSE in the regime of finite \( \gamma \) and finite \( n \), simply because the trade-off between a polynomial subspace and an infinite-dimensional nonparametric subspace exists whether the interest is the MISE or pointwise MSE.
order polynomials but use local linear or local quadratic polynomials (as discussed in Hahn, et. al, 2001; Porter, 2003; Calonico, et. al, 2014) or other smooth functions in RDD analysis. Strikingly, these recommendations largely coincide with our recommendation. Therefore, there is a theoretical basis for the widely adopted practical recommendations given in Gelman and Imbens (2019).

Beyond empirical evidence that indicates high order polynomials do not perform well, there is also simulation evidence in the literature showing that it takes a large $n$ for high order kernel density estimators to become beneficial in nonparametric regressions (see, e.g., Marron, 1994). Specifically, Marron (1994) found in simulations that the second order kernel produces a smaller MISE when the sample size is between 70 and 10000, and the fourth order kernel is dominantly better than the second order kernel when $n > 10000$. Note that the turning point $n = 10000$ is roughly consistent with our recommended rule in (3). This coincidence deserves a future investigation as our (optimal rate) achievability results in this paper concern global nonparametric procedures. Nevertheless, it is possible that a phase transition phenomenon also exists in local smoothing methods. See Section 7 for more discussions.

Of course our recommended $\gamma^*$—rule is harder to apply when a researcher has zero or little knowledge about the smoothness degree $\gamma (\geq \gamma^*)$. A recent paper by Chen et. al (2021) studies (global) 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. One interesting (but challenging) direction is to develop data-driven estimators that are adaptive to the unknown smoothness parameter and optimal (or nearly optimal) rates in the regime where both $n$ and (the unknown) smoothness parameter are finite. The challenging part of this direction is to show whether these estimators are adaptive to phase transition without taking $n$ to infinity.

We want to emphasize that the finite sample 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.

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 $\sqrt{n} (\hat{\alpha} - \alpha) = \frac{1}{\sqrt{n}} \left( \hat{f} (Z_{ij}) - f (Z_{ij}) \right)^2$, where $j$ is the index of the endogenous variables and $Z_{ij}$ is a instrumental variable for the $j$th endogenous variable.

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The author would like to thank Shakeeb Khan for pointing out this reference, the issues of high order kernel density estimators, and the broader implications of our results.

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 $(Z_{ij} \pi_j - Z_{ij} \pi_j^*)^2$ in Zhu (2018) with $\left( \hat{f} (Z_{ij}) - f (Z_{ij}) \right)^2$, where $j$ is the index of the endogenous variables and $Z_{ij}$ is a instrumental variable for the $j$th endogenous variable.
normal random variable + remainder, and the sample analogue of the MISE of the first-step nonparametric estimator enters “remainder”. This insight is revealed in Belloni, et. al (2014) despite the focus there is on sparse function approximations rather than smooth function approximations for the first step. This insight plays a crucial role in arguing for good machine learning algorithms to be applied in the first step to reduce the magnitude of “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 Outline of our theoretical contributions

This paper generalizes the standard Hölder class in the literature to the generalized Hölder class where the absolute value of the kth (k = 0,...,γ) derivative of any member is bounded by a parameter Rk and the γth derivative is Rγ+1−Lipschitz (i.e., Rk is allowed to depend on k). Like the standard Hölder class, we can decompose the generalized Hölder class into two orthogonal subspaces: the generalized polynomial subspace the generalized Hölder subspace. We also generalize the standard ellipsoid subspace of smooth functions in a similar fashion by allowing its RKHS radius to be bounded by Rγ+1. Notably, a Sobolev subspace can be expressed as an ellipsoid subspace. Like the Hölder subspace, the ellipsoid subspace is orthogonal to the polynomial subspace. The first objective of this paper is to examine the impacts of γ and {Rk}γ+1 0 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 establish the phase transition phenomenon in the regime of finite γ and finite n.

The existing literature mostly assumes that Rk 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 ˆy′ on f(ˆy; θ) to obtain estimates of the parameters θ 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)| ≤ 1 for all x on the domain and k = 0,...,γ + 1, then |y(k+1)(x)| ≤ k!; (ii) the factorial bounds are attainable by the solutions to some ODE (e.g., y′ = e−y−1/2) 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.

In contrast to the classical entropy bounds in the literature, our entropy bounds enable us to reveal the phase transition phenomenon in the regime of finite $n$ and finite $\gamma$. When metric entropy results are used to study smoothness classes, virtually every paper including recent textbooks on nonasymptotic statistics (such as Wainwright, 2019) takes $\log(\delta − \text{covering number}) \approx \delta^{-\frac{1}{\gamma+1}}$ 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 is not sharp. As a consequence, the minimax optimal rate $(\frac{1}{n})^{\frac{2\gamma+2}{2\gamma+3}}$ derived based on $\delta^{-\frac{1}{\gamma+1}}$ is not sharp unless $n$ is large relative to the order of $(\gamma + 1)^{2\gamma+3}$ (in which case, $\delta$ becomes small enough). We discover that:

1. the derivations of the lower bound on the metric entropy in Kolmogorov and Tikhomirov (1959) as well as the following literature for Hölder and ellipsoid classes ignore the polynomial subspace, which is why $\delta^{-\frac{1}{\gamma+1}}$ is not sharp even for the 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 subspace is far from being tight when $R_k$s become large enough;

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

4. the existing minimax optimal rate for MISE or its sample analogue associated with the standard smoothness classes takes the form $(\frac{1}{n})^{\frac{2\gamma+2}{2\gamma+3}}$, which is unable to reveal the phase transition phenomenon in finite samples.\(^7\)

All these issues are addressed in this paper. Particularly, in deriving the bounds for the polynomial subspace, we develop our own arguments; in deriving the bounds for the ellipsoid subspace, 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 $R_{\gamma+1}$.

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\(^6\)For the standard smoothness classes, one may use methods based on “ranks” (for the polynomial subspace) and “eigenvalues” (for the nonparametric subspace) 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 $R_k$.

\(^7\)For the non-standard Hölder class with $R_k = (k − 1)!$, 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 number, Zhu and Mirzaei (2021) simply takes the classical result $\delta^{-\frac{1}{\gamma+1}}$ from Kolmogorov and Tikhomirov (1959). The consequences are, the MSE rates derived in Zhu and Mirzaei (2021) are far from being sharp, the lower and upper error bounds have different rates, and therefore are unable to show that the phase transition necessarily exists in finite samples. See Section 5 for the details.
In our nonasymptotic analysis, none of $n$, $\gamma$ and $\{R_k\}_{k=0}^{\gamma+1}$ are taken to infinity (although our results do hold for the degenerate case of $\gamma$ being finite and $n$ tending to infinity). 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 independent of $n$, $\gamma$ and $\{R_k\}_{k=0}^{\gamma+1}$. Ideally, our proposed rule for selecting $\gamma^*$ based on (2) should reflect the universal constants. But practically speaking, as $n$ need to grow super-factorially in the smoothness degree for one extra degree to become beneficial, the universal constants essentially do not matter much once $\gamma^* \geq 3$. Therefore, the practical implications discussed in Section 1.1 would hold true regardless of the universal constant.

Deriving sharp constants for global criteria such as MISE and in the context of global nonparametric procedures is known to 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” metric procedures is known to be difficult, which is why the existing literature does not make an implication discussed in Section 1.1 would hold true regardless of the universal constant. We are only able to provide some partial answers. Nevertheless, we expect similar implications would carry over to the higher dimensional case.

2.1 Notation and definitions

Notation. Let $\lceil x \rceil$ denote the largest integer smaller than or equal to $x$. For two functions $f(n)$ and $g(n)$, let us write $f(n) \gtrsim g(n)$ if $f(n) \geq cg(n)$ for a universal constant $c \in (0, \infty)$; similarly, we write $f(n) \lesssim g(n)$ 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 $f(n) \lesssim g(n)$. Throughout this paper, we use various $c$ and $C$ letters to denote positive universal constants that are: $\gtrsim 1$ and independent of $n$, $\gamma$, $\{R_k\}_{k=0}^{\gamma+1}$ and the dimension $d$ of the covariates; 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 $B_q^J(R) := \{\theta \in \mathbb{R}^J : |\theta|_q \leq R\}$. For functions on $[a, b]$, the unweighted $L^2$-norm $|f - g|_2 := \sqrt{\int_a^b |f(x) - g(x)|^2 \, dx}$, and the weighted $L^2(\mathbb{P})$-norm $|f - g|_{2, \mathbb{P}} := \sqrt{\int_a^b \mathbb{P}(\cdot)(f(x) - g(x))^2 \, dx}$.

For functions on $[a, b]^d$, the supremum norm $|f - g|_\infty := \sup_{x \in [a, b]^d} |f(x) - g(x)|$.

Finally, the $L^2(\mathbb{P}_n)$-norm of the vector $f := \{f(x_i)\}_{i=1}^n$, denoted by $|f|_{n, 2}$, 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 $\{\eta^1, \eta^2, \ldots, \eta^N\} \subset \Lambda$ 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 $\rho(\eta, \eta^i) \leq \delta$.

\footnote{In fact, our metric entropy bounds could be expressed with explicit universal constants. 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 line to line.}
The $\delta$–covering number of $\Lambda$, denoted by $N_\rho(\delta, \Lambda)$, is the cardinality of the smallest $\delta$–cover. A set $\{\eta^1, \eta^2, ..., \eta^M\} \subset \Lambda$ is a $\delta$–packing of $\Lambda$ in the metric $\rho$ if for any distinct $i, j \in \{1, ..., M\}$, $\rho(\eta^i, \eta^j) > \delta$. 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 $N_q(\delta, \mathcal{F})$ and $M_q(\delta, \mathcal{F})$ 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 $L^2(\mathbb{P})$–norm $|\cdot|_{2,p}$.

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

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

(4)

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.

Let $p = (p_j)_{j=1}^d$ and $P = \sum_{j=1}^d p_j$ where $p_j$s are 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 $\mathcal{U}_{\gamma+1}((R_k)_{k=0}^{\gamma+1}, [-1, 1]^d)$ be the class of functions such that any function $f \in \mathcal{U}_{\gamma+1}((R_k)_{k=0}^{\gamma+1}, [-1, 1]^d)$ 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) $|D^p f(x) - D^p f(x')| \leq R_{\gamma+1} \left| x - x' \right|$ for all $p$ with $P = \gamma$ and $x, x' \in [-1, 1]^d$.

Our main results in this paper (Sections 3–5) concern $d \geq 1$, where we use the shortform $\mathcal{U}_{\gamma+1}$. Section 6 considers a general $d$, where we use the shortform $\mathcal{U}_{\gamma+1}^d$. Any function $f$ in the Hölder class, $\mathcal{U}_{\gamma+1} [-1, 1]$, can be written as

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

(5)

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

$$\mathcal{U}_{\gamma+1} = \mathcal{U}_{\gamma+1,1} + \mathcal{U}_{\gamma+1,2} := \{ f_1 + f_2 : f_1 \in \mathcal{U}_{\gamma+1,1}, f_2 \in \mathcal{U}_{\gamma+1,2} \}$$

where the polynomial subspace

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

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

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

and the Hölder subspace

$$\mathcal{U}_{\gamma+1,2} = \left\{ f \in \mathcal{U}_{\gamma+1} : f^{(k)}(0) = 0 \text{ for all } k \leq \gamma \right\}.$$
Any function \( f \) in a Sobolev class 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 \((a)_{+} = a \vee 0\). The (RK)HS norm associated with a Sobolev class takes the form
\[
|f|_H = \left( \sum_{k=0}^{\gamma} (f^{(k)}(0))^2 + \int_0^1 [f^{(\gamma+1)}(t)]^2 \right)^{1/2},
\]
(6)

Therefore, a Sobolev class can be decomposed into a polynomial subspace and a Sobolev subspace imposed with the restrictions that \( f^{(k)}(0) = 0 \) for all \( k \leq \gamma \) and \( f^{(\gamma+1)} \) belongs to the space \( L^2 [0, 1] \) (see Wahba, 1990, Chapter 1).

Let us introduce the Sobolev subspace with the restrictions at zero:
\[
S_{\gamma+1} := \{ f : [0, 1] \to \mathbb{R} | f \text{ is } \gamma + 1 \text{ times differentiable a.e.,} \]
\[
f^{(k)}(0) = 0 \text{ for all } k \leq \gamma, \text{ and} \]
\[
f^{(\gamma)} \text{ is absolutely continuous with} \]
\[
\int_0^1 [f^{(\gamma+1)}(t)]^2 dt \leq R_{\gamma+1}^2 \}.
\]

The Sobolev subspaces are special cases of the ellipsoid subspaces. We define the generalized ellipsoid subspace of smooth functions as follows:
\[
\mathcal{H}_{\gamma+1} = \left\{ f = \sum_{m=1}^{\infty} \theta_m \phi_m : \text{for } (\theta_m)_{m=1}^{\infty} \in \ell^2(\mathbb{N}) \text{ such that } \sum_{m=1}^{\infty} \frac{\theta_m^2}{\mu_m} \leq R_{\gamma+1}^2 \right\}
\]
(7)

where \( \ell^2(\mathbb{N}) := \{ (\theta_m)_{m=1}^{\infty} | \sum_{m=1}^{\infty} \theta_m^2 < \infty \} \), \( (\mu_m)_{m=1}^{\infty} \) and \( (\phi_m)_{m=1}^{\infty} \) are the eigenvalues and eigenfunctions (that forms an orthonormal basis of \( L^2 [0, 1] \)), 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 \( R_{\gamma+1} \asymp 1 \) in (7) gives the standard ellipsoid subspace. Moreover, (7) is equipped with the inner product \( \langle h, g \rangle_{\mathcal{H}} = \sum_{m=1}^{\infty} \frac{\langle h, \phi_m \rangle \langle g, \phi_m \rangle}{\mu_m} \) where \( \langle \cdot, \cdot \rangle \) is the inner product in \( L^2 [0, 1] \).

3 Covering and packing numbers

In this section, we present bounds on covering and packing numbers associated with the generalized \( U_{\gamma+1,1}, U_{\gamma+1,2} \), and \( \mathcal{H}_{\gamma+1} \). As a reminder, various \( c \) and \( C \) letters denote positive universal constants that are: \( \gtrsim 1 \) and independent of \( n, \gamma \), 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.
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

| $U_{\gamma+1,1}$ ($q \in (2, \infty)$) | $U_{\gamma+1,2}$ ($q \in (2, \infty)$) | $H_{\gamma+1}$ ($q = 2$) |
|--------------------------------------|--------------------------------------|-----------------------------|
| $\geq \begin{cases} B_2 (\delta) & \text{if } \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k! \delta} \geq 0 \\ B_1 (\delta) & \text{otherwise} \end{cases}$ | $R^* \frac{1}{\gamma^{\frac{1}{\gamma}}} \delta^{\frac{1}{\gamma+1}}$ if $R_{\gamma+1} \geq \gamma + 1$ | $R^* \frac{1}{\gamma^{\frac{1}{\gamma}}} \delta^{\frac{1}{\gamma+1}}$ if $R_{\gamma+1} \leq \gamma + 1$ |
| $\geq \max \{ B_1 (\delta), B_2 (\delta) \}$ | $R^* \frac{1}{\gamma^{\frac{1}{\gamma}}} \delta^{\frac{1}{\gamma+1}} \frac{\delta}{\gamma}$ if $R_0 \geq 1$ | $R^* \frac{1}{\gamma^{\frac{1}{\gamma}}} \delta^{\frac{1}{\gamma+1}} \frac{\delta}{\gamma}$ if $R_0 \geq 1$ |

where: $B_1 (\delta) = \sum_{k=0}^{\gamma} \log \frac{4(\gamma+1)R_k}{k! \delta}$; $B_2 (\delta) = (\frac{\gamma}{2} + 1) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} \log R_k$; $B_3 (\delta) = \sum_{k=0}^{\gamma} \log \left( 9^{-\gamma} \gamma^{-\gamma} + \sum_{k=0}^{\gamma} \log \frac{C \sum_{m=0}^{\gamma/2} R_{k+2m}}{\delta} \right)$ (with $R_{k+2m} = 0$ for $k + 2m > \gamma$); $B_4 = C' \left( \frac{\gamma}{2} + 1 \right) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} \log R_k$. $C$ and $C'$ are positive universal constants that are: $\leq 1$ and independent of $n$, $\gamma$, and $\{R_k\}_{k=0}^{\gamma}$.

3.1 The generalized polynomial subspace, $U_{\gamma+1,1}$

Lemma 3.1. (i) If $\delta$ is small enough such that $\min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k! \delta} \geq 0$, we have

$$\log N_{2,P} (\delta, U_{\gamma+1,1}) \leq \log N_{\infty} (\delta, U_{\gamma+1,1}) \leq \sum_{k=0}^{\gamma} \log \frac{4(\gamma+1)R_k}{k! \delta}. \quad (8)$$

if $\delta$ is large enough such that $\min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k! \delta} < 0$, we have

$$\log N_{2,P} (\delta, U_{\gamma+1,1}) \leq \log N_{\infty} (\delta, U_{\gamma+1,1}) \leq \left( \frac{\gamma}{2} + 1 \right) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} \log R_k. \quad (9)$$

(ii) In terms of the lower bounds, we have

$$\log M_2 (\delta, U_{\gamma+1,1}) \geq B_1 (\delta),$$
$$\log M_{\infty} (\delta, U_{\gamma+1,1}) \geq B_1 (\delta),$$

where $B_1 (\delta) = \sum_{k=0}^{\gamma} \log \left( 9^{-\gamma} \gamma^{-\gamma} + \sum_{k=0}^{\gamma} \log \frac{C \sum_{m=0}^{\gamma/2} R_{k+2m}}{\delta} \right)$ (with $R_{k+2m} = 0$ for $k + 2m > \gamma$) for some positive universal constant $C$. Let $k \in \arg \max_{k \in \{0, \ldots, \gamma\}} \frac{R_k}{k! \delta}$. If

$$\frac{R_k}{k! \delta \left( \frac{\gamma}{2} + 1 \right) \vee \sum_{k=0}^{\gamma} \frac{R_k}{k! \delta} \geq 2^{\gamma+1}, \quad (10)$$

we also have

$$\log M_2 (\delta, U_{\gamma+1,1}) \geq B_2 = C' \left( \frac{\gamma}{2} + 1 \right),$$
$$\log M_{\infty} (\delta, U_{\gamma+1,1}) \geq B_2.$$

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(iii) If the density function \( p(x) \) on \([-1, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then
\[
\log M_{2,p}(\delta, U_{\gamma+1,1}) \gtrsim \mathcal{B}_1(\delta),
\tag{12}
\]
under (\text{III}), we also have
\[
\log M_{2,p}(\delta, U_{\gamma+1,1}) \gtrsim \mathcal{B}_2.
\tag{13}
\]

**Remark.** When \( R_k = \mathcal{C} \) for \( k = 0, \ldots, \gamma \), \( \left( k + 1 \right) \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!} \asymp 1 \); when \( R_0 = \mathcal{C} \) and \( R_k \leq \mathcal{C}(k - 1)! \) for \( k = 1, \ldots, \gamma \), \( \left( k + 1 \right) \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!} \asymp \log (\gamma \vee 2) \); when \( R_k = \mathcal{C}k! \) for all \( k = 0, \ldots, \gamma \), \( \left( k + 1 \right) \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!} \asymp (\gamma \vee 1) \).

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

The lower bounds \( \mathcal{B}_1(\delta) \) and \( \mathcal{B}_2 \), as well as the upper bound \( \mathcal{B}_1(\delta) \) are original. The (less original) bound \( \mathcal{B}_2(\delta) \) generalizes the upper bound associated with the polynomial subspace in Kolmogorov and Tikhomirov (1959). It is worth pointing out that \( \mathcal{B}_2(\delta) \) holds for all \( \delta \in (0, 1) \) (not just \( \delta \) such that \( \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k!} < 0 \) but is far from being tight when \( \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k!} \geq 0 \). Obviously \( \mathcal{B}_1(\delta) \gtrsim \mathcal{B}_2(\delta) \). When it comes to deriving the upper bounds for the MISE under large enough \( R_k \), \( \mathcal{B}_1(\delta) \) will be very useful.

For the packing numbers of \( U_{\gamma+1,1} \), we also present two different lower bounds. In particular, \( \mathcal{B}_2 \) in (13) will be useful for deriving the minimax lower bounds for the MISE when \( R_k \) is relatively small, while \( \mathcal{B}_1(\delta) \) in (12) will be useful when \( R_k \) is relatively large. When deriving a lower bound for the *standard* \( U_{\gamma+1} = (U_{\gamma+1,1} + U_{\gamma+1,2}) \) under the assumption that \( R_k = \mathcal{C} \), Kolmogorov and Tikhomirov (1959) constructs a set of functions whose polynomial subspace is a singleton, and therefore the cardinality of this set only gives a lower bound for the *standard* Hölder subspace \( U_{\gamma+1,2} \). 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 \( \mathcal{B}_1(\delta) \), \( \mathcal{B}_1(\delta) \) and \( \mathcal{B}_2 \), we discard the argument in Kolmogorov and Tikhomirov (1959) and develop our own. The derivation of \( \mathcal{B}_2 \) is based on a constructive proof. To derive \( \mathcal{B}_1(\delta) \) and \( \mathcal{B}_2(\delta) \), we consider two classes (equivalent to \( U_{\gamma+1,1} \)), each in the form of a \((\gamma + 1)\)-dimensional polyhedron. The lower bound \( \mathcal{B}_1(\delta) \) is the more delicate part. In particular, for any \( f \in U_{\gamma+1,1} \), we write \( f(x) = \sum_{k=0}^{\gamma} \theta_k \phi_k(x) \), where \( (\phi_k)_{k=0}^{\gamma} \) are the Legendre polynomials. The key step is to derive sharp nonasymptotic lower bounds for the magnitude of \( \left( \tilde{\theta}_k \right)_{k=0}^{\gamma} \) in the worst case.

### 3.2 The generalized Hölder subspace, \( U_{\gamma+1,2} \)

**Lemma 3.2.** Let \( R^* = \left( \max_{k \in \{1, \ldots, \gamma+1\}} \frac{R_k}{k!} \right) \vee 1 \). We have
\[
\log N_{2,p}(\delta, U_{\gamma+1,2}) \leq \log N_{\infty}(\delta, U_{\gamma+1,2}) \gtrsim R^* \frac{1}{\gamma+1} \delta^{-\gamma+1}.
\]
We also have
\[
\log M_{\infty}(\delta, U_{\gamma+1,2}) \gtrsim \log M_{2}(\delta, U_{\gamma+1,2}) \gtrsim R^* \frac{1}{\gamma+1} \delta^{-\gamma+1}, \quad \text{if } R_0 \gtrsim 1, \delta \in (0, 1);
\]
\[
\log M_{\infty}(\delta, U_{\gamma+1,2}) \gtrsim \log M_{2}(\delta, U_{\gamma+1,2}) \gtrsim (R^* R_0)^{1/\gamma} \delta^{-\gamma+1}, \quad \text{if } R_0 \gtrsim 1, \delta \in (0, 1).
\]

If the density function \( p(x) \) on \([-1, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then
\[
\log M_{2,p}(\delta, U_{\gamma+1,2}) \gtrsim \frac{R^*}{\gamma+1} \delta^{-\gamma+1}, \quad \text{if } R_0 \gtrsim 1, \delta \in (0, 1);
\]
\[
\log M_{2,p}(\delta, U_{\gamma+1,2}) \gtrsim (R^* R_0)^{1/\gamma} \delta^{-\gamma+1}, \quad \text{if } R_0 \gtrsim 1, \delta \in (0, 1).
\]
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 $R_k \leq Ck!$ for all $k = 1, \ldots, \gamma + 1$, $R^\gamma \geq 1$ if $R_k \leq Ck!$ for all $k = 1, \ldots, \gamma + 1$, $R^\gamma \geq 1$; for example, taking $R_k \geq C(k!)^2$ for all $k = 1, \ldots, \gamma + 1$ yields $R^\gamma \geq \gamma$.

Given Lemmas 3.1 and 3.2, we have

$$\log N_2 (2\delta, \mathcal{U}_{\gamma+1}) \leq \log N_\infty (2\delta, \mathcal{U}_{\gamma+1}) \leq \begin{cases} \frac{B_1 (\delta)}{B_2 (\delta)} + R^\gamma \frac{1}{\gamma + 1} & \text{if } \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k!\delta} \geq 0 \\ \frac{B_1 (\delta)}{B_2 (\delta)} + R^\gamma \frac{1}{\gamma + 1} & \text{if } \min_{k \in \{0, \ldots, \gamma\}} \log \frac{4(\gamma+1)R_k}{k!\delta} < 0 \end{cases}$$

and

$$\log M_\infty (\delta, \mathcal{U}_{\gamma+1}) \geq \log M_2 (\delta, \mathcal{U}_{\gamma+1}) \geq \begin{cases} \max \left\{ \frac{B_1 (\delta)}{B_2 (\delta)} \cdot B_2^2, R^\gamma \frac{1}{\gamma + 1} \right\} & \text{if } R_0 \geq 1 \\ \max \left\{ \frac{B_1 (\delta)}{B_2 (\delta)} \cdot B_2, (R^\gamma R_0)^\frac{1}{\gamma + 1} \right\} & \text{if } R_0 \geq 1 \end{cases}$$

The results above are obvious. To cover $\mathcal{U}_{\gamma+1}$ within $2\delta$-precision, we find a smallest $\delta$-cover of $\mathcal{U}_{\gamma+1,1}$, $\{f_{1,1}, f_{1,2}, \ldots, f_{1,N_1}\}$, and a smallest $\delta$-cover of $\mathcal{U}_{\gamma+1,2}$, $\{f_{2,1}, f_{2,2}, \ldots, f_{2,N_2}\}$. Given that any $f \in \mathcal{U}_{\gamma+1}$ can be expressed by $f = f_1 + f_2$ for some $f_1 \in \mathcal{U}_{\gamma+1,1}$ and $f_2 \in \mathcal{U}_{\gamma+1,2}$, there exist some $f_{1,i}$ and $f_{2,i}$ from the covering sets such that

$$|f_1 + f_2 - f_{1,i} - f_{2,i}|_\infty \leq |f_1 - f_{1,i}|_\infty + |f_2 - f_{2,i}|_\infty \leq 2\delta,$$

$$|f_1 + f_2 - f_{1,i} - f_{2,i}|_\infty \leq |f_1 - f_{1,i}|_\infty + |f_2 - f_{2,i}|_\infty \leq 2\delta.$$

Consequently, we obtain

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

$$\log N_2 (2\delta, \mathcal{U}_{\gamma+1}) \leq \log N_2 (\delta, \mathcal{U}_{\gamma+1,1}) + \log N_2 (\delta, \mathcal{U}_{\gamma+1,2}).$$

In terms of $\log M_q (\delta, \mathcal{U}_{\gamma+1})$, we have

$$\log M_q (\delta, \mathcal{U}_{\gamma+1}) \geq \max \{ \log M_q (\delta, \mathcal{U}_{\gamma+1,1}), \log M_q (\delta, \mathcal{U}_{\gamma+1,2}) \}, \quad q \in \{2, \infty\}.$$

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 $R_k = C$) takes the form $\delta^\frac{1}{\gamma + 1}$. This result is inherited later in papers and textbooks including the more recent textbook on nonasymptotic statistics by Wainwright (2019). The derivation of Kolmogorov and Tikhomirov (1959) ignores the polynomial subspace and therefore the bound $\delta^\frac{1}{\gamma + 1}$ is not sharp when $\delta$ is not small enough.

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

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

$$\log N_2 (\delta, \mathcal{H}_{\gamma+1}) \asymp \left( R_{\gamma+1} \delta^{-1} \right)^\frac{1}{\gamma + 1}.$$  

If $R_{\gamma+1} \lesssim \gamma + 1$, we have

$$\log N_2 (\delta, \mathcal{H}_{\gamma+1}) \lesssim \delta^\frac{1}{\gamma + 1},$$

$$\log N_2 (\delta, \mathcal{H}_{\gamma+1}) \gtrsim \left( R_{\gamma+1} \delta^{-1} \right)^\frac{1}{\gamma + 1}. \quad (15) (16)$$
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 $\log N_{2,F}(\delta, \mathcal{H}_{\mathcal{Y} + 1})$.

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 $\log N_{2}(\delta, \mathcal{H}_{\mathcal{Y} + 1})$ in Wainwright (2019) from $(\gamma \vee 1) \delta^{-\frac{1}{\gamma + 1}}$ to $\delta^{-\frac{1}{\gamma + 1}}$; in particular, the upper and lower bounds in Wainwright (2019) (the last two inequalities on p.131) scale as $(\gamma \vee 1) \delta^{-\frac{1}{\gamma + 1}}$ and $\delta^{-\frac{1}{\gamma + 1}}$, respectively, while our upper and lower bounds in Lemma 3.3 have the same scaling $\delta^{-\frac{1}{\gamma + 1}}$. 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 Mitryagin (1961). 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 $(R_{\gamma + 1} \delta^{-1})^{-\frac{1}{\gamma + 1}}$. Note that $(R_{\gamma + 1} \delta^{-1})^{-\frac{1}{\gamma + 1}} \propto \delta^{-\frac{1}{\gamma + 1}}$ when $R_{\gamma + 1} \propto 1$. 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 $(R_{\gamma + 1} \delta^{-1})^{-\frac{1}{\gamma + 1}}$.

4 Minimax optimal rates and phase transition in standard cases

In this section, we illustrate the phase transition phenomenon associated with the most commonly seen smoothness classes in the literature.

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

$$\mathfrak{s}_{\gamma + 1} := \{f : [0, 1] \to \mathbb{R} | f is \ \gamma + 1 \ times \ differentiable \ a.e., \ \ f^{(\gamma)} is \ absolutely \ continuous, \ \ |f|_{\mathcal{H}} \leq R_{\gamma + 1} = \overline{C}\}$$

where $|.|_{\mathcal{H}}$ is the norm defined in (1).

When we write $\mathcal{U}_{\gamma + 1}$ or $\mathfrak{s}_{\gamma + 1}$ in this section, $\mathcal{U}_{\gamma + 1}$ refers to the standard Hölder class and $\mathfrak{s}_{\gamma + 1}$ refers to the standard Sobolev class. The regression model (1) is subject to the following assumption.

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

Remark. In the literature on minimax lower bounds, when both $\{X_i\}_{i=1}^{n}$ and $\{\varepsilon_i\}_{i=1}^{n}$ are stochastic, the normality assumption on $\{\varepsilon_i\}_{i=1}^{n}$ and the assumption of $\{\varepsilon_i\}_{i=1}^{n}$ being independent of $\{X_i\}_{i=1}^{n}$ are the most common for technical reasons; see, e.g., Yang and Barron (1999), Raskutti, et al. (2011). To relax the normality of $\{\varepsilon_i\}_{i=1}^{n}$, one could assume $\{X_i\}_{i=1}^{n}$ 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). Essentially,

\[\text{In the cases of Sobolev classes, we consider the interval } [0, 1] \text{ (instead of } [-1, 1]). \text{ This is purely for simplifying notations and also consistent with the literature.}\]
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. 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 minimax upper bounds, the normality of $\{\varepsilon_i\}_{i=1}^n$ 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 minimax 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 $\{\varepsilon_i\}_{i=1}^n$ and $\{X_i\}_{i=1}^n$ for the minimax lower and upper bounds.

For the minimax upper bounds, we consider the constrained nonparametric least squares estimator (CNLS)

$$\hat{f} \in \arg\min_{f \in F} \frac{1}{2n} \sum_{i=1}^n (y_i - \hat{f}(x_i))^2.$$  \hspace{1cm} (17)

The CNLS construction is commonly seen in the minimax optimality literature (e.g., Raskutti, et. al 2011). We consider either $F = U_{\gamma+1}$ or $F = S_{\gamma+1}$. 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 (17) via kernel functions. Let the matrix $K_{\gamma+1} \in \mathbb{R}^{n \times n}$ consist of entries $\frac{1}{n}K_{\gamma+1}(x_i, x_j)$, taking the form

$$K_{\gamma+1}(x_i, x_j) = 1 + (x_i \wedge x_j) \quad \text{for } \gamma = 0,$$

$$K_{\gamma+1}(x_i, x_j) = \sum_{k=0}^{\gamma} \frac{x_i^k x_j^k}{k! k!} + \int_0^1 \frac{(x_i - t)^{\gamma}}{\gamma!} \frac{(x_j - t)^{\gamma}}{\gamma!} dt \quad \text{for } \gamma > 0,$$

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

When $F = S_{\gamma+1}$ in (17), $\hat{f}$ can be written as

$$\hat{f} = \frac{1}{\sqrt{n}} \sum_{j=1}^n \pi_j K_{\gamma+1}(:, x_j)$$  \hspace{1cm} (20)

where

$$\pi := \{\pi_j\}_{j=1}^n = \arg\min_{\pi \in \mathbb{R}^n} \frac{1}{2n} \sum_{i=1}^n \left( y_i - \frac{1}{\sqrt{n}} \sum_{j=1}^n \pi_j K_{\gamma+1}(x_i, x_j) \right)^2$$  \hspace{1cm} (21)

$$\text{s.t. } \pi^T K_{\gamma+1} \pi \leq C^2.$$  \hspace{1cm} (22)
In particular, (22) comes from the representation $|\tilde{f}|^2_H = \pi^T \mathbb{K}_{\gamma+1} \pi$ when $F = \overline{S}_{\gamma+1}$ in (17) and $\tilde{f}$ takes the form $\tilde{f} = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \pi_j \mathcal{K}_{\gamma+1}(\cdot, x_j)$.

By the Lagrangian duality, solving (21) is equivalent to solving

$$\hat{\pi} = \arg \min_{\pi \in \mathbb{R}^n} \frac{1}{2n} \sum_{i=1}^{n} \left(y_i - \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \hat{\pi}_j \mathcal{K}_{\gamma+1}(x_i, x_j)\right)^2 + \lambda \pi^T \mathbb{K}_{\gamma+1} \pi$$

(23)

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

$$\hat{\pi} = (\mathbb{K}_{\gamma+1} + \lambda I_n)^{-1} \frac{Y}{\sqrt{n}}.$$  

(24)

where $Y = \{y_i\}_{i=1}^{n}$. The KRR estimators associated with $\overline{S}_{\gamma+1}$ are equivalent to the smoothing splines methods and also closely related to 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.

The proofs for the minimax optimality results in this section as well as Section 5 are based on techniques from empirical processes, machine learning theory, and information theory. The key to show the phase transition phenomenon using these techniques lies in sharp bounds for metric entropy established in Section 3. Even for the standard smoothness classes, the existing minimax optimality results are unable to reveal the phase transition phenomenon in finite samples because the classical metric entropy bound $\frac{1}{(\gamma+1)}$ applied into these techniques ignores the polynomial subspace.

4.1 Mean integrated squared error

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

$$A^\gamma (\gamma + 1) \lesssim \frac{n}{\sigma^2} \lesssim (\gamma + 1)^{2\gamma+3},$$

(25)

we have

$$\inf_{\tilde{f}} \sup_{f \in \overline{S}_{\gamma+1}} \mathbb{E} \left( |\tilde{f} - f|^2_{2,F} \right) \asymp \frac{\sigma^2 (\gamma + 1)}{n},$$

$$\inf_{\tilde{f}} \sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( |\tilde{f} - f|^2_{2,F} \right) \asymp \frac{\sigma^2 (\gamma + 1)}{n}.$$  

On the other hand, if

$$\frac{n}{\sigma^2} \asymp (\gamma + 1)^{2\gamma+3},$$

(26)

then we have

$$\inf_{\tilde{f}} \sup_{f \in \overline{S}_{\gamma+1}} \mathbb{E} \left( |\tilde{f} - f|^2_{2,F} \right) \asymp \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}},$$

$$\inf_{\tilde{f}} \sup_{f \in \mathcal{U}_{\gamma+1}} \mathbb{E} \left( |\tilde{f} - f|^2_{2,F} \right) \asymp \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}.$$
Moreover, $\frac{\sigma^2(\gamma+1)}{n} \lesssim \left(\frac{\sigma^2}{n}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \under \frac{n}{\sigma^2} \lesssim (\gamma+1)^{2\gamma+3}$ and $\frac{\sigma^2(\gamma+1)}{n} \lesssim \left(\frac{\sigma^2}{n}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \under \frac{n}{\sigma^2} \lesssim (\gamma+1)^{2\gamma+3}$.

The proof for Theorem 4.1 is given in Section B.1, which relies on the constructions behind the bound $B_3$ in Lemma 3.1, as well as the bounds in Lemmas 3.2-3.3.

The proof for Theorem 4.1 applies a version of the Fano’s inequality, which converts the problem into a multiple classification problem that tries to distinguish among $M$ members in the function class of interest. The set of $M$ members need be sufficiently large and is naturally connected with a packing set of the function class. As discussed earlier, the derivations of the classical lower bound $\sigma_2^{\gamma+1}$ for the packing number of $\mathcal{U}_{\gamma+1}$ or $\mathcal{F}_{\gamma+1}$ ignore the polynomial subspace. Using $M \asymp \delta^{\gamma+1}$ to derive the minimax lower bound (as in the existing literature) results in a rate $\left(\frac{\sigma^2}{n}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}$ that is not tight when $n$ is not large enough. More specifically, if $\frac{n}{\sigma^2} \lesssim (\gamma+1)^{2\gamma+3}$, the error rate $\frac{\sigma^2(\gamma+1)}{n}$ from distinguishing any pair of members in the packing set of the $\gamma$th degree polynomial subspace dominates the error rate $\left(\frac{\sigma^2}{n}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}$ from distinguishing any pair in the packing set of the nonparametric subspace; as a result, the sharp lower bound should take the form $\frac{\sigma^2(\gamma+1)}{n}$ instead of $\left(\frac{\sigma^2}{n}\right)^{\frac{2(\gamma+1)}{\gamma+1}+1}$. Once $\frac{n}{\sigma^2} \lesssim (\gamma+1)^{2\gamma+3}$, the dominant error rate switches from $\frac{\sigma^2(\gamma+1)}{n}$ to $\left(\frac{\sigma^2}{n}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}$.

For audience who is not familiar with the minimax lower bound literature, the “max” part can mislead one to conclude that this type of analysis is conservative as it deals with the worst-case scenario. In fact, the worst-case scenarios in many problems including those in this paper turn out to be “common” cases as the rates of the minimax lower bounds can be achieved by common nonparametric procedures. Take (17) with $\mathcal{F} = \mathcal{F}_{\gamma+1}$ and (20) as an example: when estimating a component from the $\gamma$th degree polynomial subspace of $\mathcal{F}_{\gamma+1}$, one should expect an error rate of $\frac{\sigma^2(\gamma+1)}{n}$, and in estimating a component from the nonparametric subspace of $\mathcal{F}_{\gamma+1}$, one should expect an error rate of $\left(\frac{\sigma^2}{n}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}$. In the following, we show the achievability results.

**Theorem 4.2** (upper bounds for standard Sobolev). Suppose Assumption 1 holds. Let $\hat{f}$ be (20) where $\hat{\pi}$ is given by (24) with $\lambda \asymp \left(\frac{\gamma+1}{\gamma+1} \vee \left(\frac{1}{n}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}\right)$. If

$$ (\gamma+1) \lesssim \frac{n}{\sigma^2} \lesssim (\gamma+1)^{2\gamma+3}, \tag{27} $$

we have

$$ \sup_{f \in \mathcal{F}_{\gamma+1}} \mathbb{E}\left(\left|\hat{f} - f\right|^2\right) \lesssim r_1^2 + \exp \{-cnr_1^2\} $$

where $r_1^2 = \frac{\sigma^2(\gamma+1)}{n}$. On the other hand, if

$$ \frac{n}{\sigma^2} \lesssim (\gamma+1)^{2\gamma+3}, \tag{28} $$

then we have

$$ \sup_{f \in \mathcal{F}_{\gamma+1}} \mathbb{E}\left(\left|\hat{f} - f\right|^2\right) \lesssim r_2^2 + \exp \{-cnr_2^2\}, $$

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Table 2: Minimax optimal MISE rates of the standard Sobolev and standard Hölder

|                | standard Sobolev | standard Hölder |
|----------------|------------------|----------------|
| MISE           | \(4^{\gamma}(\gamma + 1) \gtrless \frac{\sigma^2}{n} \gtrless \frac{n}{\sigma^2} \gtrless (\gamma + 1)^{2\gamma + 3} \times \left(\frac{\sigma^2}{n}\right)^{2\gamma + 3}\) | \(4^{\gamma}(\gamma + 1) \gtrless \frac{\sigma^2}{n} \gtrless (\gamma + 1)^{2\gamma + 3} \times \left(\frac{\sigma^2}{n}\right)^{2\gamma + 3}\) |

where \(r^2_1 = \left(\frac{\sigma^2}{n}\right)^{2\gamma + 3}\).

The proof for Theorem 4.2 is given in Section B.3.

Consider two smoothness parameters \(\gamma_1\) and \(\gamma_2\), such that \(\gamma_1 < \gamma_2\), where \(S_{\gamma_2+1} \subset S_{\gamma_1+1}\). If \(4^{\gamma_2}(\gamma_2 + 1) \gtrless n \gtrless (\gamma_1 + 1)^{2\gamma_1+3}\), Theorems 4.1 and 4.2 together imply that the slower minimax lower rate \(\frac{\sigma^2}{n}(\gamma + 1)^{2\gamma + 3}\) (with “sup” taken over \(f \in S_{\gamma_2+1}\)) is achieved by (20) constrained to be in the smaller class \(S_{\gamma_2+1}\), while the faster minimax lower rate \(\frac{\sigma^2}{n}(\gamma + 1)^{2\gamma + 3}\) (with “sup” taken over \(f \in S_{\gamma_1+1}\)) is achieved by (20) constrained to be in the larger class \(S_{\gamma_1+1}\). This phenomenon is opposite to the common wisdom based on classical asymptotic rates. As we have discussed in the introduction, the “counter-intuitiveness” can be explained with the tension between the approximation of \(f_1\) and the approximation of \(f_2\), where \(f = f_1 + f_2\), \(f_1\) lies in the polynomial subspace and \(f_2\) lies in the nonparametric subspace.

Like the standard Sobolev class \(S_{\gamma+1}\), we can show a similar achievability result for the standard Hölder class \(U_{\gamma+1}\).

**Theorem 4.3** (upper bounds for standard Hölder). Suppose Assumption 1 holds. Let \(\hat{f}\) be (17) with \(\mathcal{F} = U_{\gamma+1}\). If

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

we have

\[
\sup_{f \in U_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|^2 \right) \gtrless r^2_1 + \exp \left\{ -cnr^2_1 \right\}
\]

where \(r^2_1 = \frac{\sigma^2}{n} \gtrless (\gamma + 1)^{2\gamma + 3}\). On the other hand, if

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

then we have

\[
\sup_{f \in U_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|^2 \right) \gtrless r^2_2 + \exp \left\{ -cnr^2_2 \right\},
\]

where \(r^2_2 = \left(\frac{\sigma^2}{n}\right)^{2\gamma + 3}\).

The proof for Theorem 4.3 is given in Section B.4.

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. As we have discussed in Section 1.1,
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 SMSE.

**Corollary 4.1.** Suppose the conditions in Theorem 4.2 hold. Under (27), we have

\[ |\hat{f} - f|^2_n \precsim r_1^2 \text{ for any } f \in S_{\gamma+1}, \]

with probability at least \(1 - c_0 \exp\{-cnr_1^2\}\). Under (28), we have

\[ |\hat{f} - f|^2_n \precsim r_2^2 \text{ for any } f \in S_{\gamma+1}, \]

with probability at least \(1 - c_0 \exp\{-cnr_2^2\}\).

**Corollary 4.2.** Suppose the conditions in Theorem 4.3 hold. Under (29), we have

\[ |\hat{f} - f|^2_n \precsim r_1^2 \text{ for any } f \in U_{\gamma+1}, \]

with probability at least \(1 - c_0 \exp\{-cnr_1^2\}\). Under (30), we have

\[ |\hat{f} - f|^2_n \precsim r_2^2 \text{ for any } f \in U_{\gamma+1}, \]

with probability at least \(1 - c_0 \exp\{-cnr_2^2\}\).

### 4.3 Practical implications

The practical importance of our results in Section 4.2 lies in the growth rate of the sample size \(n\) (i.e., \((\gamma+1)^{2\gamma+3}\)) at which the minimax optimal rate transitions from \(\frac{\gamma+1}{n}\) to \(\left(\frac{1}{n}\right)^{\frac{2\gamma+3}{2\gamma+5}}\). Notably, our results suggest a way to select the degree of smoothness for the nonparametric approximation of \(f\) if a researcher knows a priori or from earlier experience that \(f\) is from a smoothness class up to the degree \(\gamma\). Then we can find \(\gamma^* \leq \gamma\) such that

\[ n \in \left[ (\gamma^* + 1)^{2\gamma^*+3}, (\gamma^* + 2)^{2\gamma^*+5} \right]. \]

**Case 1.** If

\[ n \in \left[ (\gamma^* + 1)^{2\gamma^*+3}, (\gamma^* + 2)^{2\gamma^*+3} \right], \]

choose the \((\gamma^* + 1)\)th degree smoothness in estimation, which would yield an error converging to zero at the rate \(n^{-\frac{2(\gamma^*+1)}{2\gamma^*+3}}\) as \(n \geq (\gamma^* + 1)^{2\gamma^*+3}\) and \(n^{-\frac{2(\gamma^*+2)}{2\gamma^*+5}} \geq \frac{\gamma^*+1}{n}\). The part \(“(\gamma^* + 2)^{2\gamma^*+3}”\) comes from the following fact: whenever \(n \geq (\gamma^* + 2)^{2\gamma^*+3}\), \(n^{-\frac{2(\gamma^*+1)}{2\gamma^*+3}} \leq \frac{\gamma^*+2}{n}\); therefore, choosing the \((\gamma^* + 1)\)th degree smoothness in estimation yields an error converging to zero at a rate faster than choosing the \((\gamma^* + 2)\)th degree smoothness. The latter has an error converging to zero at the rate \(n^{-\frac{2(\gamma^*+2)}{2\gamma^*+5}}\) as \(n \geq (\gamma^* + 2)^{2\gamma^*+3} \leq (\gamma^* + 2)^{2\gamma^*+5}\) and \(n^{-\frac{2(\gamma^*+2)}{2\gamma^*+5}} \geq n^{-\frac{2(\gamma^*+2)}{2}\gamma^*+5}}\).

**Case 2.** If
choose the \((\gamma^* + 2)\)th degree smoothness in estimation, which would yield an error converging to zero at the rate \(\frac{\gamma^*}{n}\) as \(n \leq (\gamma^* + 2)^{\gamma^* + 5}\) and \(\frac{\gamma^*^2}{n} \geq n^{-\frac{2(\gamma^* + 2)}{2\gamma^* + 3}}\). When \(n \geq (\gamma^* + 2)^{\gamma^* + 3}\), \(n^{-\frac{2(\gamma^* + 1)}{2\gamma^* + 3}} \geq \gamma^* + 2\); therefore, choosing the \((\gamma^* + 2)\)th degree smoothness in estimation yields an error converging to zero at a rate faster than choosing the \((\gamma^* + 1)\)th degree smoothness.

Because our achievability results in Theorem 4.2 concern \((20)\), our recommended rule above applies most naturally to the global nonparametric estimators such as KRR and smoothing splines. Nevertheless, our recommended rule could potentially be applied to local polynomials (see Section 7 for more discussions).

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 \(\mathcal{F}_1(\delta), \mathcal{B}_1(\delta)\) and \(\mathcal{B}_2\) 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 \(\mathcal{B}\) based on the kernel function \(K(\cdot, \cdot)\) associated with \(\mathcal{H}_{\gamma+1}\) in (7), where \(\hat{\pi}\) is given by (24) with \(\lambda \asymp \left(\frac{1}{2}\right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}\). 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

\[
\inf_{f} \sup_{f \in \mathcal{H}_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2, \mathcal{F}}^2 \right) \lesssim r^2,
\]

where \(r^2 = R_{\gamma+1}^{\frac{2(\gamma+1)}{2\gamma+1}} \left( \frac{a^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}\).

(ii) Let \(\hat{f}\) be (17) with \(\mathcal{F} = \mathcal{U}_{\gamma+1, 2}\). If \(R_0 \gtrsim 1\), we have

\[
\inf_{f} \sup_{f \in \mathcal{U}_{\gamma+1, 2}} \mathbb{E} \left( \left| \hat{f} - f \right|_{2, \mathcal{P}}^2 \right) \lesssim r^2,
\]

where \(r^2 = (R^*)^{\frac{2}{n(\gamma + 1)}} \left( \frac{a^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}}\) and \(R^* = \left( \max_{k \in \{1, \ldots, \gamma+1\}} \frac{R_k}{(k-1)!} \right) \vee 1\).

The proof for Theorem 5.1 is given in Section 3.5.

Theorems 4.1-4.3 suggest that the “blessing of smoothness” arises when \(n\) is large relative to the order of \((\gamma + 1)^{2\gamma+3}\), 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 \(\left( \frac{a^2}{n} \right)^{\frac{2\gamma+3}{2\gamma+1}}\), which decreases in \(\gamma\). Theorem 5.1 suggests that the “blessing of smoothness” may also arise when a smoothness
class is imposed with the restrictions that \( f^{(k)}(0) = 0 \) for all \( k \leq \gamma \). In these cases, there is no phase transition phenomenon in the minimax optimal MISE rates as the polynomial subspace is a singleton \( \{0\} \); if \( R_{\gamma+1}^{2\gamma+3} = 1 \) in the case of \( \mathcal{H}_{\gamma+1} \) and \( (R^*)^{2\gamma+3} = 1 \) in the case of \( \mathcal{U}_{\gamma+1,2} \), the minimax optimal rate for the MISE is \( \left( \frac{\sigma^2}{n} \right)^{\frac{2\gamma+3}{2\gamma+3}} \).

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 \( \left( \frac{\sigma^2}{n} \right)^{\frac{2\gamma+3}{2\gamma+3}} \) by \( R^{2\gamma+3} \) 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 exploited using the bounds in Section 3. We focus on the Hölder classes which reveal an interesting contrast coming from the polynomial subspace when \( R_k \) is increased from \( \overline{C} (k-1)! \) to \( \overline{C} k! \).

**Theorem 5.2.** Suppose Assumption 1 holds, \( R_0 = \overline{C} \) and \( R_k \) can be any value in \( [\overline{C}, \overline{C} (k-1)!] \) for \( k = 1, \ldots, \gamma + 1 \). Let \( R^* := 1 \vee \sum_{k=0}^{\gamma} \frac{R_k}{k!} \). If

\[
4^\gamma (\gamma + 1) R^{12} \lesssim \frac{n}{\sigma^2} \lesssim (\gamma + 1)^{2\gamma+3},
\]

we have

\[
\inf \sup \mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,\mathbb{P}} \right) \gtrsim \frac{\sigma^2 (\gamma + 1)}{n}.
\]

Let \( \hat{f} \) be (17) with \( \mathcal{F} = \mathcal{U}_{\gamma+1} \). If

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

we have

\[
\sup \mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,\mathbb{P}} \right) \gtrsim r_1^2 + \exp \left\{ -cnr_1^2 \right\}
\]

where \( r_1^2 = \frac{\sigma^2(\gamma+1)}{n} \), and \( r_1^2 \gtrsim \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \) under (32).

On the other hand, if

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

then we have

\[
\inf \sup \mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,\mathbb{P}} \right) \gtrsim r_2^2,
\]

\[
\sup \mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,\mathbb{P}} \right) \gtrsim r_2^2 + \exp \left\{ -cnr_2^2 \right\},
\]

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where \( r_2^2 = \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \), and \( r_2^2 \gtrsim \frac{\sigma^2(\gamma+1)}{n} \) under (34).

**Remark.** When \( R_0, R_1 = \overline{C} \) and \( R_k \leq \overline{C}(k-2)! \) for all \( k = 2, \ldots, \gamma+1 \), the part “4\( \gamma \) \((\gamma + 1) R_{12}^2 \lesssim \frac{n}{\sigma^2} \)” in (31) becomes 4\( \gamma \) \((\gamma + 1) \gtrsim \frac{n}{\sigma^2} \); when \( R_0 = \overline{C} \) and \( R_k = \overline{C}(k-1)! \) for all \( k = 1, \ldots, \gamma+1 \), the part “4\( \gamma \) \((\gamma + 1) R_{12}^2 \lesssim \frac{n}{\sigma^2} \)” in (31) becomes 4\( \gamma \) \((\gamma + 1) (\log (\gamma \vee 2))^2 \lesssim \frac{n}{\sigma^2} \). We can improve this condition to 4\( \gamma \) \((\gamma + 1) \log (\gamma \vee 2)^2 \lesssim \frac{n}{\sigma^2} \) using the bound \( B_1(\delta) \) 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 \( B_2 \) in Lemma 3.1, which gives “4\( \gamma \) \((\gamma + 1) R_{12}^2 \lesssim \frac{n}{\sigma^2} \)” in (31).

The proof for Theorem 5.2 is given in Section B.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 \( U_{\gamma+1, 1} \) under \( R_k = (k-1)! \). If this result is used to derive an upper bound for the MISE, we would have obtained (33) with \( r_0^2 = \frac{\sigma^2(\gamma+1)\log(\gamma+2)}{n} \). With the new bound \( B_1(\delta) \) developed in our Lemma 3.1, the upper bound for the MISE shown in Theorem 5.2 improves \( \frac{\sigma^2(\gamma+1)^2\log(\gamma+2)}{n} \) by a factor of \( (\gamma + 1) \log (\gamma \vee 2) \). For the lower bound on the covering number of \( U_{\gamma+1} \) under \( R_k = (k-1)! \), Zhu and Mirzaei (2021) simply takes the classical result \( \delta^{-\frac{1}{\gamma+1}} \). As discussed in Section 4.2, this result ignores the polynomial subspace and is unable to reveal the phase transition phenomenon when applied to derive the minimax lower bound on the MISE.

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

\[
4\gamma (\gamma + 1) \log (\gamma \vee 2) \lesssim \frac{n}{\sigma^2} \gtrsim ((\gamma + 1) \log (\gamma \vee 2))^{2\gamma+3},
\]

we have

\[
\inf_{f} \sup_{f' \in U_{\gamma+1}} \mathbb{E}\left( |\hat{f} - f|^2_{2,\mathcal{F}} \right) \gtrsim \frac{\sigma^2(\gamma + 1) \log (\gamma \vee 2)}{n}.
\]

Let \( \hat{f} \) be (17) with \( \mathcal{F} = U_{\gamma+1} \). If

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

we have

\[
\sup_{f \in U_{\gamma+1}} \mathbb{E}\left( |\hat{f} - f|^2_{2,\mathcal{F}} \right) \lesssim r_1^2 + \exp \{ -cnr_1^2 \}
\]

where \( r_1^2 = \frac{\sigma^2(\gamma+1)\log(\gamma+2)}{n} \), and \( r_1^2 \gtrsim \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{2(\gamma+1)+1}} \) under (36).

On the other hand, if

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

then we have

\[
\inf_{f} \sup_{f' \in U_{\gamma+1}} \mathbb{E}\left( |\hat{f} - f|^2_{2,\mathcal{F}} \right) \gtrsim r_2^2,
\]

\[
\sup_{f \in U_{\gamma+1}} \mathbb{E}\left( |\hat{f} - f|^2_{2,\mathcal{F}} \right) \gtrsim r_2^2 + \exp \{ -cnr_2^2 \},
\]

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Table 3: Minimax optimal MISE rates of the generalized $H_{γ+1}$ and $U_{r+1,2}$

|                      | $H_{γ+1}$                      | $U_{r+1,2}$                      |
|----------------------|--------------------------------|----------------------------------|
| MISE                 | $\asymp R_{γ+1}^2 \left( \frac{σ^2}{n} \right) \frac{(γ+1)^{2γ+3}}{\sqrt{n}}$ | $\asymp (R^*) \frac{(γ+1)^{2γ+3}}{\sqrt{n}}$ |

where $R^* = \left( \max_{k \in \{1,\ldots,γ+1\}} \frac{R_k}{|k-1|!} \right) \lor 1$.

Table 4: Minimax optimal MISE rates of non-standard $U_{r+1}$

|                      | $R_k = \mathcal{C}$, $R_k \in [\mathcal{C}, \mathcal{C}(k-1)!]$ $\forall k = 1,\ldots,γ + 1$ | $R_k = \mathcal{C}! \forall k = 0,\ldots,γ + 1$ |
|----------------------|-------------------------------------------------|-----------------------------------------------|
| MISE                 | $\frac{n_1}{σ^2} \asymp (γ + 1)^{2γ+3}$ | $\frac{n_1}{σ^2} \asymp \frac{(γ + 1)^{2γ+3}}{\sqrt{n}}$ | $\frac{n_2}{σ^2} \asymp \frac{(γ + 1)^{2γ+3}}{\sqrt{n}}$ |
| $\frac{n_1}{σ^2} \asymp \frac{σ^2(γ+1)}{n}$ | $\frac{n_2}{σ^2} \asymp \frac{σ^2(γ+1)(γ+2)}{n}$ | $\frac{n_2}{σ^2} \asymp \frac{σ^2(γ+1)(γ+2)}{n}$ |
| $\frac{n_1}{σ^2} \asymp \frac{σ^2(γ+1)(γ+2)}{n}$ | $\frac{n_2}{σ^2} \asymp \frac{σ^2(γ+1)(γ+2)}{n}$ | $\frac{n_2}{σ^2} \asymp \frac{σ^2(γ+1)(γ+2)}{n}$ |

where $n_1 := 4γ (γ + 1) R^2$, $R^1 := 1 \lor \sum_{k=0}^{γ} \frac{R_k}{k!}$, and $n_2 := 4γ (γ + 1) log (γ \lor 2)$.

where $r_2^2 = \left( \frac{σ^2}{n} \right) \frac{(γ+1)^{2γ+3}}{γ}$, and $r_2^2 \asymp \frac{σ^2(γ+1)(γ+2)}{n}$ under $\mathcal{C}$.

The proof for Theorem 5.3 is given in Section 13.7.

A couple of interesting facts are revealed by Theorems 5.2-5.3. First, the minimax optimal MISE rates are the same when $R_k$ takes any value in $[\mathcal{C}, \mathcal{C}(k-1)!]$. Second, as $R_k$ is increased from $\mathcal{C}(k-1)!$ to $\mathcal{C}k!$, the minimax optimal rate is increased from $\frac{σ^2(γ+1)}{n}$ to $\frac{σ^2(γ+1)(γ+2)}{n}$ when the sample size is not large enough such that the component in the polynomial subspace dominates. Once $n \asymp (γ + 1)^{2γ+3}$ in the case of $R_k = \mathcal{C}(k-1)!$, and $n \asymp ((γ + 1) log (γ \lor 2))^{2γ+3}$ in the case of $R_k = \mathcal{C}k!$, the optimal rate becomes $\left( \frac{σ^2}{n} \right) \frac{(γ+1)^{2γ+3}}{γ}$ as now the component in the nonparametric subspace dominates.

The terms $(k!)_{k=0}^γ$ in (5) play a more important role on the size of the polynomial subspace when $R_k$ becomes large enough, which is why $\overline{B}_1(δ)$ and $\overline{B}_2(δ)$ in Lemma 3.1 are very useful for deriving the minimax optimal rate for the MISE under large $R_k$. In particular, in dealing with the polynomial subspace, Theorems 4.1-4.3 rely on the bounds $\overline{B}_2(δ)$ and $B_3$ in Lemma 3.1, Theorem 5.2 relies on $\overline{B}_1(δ)$ and $B_2$, and Theorem 5.3 relies on $\overline{B}_1(δ)$ and $B_3(δ)$. The use of various bounds in Lemma 3.1 to control for the polynomial subcomponent suggests the intricacy of deriving the minimax optimal MISE rates when $n$ is not taken to infinity. For example, the intuition for “$(γ + 1) log (γ \lor 2)$” in Theorem 5.3 may be explained by that the metric entropy of $U_{γ+1,1}$ with respect to the $L^q$-norm ($q \in \{2, \infty\}$) under $R_k = \mathcal{C}k!$ behaves the same way as the metric entropy of an $l_1$-ball with respect to the $l_1$-norm. However, if this intuition is applied to the case where $R_0 = \mathcal{C}$ and $R_k = \mathcal{C}(k-1)!$, then we would expect to see “$(γ + 1) log (2 \lor log (γ \lor 2))$” in the minimax optimal rates. It turns out that the correct order is “$γ + 1$” (as in Theorem 5.2) rather than “$(γ + 1) log (2 \lor log (γ \lor 2))$”.

Tables 3 and 4 summarize the results in this section for easy reference.

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 $γ$ and the dimension $d$. We provide below some partial results about the higher dimensional generalized Hölder class.
Given any function $f \in \mathcal{U}_{d, \gamma+1}$, we have
\[
    f(x) = \sum_{k=0}^{\gamma} \sum_{p:P=k} \frac{x^p D^p f(0)}{k!} + \sum_{p:P=\gamma} \frac{x^p D^p f(z)}{\gamma!} - \sum_{p:P=\gamma} \frac{x^p D^p f(0)}{\gamma!}
\]
for some intermediate value $z$. Similar to Section 2, we have the following decomposition:
\[
    \mathcal{U}_{d, \gamma+1} = \mathcal{U}_{d, \gamma+1, 1} + \mathcal{U}_{d, \gamma+1, 2} := \{ f_1 + f_2 : f_1 \in \mathcal{U}_{d, \gamma+1, 1}, f_2 \in \mathcal{U}_{d, \gamma+1, 2} \}
\]
where
\[
    \mathcal{U}_{d, \gamma+1, 1} = \left\{ f = \sum_{k=0}^{\gamma} \sum_{p:P=k} x^p \theta_{(p,k)} : \{ \theta_{(p,k)} \}_{(p,k)} \in \mathcal{P}_\Gamma, x \in [-1,1]^d \right\}
\]
with the $\Gamma := \sum_{k=0}^{\gamma} \left( \frac{d + k - 1}{d - 1} \right)$-dimensional polyhedron
\[
\mathcal{P}_\Gamma = \left\{ \{ \theta_{(p,k)} \}_{(p,k)} \in \mathbb{R}^\Gamma : \text{for any given } k \in \{0,...,\gamma\}, \theta_{(p,k)} \in \left[ \frac{-R_k}{k!}, \frac{R_k}{k!} \right] \text{ for all } p \text{ with } P \leq k \right\}
\]
where $\theta = \{ \theta_{(p,k)} \}_{(p,k)}$ denotes the collection of $\theta_{(p,k)}$ over all $(p,k)$ configurations. And,
\[
    \mathcal{U}_{d, \gamma+1, 2} = \left\{ f \in \mathcal{U}_{d, \gamma+1} : D^p f(0) = 0 \text{ for all } p \text{ with } P \leq k, k = 0,...,\gamma \right\}.
\]

**Lemma 6.1.** Let $R^* = \left( \max_{k \in \{1,...,\gamma+1\}} \frac{D^*_{k-1} R_k}{(k-1)!} \right) \lor 1$. We have
\[
    \log N_{2,p} \left( \delta, \mathcal{U}_{d, \gamma+1, 2} \right) \leq \log N_{\infty} \left( \delta, \mathcal{U}_{d, \gamma+1, 2} \right) \sim d^d R^*_{\gamma+1} \delta^{\gamma+1},
\]
\[
    \log M_{2} \left( \delta, \mathcal{U}_{d, \gamma+1, 2} \right) \sim \log M_{2} \left( \delta, \mathcal{U}_{d, \gamma+1, 2} \right) \sim d^d R^*_{\gamma+1} \delta^{\gamma+1}.
\]

**Remark.** With Lemma 6.1, we can easily establish the minimax optimal MSE rate for $\mathcal{U}_{d, \gamma+1, 2}$, using arguments almost identical to those for Theorem 5.1.

The proof for Lemma 6.1 is given in Section D.1.

**Lemma 6.2.** If $\delta$ is small enough such that $\min_{k \in \{0,...,\gamma\}} \log \frac{4(\gamma+1) D^*_{k} R_k}{\delta k!} \geq 0$, 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 $D^*_k = \left( \frac{d + k - 1}{d - 1} \right)$; if $\delta$ is large enough such that $\min_{k \in \{0,...,\gamma\}} \log \frac{4(\gamma+1) D^*_{k} R_k}{\delta k!} < 0$, we have
\[
    \log N_{2,p} \left( \delta, \mathcal{U}_{d, \gamma+1, 1} \right) \leq \log N_{\infty} \left( \delta, \mathcal{U}_{d, \gamma+1, 1} \right) \sim \left( \sum_{k=0}^{\gamma} D^*_k \right) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} D^*_k \log R_k.
\]

**Remark.** The bound (40) 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 $\sum_{k=1}^{\gamma} d^k \times d^\gamma$. 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 $\frac{\sigma^2}{n} \sum_{k=0}^{\gamma} D_k^*$ 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

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

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 $\log M_2 (\delta, \mathcal{U}_{\gamma+1,1})$. However, this extension is very intensive. Arguments similar to those for $B_2$ in Lemma 3.1 will not lead to a useful bound for $\mathcal{U}_{\gamma+1,1}$, despite the lack of lower bounds, we can still gain some insights from Lemma 6.2, as it implies

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

where $r^2 = \frac{\sigma^2}{n} \sum_{k=0}^{\gamma} D_k^*$ and $\hat{f}$ is the estimator in (11) with $\mathcal{F} = \mathcal{U}_{\gamma+1,1}$. 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 $\mathcal{U}_{\gamma+1,1}$ has $D_k^*$ distinct $k$th partial derivatives. Therefore, there is a good reason to think the rate $r^2$ is minimax optimal.

Suppose $R_k = 1$ for all $k = 0, \ldots, \gamma + 1$. If $d$ is small relative to $\gamma$ and $n$, Lemma 6.1 implies that the minimax optimal rate concerning $\mathcal{U}_{\gamma+1,2}$ is roughly $(\frac{\sigma^2}{n})^{\frac{2\gamma + 2 + d}{2\gamma + 2 + d}}$, the classical rate for $\mathcal{U}_{\gamma+1}$ derived under the regime where $\gamma$ and $d$ are finite but $n \to \infty$. Observe that $\frac{\sigma^2}{n} \sum_{k=0}^{\gamma} D_k^* \lesssim \left( \frac{\sigma^2}{n} \right)^{\frac{2\gamma + 2 + d}{2\gamma + 2 + d}}$ whenever $\frac{\sigma^2}{n} \lesssim (\sum_{k=0}^{\gamma} D_k^*)^{\frac{2\gamma + 2 + d}{d}}$, and $\frac{\sigma^2}{n} \sum_{k=0}^{\gamma} D_k^* \lesssim \left( \frac{\sigma^2}{n} \right)^{\frac{2\gamma + 2 + d}{2\gamma + 2 + d}}$ whenever $\frac{\sigma^2}{n} \lesssim (\sum_{k=0}^{\gamma} D_k^*)^{\frac{2\gamma + 2 + d}{d}}$. Therefore, the classical asymptotic minimax rate $\left( \frac{\sigma^2}{n} \right)^{\frac{2\gamma + 2 + d}{2\gamma + 2 + d}}$ could be an underestimate of the MISE in finite sample settings where $n$ is not large enough.

7 Conclusion and future directions

When the regression function belongs to a smooth class consisting of univariate functions with derivatives up to the $(\gamma + 1)$th order bounded in absolute values by a common constant everywhere or a.e., it is well known that the minimax optimal rate of convergence in MISE is $(\frac{1}{n})^{\frac{2\gamma + 2 + d}{2\gamma + 2 + d}}$ when $\gamma$ is finite and the sample size $n \to \infty$. This paper shows that the MISE increases in $\gamma$ when the sample size $n$ is small relative to the order of $(\gamma + 1)^{2\gamma + 3}$ (e.g., $(\gamma + 1)^{2\gamma + 3} = 262144$ when $\gamma = 3$), and decreases in $\gamma$ when $n$ is large relative to the order of $(\gamma + 1)^{2\gamma + 3}$. In particular, this phase transition property is shown to be achieved by common nonparametric procedures. In data sets with fewer than hundreds of thousands observations, our results suggest that one should not exploit beyond the third or fourth degree of smoothness.

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 the most commonly seen smoothness classes and also several non-standard smoothness classes in the nonasymptotic setting where \( n \) is not taken to infinity (although our results do hold when \( n \) tends to infinity).

In the introduction, we have discussed the connections between our theoretical results and the empirical findings in Gelman and Imbens (2019). Based on their empirical evidence, Gelman and Imbens (2019) recommend researchers to avoid using high order polynomials but use local linear or local quadratic polynomials or other smooth functions in RDD analysis. We have discussed in Section 1.1 how these recommendations largely coincide with our recommendation based on (2).

To some extent, our results provide a theoretical basis for the widely adopted practical recommendations given in Gelman and Imbens (2019). The phrase “to some extent” means the following.

Gelman and Imbens (2019) concern the MSE of the high order polynomial implementation at a point. The minimax optimality of pointwise MSE and the global MISE (concerning an entire function) would involve different proofs, and the proof for the pointwise problem is typically simpler. As we point out in footnote 3, it is well known that the minimax optimal MISE rate coincides with the minimax optimal pointwise MSE rate in the regime where \( \gamma \) is finite and \( n \to \infty \) (see Tsybakov, 2009). We do not expect that the minimax optimal rates would differ between MISE and pointwise MSE in the regime of finite \( \gamma \) and finite \( n \), simply because the trade-off between a polynomial subspace and an infinite-dimensional nonparametric subspace exists whether the interest is the MISE or pointwise MSE. Based on this fact, we make a conjecture about estimating functions (in the smoothness classes) at a point: the minimax optimal rate for MSE at a point exhibits the same phase transition phenomenon.

Simulation evidence in the literature (as discussed in Section 1.1) indicates that a phase transition phenomenon is also likely to exist in local smoothing methods such as kernel density estimators and local polynomials. For this problem, we could consider \([1]\) where \( X_i = \frac{i}{n} \) for \( i = 1, \ldots, n \) and \( \{\varepsilon_i\}_{i=1}^n \) 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 \( \{\varepsilon_i\}_{i=1}^n \) (see the remark following Assumption 1 in Section 4). Like how we establish the results in this paper, we would first show that the minimax lower bound under the different setup exhibits a phase transition property, and then show that this property is achieved by a local smoothing method. 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 minimax upper bound \( \left( \frac{1}{n} \right)^{\frac{2\gamma+3}{2\gamma+2}} \). This eigenvalue condition in Tsybakov (2009) requires a large enough \( n \) and a sufficient condition given in Tsybakov (2009) is that \( n \to \infty \).

The aforementioned future directions continue the theme of phase transitions in optimal estimation. A different direction would be to investigate whether a phase transition property exists in optimal inference problems in economics (e.g., Armstrong and Kolesár, 2018; Chen et. al, 2021). Optimal inference theory concerns criteria that are different from MISE or pointwise MSE studied in the estimation theory. Therefore, the phase transition property could differ between optimal inference theory and optimal estimation theory.
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 $k \in \{0,\ldots,\gamma\}$ only. We first derive an upper bound for $N_{\infty}(\delta, U_{\gamma+1,1})$. Because the weighted $L^2(P)$-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 $\|\cdot\|_2$, we have

$$N_2(P, \delta, U_{\gamma+1,1}) \leq N_{\infty}(\delta, U_{\gamma+1,1}).$$

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

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

As a consequence, we have

$$\log N_1(\delta, \mathcal{P}_\gamma) \leq \sum_{k=0}^\gamma \log \frac{4R_k}{a_k k! \delta} = -\sum_{k=0}^\gamma \log a_k + \sum_{k=0}^\gamma \log \frac{4R_k}{k! \delta}. \quad (41)$$

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

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

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,

$$\log N_{2,p}(\delta, U_{\gamma+1,1}) \leq \log N_{\infty}(\delta, U_{\gamma+1,1}) \leq \sum_{k=0}^{\gamma} \log \frac{4(\gamma + 1) R_k}{k!\delta}. \quad (42)$$

If $\delta$ is large enough such that $\min_{k \in \{0, ..., \gamma\}} \log \frac{4(k+1)R_k}{k!\delta} < 0$, we can evoke the counting argument in Kolmogorov and Tikhomirov (1959) to obtain

$$\log N_{2,p}(\delta, U_{\gamma+1,1}) \leq \log N_{\infty}(\delta, U_{\gamma+1,1}) \leq \left(\frac{\gamma}{2} + 1\right) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} \log R_k. \quad (43)$$

**The lower bound.** We first derive a lower bound for $M_2(\delta, U_{\gamma+1,1})$. Let $(\phi_k)_{k=0}^{\gamma}$ be the Legendre polynomials on $[-1, 1]$. For any function $f \in U_{\gamma+1,1}$, we can write

$$f(x) = \sum_{k=0}^{\gamma} \tilde{\theta}_k \phi_k(x) \quad (44)$$

such that

$$\tilde{\theta}_k = \frac{(2k+1)}{2} \int_{-1}^{1} f(x) \phi_k(x) dx. \quad (45)$$

In Lemma A.1 of Section A.2, we show that

$$\tilde{\theta}_k = \left( k + \frac{1}{2} \right) \sum_{m=0}^{\lfloor \gamma/2 \rfloor} \frac{f(k+2m)(0)}{2^{k+2m}m! \left(\frac{1}{2}\right)^{k+m+1}}$$

where $(a)_k = a(a+1) \cdots (a+k-1)$ is known as the Pochhammer symbol. Recall $|f^{(k)}(0)| \leq R_k$ for $k = 0, ..., \gamma$ and $f^{(k)}(0) = 0$ for $k > \gamma$. We can rewrite

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

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

$$\mathcal{P}_\gamma^L = \left\{ \left( \tilde{\theta}_k \right)_{k=0}^{\gamma} \in \mathbb{R}^{\gamma+1} : \tilde{\theta}_k \in [-R_k, R_k] \right\}$$

where $\overline{R}_k := \sum_{m=0}^{\lfloor \gamma/2 \rfloor} b_{k,m} R_{k+2m}$ and $b_{k,m} = \frac{k+1}{2^{k+2m}m! \left(\frac{1}{2}\right)^{k+m+1}}$. If we can bound $\overline{R}_k$ from below by $\overline{R}_k$, then we have

$$\mathcal{P}_\gamma^L \supseteq \mathcal{P}_\gamma^L = \left\{ \left( \tilde{\theta}_k \right)_{k=0}^{\gamma} \in \mathbb{R}^{\gamma+1} : \tilde{\theta}_k \in [-\overline{R}_k, \overline{R}_k] \right\}. \quad (46)$$

Let us derive $\overline{R}_k$. Because $f^{(l)}(0) = 0$ for $l > \gamma$,

$$\frac{f^{(k+2m)}(0)}{2^{k+2m}m! \left(\frac{1}{2}\right)^{k+m+1}} = 0 \quad \text{if } k + 2m > \gamma.$$ 

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
\[
\left( \frac{1}{2} \right)^{k+m+1} = \frac{1 \cdot 1 + 2 \cdot 2 \cdot \ldots \cdot 1 + 2(k+m)}{2 \cdot 2 \cdot \ldots \cdot 2} \leq \frac{2 \cdot 2 \cdot \ldots \cdot 2 + 2(k+m)}{2} = (k+m+1)!
\]

where \( k + m + 1 \leq \frac{3\gamma}{2} + 1 \). Hence, we have

\[
m! \left( \frac{1}{2} \right)^{k+m+1} \leq m!(k+m+1)! \leq 1 \cdot \left( \frac{3\gamma}{2} + 1 \right)^{\gamma} \leq (3\gamma)^{\gamma}.
\]

As a result, we have

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

Note that for any \( f, g \in U_{\gamma+1,1} \) where \( f(x) = \sum_{k=0}^{\gamma} \tilde{\theta}_k \phi_k(x) \) 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 (46) and (48), to construct a packing set of \( U_{\gamma+1,1} \) 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

\[
\log M_2 (\delta, U_{\gamma+1,1}) \geq \sum_{k=0}^{\gamma} \log \sqrt{\frac{2(\gamma+1) R_k}{2k+1}}.
\]

Bounds (50) and (47) together give

\[
\log M_2 (\delta, U_{\gamma+1,1}) \geq \sum_{k=0}^{\gamma} \log (9^{-\gamma} 2^{\gamma}) + \sum_{k=0}^{\gamma} \log C \sum_{m=0}^{\gamma/2} \frac{R_{k+2m}}{\delta} =: B_1 (\delta)
\]

for some positive universal constant \( C \).

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

\footnote{In fact, we can make the same statement about an exactly \( \delta \)-separated set, i.e., \( = \delta^2 \) rather than \( > \delta^2 \) in (49).}
Let $\tilde{k} \in \arg \max_{k \in \{0, \ldots, \gamma\}} \frac{R_k}{k!}$. We consider a $3\delta \left( \tilde{k} + 1 \right) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!}$ grid of points on $\left[ -\frac{R_{\tilde{k}}}{k!}, \frac{R_{\tilde{k}}}{k!} \right]$ (that is, each point is $3\delta \left( \tilde{k} + 1 \right) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!}$ apart) and denote the collection of these points by $(\theta^*_{i,k})_{i=1}^{M_0}$ where $M_0 = \frac{cR_{\tilde{k}}}{k! \delta (k+1) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!}}$.

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

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

(52)

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

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

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

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

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,

$$\log M_2 (\delta, U_{\gamma+1,1}) \gtrsim \gamma + 1 =: B_2.$$  

Note that the lower bound $\log M_2 (\delta, U_{\gamma+1,1}) \gtrsim \gamma + 1$ holds for all $\delta$ such that $\frac{cR_{\tilde{k}}}{k! \delta (k+1) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!}} \geq 2^{\gamma+1}$ and $3\delta \left( \tilde{k} + 1 \right) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!} \leq 2^{\frac{R_{\tilde{k}}}{k!}}$.

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

$$\log M_\infty (\delta, U_{\gamma+1,1}) \gtrsim \gamma + 1$$

for all $\delta$ such that $\frac{R_{\tilde{k}}}{k! \delta (k+1) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!}} \gtrsim 2^{\gamma+1}$ and $\delta \left( \tilde{k} + 1 \right) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!} \gtrsim \frac{R_{\tilde{k}}}{k!}$ and also

$$\log M_\infty (\delta, U_{\gamma+1,1}) \gtrsim B_1 (\delta).$$

---

11The 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 $b = 1$.

12Note that these two conditions can be reduced to $\frac{R_{\tilde{k}}}{k! \delta (k+1) \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!}} \gtrsim 2^{\gamma+1}$.  

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30
Finally, if the density function \( p(x) \) on \([-1, 1]\) is bounded away from zero, i.e., \( p(x) \geq c > 0 \), then
\[
\log M_{2,p}(\delta, \mathcal{U}_{\gamma+1,1}) \asymp \log M_{2}(\delta, \mathcal{U}_{\gamma+1,1})
\]
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 \( f \in \mathcal{U}_{\gamma+1,1} [-1, 1] \), we have \( f(x) = \sum_{k=0}^{\gamma} \theta_k \phi_k(x) \) such that
\[
\tilde{\theta}_k = \left( k + \frac{1}{2} \right) \sum_{m=0}^{[\gamma/2]} \frac{f(k+2m)(0)}{2^{2k+m}m! \left( \frac{1}{2} \right)^{k+m+1}}
\]
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
\[
x^k = \frac{1}{2^k} \sum_{m=0}^{\lfloor k/2 \rfloor} \frac{k - 2m + \frac{1}{2} \phi_{k-2m}(x)}{m! \left( \frac{1}{2} \right)^{k-m+1}}.
\]

(53)

First, let us consider the case where \( \gamma \) is odd. Applying (53) gives
\[
f(x) = \sum_{k=0}^{\gamma} \frac{f(k)(0)}{2^k} \sum_{m=0}^{\lfloor k/2 \rfloor} \frac{k - 2m + \frac{1}{2} \phi_{k-2m}(x)}{m! \left( \frac{1}{2} \right)^{k-m+1}}
\]
\[
= \sum_{k=0}^{\gamma/2} \frac{f(2k)(0)}{2^k} \sum_{m=0}^{k} \frac{2k - 2m + \frac{1}{2} \phi_{2k-2m}(x)}{m! \left( \frac{1}{2} \right)^{2k-m+1}}
\]
\[
+ \sum_{k=0}^{\gamma/2} \frac{f(2k+1)(0)}{2^{2k+1}} \sum_{m=0}^{k} \frac{2k - 2m + \frac{3}{2} \phi_{2k-2m+1}(x)}{m! \left( \frac{1}{2} \right)^{2k-m+2}}
\]
\[
= \sum_{m=0}^{\gamma/2} \sum_{l=0}^{\gamma/2} \frac{2l + \frac{1}{2} \phi_{2l}(x)}{m! \left( \frac{1}{2} \right)^{2l+m+1}}
\]
\[
= \sum_{m=0}^{\gamma/2} \sum_{l=0}^{\gamma/2} \frac{2l + \frac{3}{2} \phi_{2l+1}(x)}{m! \left( \frac{1}{2} \right)^{2l+2m+1}}
\]
\[
= \sum_{l=0}^{\gamma/2} \sum_{m=0}^{\gamma/2} \frac{2l + \frac{3}{2} \phi_{2l+1}(x)}{m! \left( \frac{1}{2} \right)^{2l+2m+1}}
\]

(54)
which gives the claim in Lemma A.1.

For the case of even \(\gamma\), note that the term in (54) takes the form

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

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

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

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

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

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

(55)

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

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

(56)

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 \( \left( \max_{k \in \{1, \ldots, \gamma + 1\}} \frac{R_k}{(k-1)!} \right) \lor 1 =: R^* \). Consider \(|\Delta| \leq (R^{* - 1} \delta)^{\frac{1}{\gamma + 1}}\) and \(\delta_k = R^* \frac{k^{\gamma}}{k!} \delta^{1 - \frac{i}{\gamma + 1}}\) for \(k = 0, \ldots, \gamma\). Then,

\[
|f(x + \Delta) - g(x - \Delta)| \leq \delta \sum_{k=0}^{\gamma} \left( R^* \frac{k^{\gamma}}{k!} \frac{1}{k!} \right) + 2R^* |\Delta|^{\gamma + 1} \leq \delta \sum_{k=0}^{\gamma} \frac{1}{k!} + 2\delta \leq 5\delta. \tag{57}
\]

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

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

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

It suffices to cover the \(k\)th derivatives of functions in \(\mathcal{U}_{\gamma + 1, 2}\) within \(\delta_k\) precision at each grid point. Then by (57), we obtain a \(5\delta\)-cover of \(\mathcal{U}_{\gamma + 1, 2}\). Following the arguments in Kolmogorov and Tikhomirov (1959), bounding \(N_\infty(\delta, \mathcal{U}_{\gamma + 1, 2})\) can be reduced to bounding the cardinality of

\[
\Lambda = \left\{ \left( \left[ \frac{f^{(k)}(x_i)}{\delta_k} \right]^{-\gamma} \right), -s \leq i \leq s, 0 \leq k \leq \gamma \mid f \in \mathcal{U}_{\gamma + 1, 2} \right\}
\]

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

Taking (56) 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,

\[
\begin{align*}
&\left| f^{(i)}(x_i) - \sum_{k=0}^{\gamma-i} \frac{\Delta_k}{k!} B_{i+k,i-1} \right| \\
\leq &\left| f^{(i)}(x_i) - \sum_{k=0}^{\gamma-i} \frac{\Delta_k}{k!} f^{(i+k)}(x_{i-1}) \right| + \left| \sum_{k=0}^{\gamma-i} \frac{\Delta_k}{k!} \left( f^{(i+k)}(x_{i-1}) - B_{i+k,i-1} \right) \right| \\
\leq &\frac{|\Delta|^{\gamma+1-i}}{(\gamma-i)!} R_{\gamma+1-i} + \sum_{k=0}^{\gamma-i} \frac{|\Delta_k|}{k!} \delta_{i+k} \\
\leq &\left( R^{* - 1} \delta \right)^{1 - \frac{i}{\gamma + 1}} R^*_{\gamma+1-i} + \sum_{k=0}^{\gamma-i} \frac{1}{k!} \left( R^{* - 1} \delta \right)^{1 - \frac{i}{\gamma + 1}} R^* \delta^{1 - \frac{i}{\gamma + 1}} \\
\leq & R^* \delta^{1 - \frac{i}{\gamma + 1}} + R^* \delta^{1 - \frac{i}{\gamma + 1}} \sum_{k=0}^{\gamma-i} \frac{1}{k!} \leq 4\delta_i.
\end{align*}
\]
Hence, the number of possible values of \( \left( \frac{f_k(x_1)}{\delta_k} \right)^\gamma \) is at most 4 given the value of \( \left( \frac{f_k(x_{i+1})}{\delta_k} \right)^\gamma \). Consequently, we have

\[
\text{card} (\Lambda) \lesssim 4^{2s} \lesssim 16(R^{-1}\delta)^{-1} \frac{1}{\gamma+1}
\]

which implies

\[
\log N_2(\delta, U_{\gamma+1,2}) \leq \log N_\infty(\delta, U_{\gamma+1,2}) \lesssim R^{1+1}\delta^{-\gamma-1}.
\] (58)

**The lower bound.** In the derivation of the lower bound, Kolmogorov and Tikhomirov (1959) considers a \( \delta^{-1} \) -grid of points

\[
\cdots < a_1 < \overline{a}_1 < a_2 < \overline{a}_2 < \cdots < a_{2s} < \overline{a}_{2s}
\]

where \( \overline{a}_i - a_i = \delta^{-1} \) and \( s \geq \delta^{-1+1} \). Recall that we have previously considered a \( (R^{-1}\delta)^{-1} \) -grid of points in \([-1, 1]\) in the derivation of the upper bound for \( \log N_\infty(\delta, U_{\gamma+1,2}) \). To obtain a lower bound for \( \log M_\infty(\delta, U_{\gamma+1,2}) \) with the same scaling as our upper bound, the key modification we need is to replace the \( \overline{a}_i - a_i = \delta^{-1} \) with \( \overline{a}_i - a_i = (R^{-1}\delta)^{-1} \) and \( s \geq \delta^{-1+1} \) with \( s \sim R^1\delta^{-\gamma-1} \). The rest of the arguments are similar to those in Kolmogorov and Tikhomirov (1959). In particular, let us consider

\[
f_\lambda(x) = R^s \sum_{i=1}^{2s} \lambda_i (\overline{a}_i - a_i)^{\gamma+1} h_0 \left( \frac{x - \overline{a}_i}{\overline{a}_i - a_i} \right)
\]

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 \( U_{\gamma+1,2} \); (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 \( h_0(x) = \begin{cases} 0 & \text{if } x \notin (0, 1) \\ \left( -\frac{1}{2} e^{\frac{1}{1-x}} - 1 \right) & \text{if } x \in (0, 1) \end{cases} \) for some properly chosen constant \( b \) that can only depend on \( R_0 \). Note that the functions \( h(x) := R^s (\overline{a}_i - a_i)^{\gamma+1} h_0 \left( \frac{x - \overline{a}_i}{\overline{a}_i - a_i} \right) \) and also \( f_\lambda(x) \) belong to \( U_{\gamma+1,2} \) if \( \delta \in (0, 1) \). For any distinct \( \lambda, \lambda' \in \{0, 1\}^{2s} \), we have

\[
|f_\lambda - f_{\lambda'}|_\infty = R^s (\overline{a}_i - a_i)^{\gamma+1} h_0 \left( \frac{1}{2} \right) = R_0 \delta.
\]

If \( R_0 \gtrsim 1 \), then \( R_0 \delta \gtrsim \delta \) and

\[
\log M_\infty(\delta, U_{\gamma+1,2}) \gtrsim R^1 \delta^{-\gamma-1}.
\]

If \( R_0 \lesssim 1 \), then we obtain

\[
\log M_\infty(R_0 \delta, U_{\gamma+1,2}) \gtrsim R^1 \delta^{-\gamma-1}
\]

which implies that

\[
\log M_\infty(\delta, U_{\gamma+1,2}) \gtrsim R^1 \left( \frac{\delta}{R_0} \right)^{-\gamma-1}.
\]

Standard argument in the literature based on the Vasharmov-Gilbert Lemma further gives

\[
\log M_2(\delta, U_{\gamma+1,2}) \gtrsim \begin{cases} R^1 \delta^{-\gamma-1} \delta^{-\gamma+1} & \text{if } R_0 \gtrsim 1 \\ (R^1 R_0)^{1+1} \delta^{-\gamma+1} & \text{if } R_0 \lesssim 1 \end{cases}
\] (59)

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 $U_{\gamma+1,1}$ and $U_{\gamma+1,2}$ on $[\gamma + 1]$. 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 $\log N_2 (\delta, H_{\gamma+1})$ in Wainwright (2019) from $(\gamma \vee 1) \bigwedge \frac{1}{\gamma+1}$ 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 $R_{\gamma+1} \asymp \gamma + 1$, we consider two different truncations, one giving the upper bound $\delta^{-\frac{1}{\gamma+1}}$ and the other giving the lower bound $(R_{\gamma+1} \delta^{-1})^{-\frac{1}{\gamma+1}}$. Note that $(R_{\gamma+1} \delta^{-1})^{-\frac{1}{\gamma+1}} \asymp \delta^{-\frac{1}{\gamma+1}}$ when $R_{\gamma+1} \asymp 1$. For the case of $R_{\gamma+1} \asymp \gamma + 1$, we use only one truncation to show that both the upper bound and the lower bound scale as $(R_{\gamma+1} \delta^{-1})^{-\frac{1}{\gamma+1}}$.

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

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

Let us introduce the $M$-dimensional ellipsoid

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

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. \(B_2 M (w_{\gamma+1} R_{\gamma+1} \delta) \subseteq E_{\gamma+1};\)  
2. \(\mu_{M-1} = (c (M - 1))^{-2(\gamma+1)} > w_{\gamma+1}^2 \delta^2 \text{ and } \mu_{M-1} = (c (M + 1))^{-2(\gamma+1)} < w_{\gamma+1}^2 \delta^2, \text{ which yield}\)

$$M \asymp (w_{\gamma+1} \delta)^{-\frac{1}{\gamma+1}}.$$ \hspace{1cm} (61)

Note that (60), (61), and the fact $E_{\gamma+1} \supseteq E_{\gamma+1}$ give

$$\log N_2 (\delta, E_{\gamma+1}) \geq \log N_2 (\delta, E_{\gamma+1}) \supseteq M \log (w_{\gamma+1} R_{\gamma+1}) \asymp (w_{\gamma+1} \delta)^{-\frac{1}{\gamma+1}} \log (w_{\gamma+1} R_{\gamma+1}).$$ \hspace{1cm} (62)

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
\[
N_2 (\delta, \mathcal{E}_{\gamma+1} ) \leq \frac{\text{vol} (\frac{2}{\delta} \mathcal{E}_{\gamma+1} + B^M_2 (1))}{\text{vol} (B^M_2 (1))}
\]
\[
\leq \left( \frac{2}{\delta} \right)^M \frac{\text{vol} (\mathcal{E}_{\gamma+1} + B^M_2 (\frac{\delta}{2}))}{\text{vol} (B^M_2 (1))}
\]
\[
\leq \left( \frac{2}{\delta} \right)^M \max \left\{ \frac{\text{vol} (2 \mathcal{E}_{\gamma+1})}{\text{vol} (B^M_2 (1))} , \frac{\text{vol} (2B^M_2 (\frac{\delta}{2}))}{\text{vol} (B^M_2 (1))} \right\}
\]
\[
\leq \max \left\{ \left( \frac{4R_{\gamma+1}}{\delta} \right)^M \prod_{m=1}^M \sqrt{\mu_m}, 2^M \right\}
\]  
(63)

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

\[
\log \left[ \left( \frac{4R_{\gamma+1}}{\delta} \right)^M \prod_{m=1}^M \sqrt{\mu_m} \right] \leq M (\log (4R_{\gamma+1}) + \gamma + 1) +
\]
\[
M \left( \log \frac{1}{\delta} - (\gamma + 1) \log (cM) \right)
\]
\[
\leq M (\log (4R_{\gamma+1}) + \gamma + 1) +
\]
\[
M \left( \log \frac{1}{\delta} - (\gamma + 1) \log (cM) + \log \frac{1}{w_{\gamma+1}} - \log \frac{1}{w_{\gamma+1}} \right)
\]
\[
\leq M (\log 4R_{\gamma+1} + \gamma + 1) + M \log w_{\gamma+1}
\]
\[
\lesssim M \log (w_{\gamma+1} (\gamma + 1) \vee R_{\gamma+1} )
\]  
(64)

where we have used the fact $\mu_M = (cM)^{-2(\gamma+1)} \leq w_{\gamma+1}^2 \delta^2$ in the second inequality. Inequalities (61), (63) and (64) together yield

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

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

\[
\sum_{m=M+1}^{\infty} \theta_m^2 \leq \mu_M \sum_{m=M+1}^{\infty} \frac{\theta_m^2}{\mu_m} \leq w_{\gamma+1}^2 R_{\gamma+1}^2 \delta^2 .
\]  
(65)

To cover $\mathcal{E}_{\gamma+1}$ within $(1 + w_{\gamma+1}^2 R_{\gamma+1}^2)^{\frac{1}{2}} \delta$—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

\[
|\theta - \theta_i|^2_2 \leq \sum_{m=1}^M (\theta_m - \theta_m^i)^2 + w_{\gamma+1}^2 R_{\gamma+1}^2 \delta^2 \leq (1 + w_{\gamma+1}^2 R_{\gamma+1}^2) \delta^2
\]

where we have used (65). Consequently, we have

\[
\log N_2 (\delta, \mathcal{E}_{\gamma+1} ) \sim \log N_2 \left( \delta \left( 1 + w_{\gamma+1}^2 R_{\gamma+1}^2 \right)^{\frac{1}{2}}, \mathcal{E}_{\gamma+1} \right)
\]
\[
\sim \left( w_{\gamma+1} \delta \left( 1 + w_{\gamma+1}^2 R_{\gamma+1}^2 \right)^{\frac{1}{2}} \right)^{-1} \max \{ \log (w_{\gamma+1} ((\gamma + 1) \vee R_{\gamma+1})), \log 2 \} .
\]  
(66)
Case 1: \( R_{\gamma+1} \gtrapprox \gamma + 1 \). Setting \( w_{\gamma+1} \propto R_{\gamma+1}^{-1} \) in (62) and (66) solves
\[
\left( \frac{w_{\gamma+1} \delta \left( 1 + w_{\gamma+1}^2 R_{\gamma+1}^2 \right)}{\gamma + 1} \right)^{\frac{1}{\gamma + 1}} \max \{ \log (w_{\gamma+1} ((\gamma + 1) \lor R_{\gamma+1})), \log 2 \} \\
\approx \left( w_{\gamma+1} \delta \right)^{\frac{1}{\gamma + 1}} \log (w_{\gamma+1} R_{\gamma+1})
\]
and gives
\[
\log N_2(\delta, \mathcal{E}_{\gamma+1}) \gtrapprox (R_{\gamma+1}^{-1} \delta)^{\frac{1}{\gamma + 1}}.
\]
Case 2: \( R_{\gamma+1} \lesssim \gamma + 1 \). Setting \( w_{\gamma+1} \propto (\gamma + 1)^{-1} \) in (66) gives
\[
\log N_2(\delta, \mathcal{E}_{\gamma+1}) \lesssim \delta^{\frac{1}{\gamma + 1}}.
\]
Note that the lower bound obtained by setting \( w_{\gamma+1} \propto (\gamma + 1)^{-1} \) in (62) is not particularly useful. Instead, we consider a different truncation with \( w_{\gamma+1} \propto R_{\gamma+1}^{-1} \). Then (62) with \( w_{\gamma+1} \propto R_{\gamma+1}^{-1} \) gives
\[
\log N_2(\delta, \mathcal{E}_{\gamma+1}) \gtrapprox R_{\gamma+1}^{\frac{1}{\gamma + 1}} \delta^{\frac{1}{\gamma + 1}}.
\]

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

Standard Sobolev \( \overline{\mathcal{S}}_{\gamma+1} \). We apply Lemma C.1(i) in Section C and some of the constructions in Section B.2. To construct \( \mathcal{M} \), we construct \( \mathcal{M}_1 \) (which is a set in the polynomial subspace) and \( \mathcal{M}_2 \) (which is a set in the Sobolev subspace), and then take \( \mathcal{M} = \mathcal{M}_1 \times \mathcal{M}_2 \). By (84) in Section C, for a set \( \{ f_1, f_2, \ldots, f^M \} = \mathcal{M} \subseteq \overline{\mathcal{S}}_{\gamma+1} \), we have
\[
D_{KL}(\mathbb{P}_j \times \mathbb{P}_X \parallel \mathbb{P}_1 \times \mathbb{P}_X) = \frac{n}{2\sigma^2} \left| f^j - f^l \right|^2_{2,\mathbb{P}} \\
\leq \frac{n}{\sigma^2} \left( \left| f^j_1 - f^l_1 \right|^2_{2,\mathbb{P}} + \left| f^j_2 - f^l_2 \right|^2_{2,\mathbb{P}} \right)
\]
where the inequality follows from that any \( f \in \mathcal{M} \) can be expressed by \( f = f_1 + f_2 \) such that \( f_1 \in \mathcal{M}_1 \) and \( f_2 \in \mathcal{M}_2 \). To construct \( \mathcal{M}_1 \), let us consider the \( \delta \)–packing set consisting of \( M_0 \) elements in the form (52) for \( \mathcal{U}_{\gamma+1}^* \) in (70). To construct \( \mathcal{M}_2 \), let us consider the \( \delta \)–separated subset of \( \mathcal{S}_{\gamma+1}^* \) in (71); in other words, each element in this subset is \( \delta \)–apart. Because of (72), \( \mathcal{M} = \mathcal{M}_1 \times \mathcal{M}_2 \) is clearly a packing subset of \( \overline{\mathcal{S}}_{\gamma+1} \).
Let us start with $M_1$. Following the notation in Section A.1 (the derivations for $B_2$), we have

$$\left| f_{2,j} - f_{M_1} \right|^2_{2,p} = \left| f_{1,j} - f_{1} \right|^2_{2,p}$$

$$= \int_0^1 \left[ (\theta_{\tilde{k}}^j - \theta_{\tilde{l}}^j) x^k + \sum_{k=0}^{\gamma} \left( 1 \{ \lambda_{j,k} \neq \lambda_{l,k} \} \theta_{\tilde{k}}^j x^k \right) \right]^2 p(x) dx$$

$$\lesssim \left( \theta_{\tilde{k}}^j - \theta_{\tilde{l}}^j \right)^2 + \left( \sum_{k=0}^{\gamma} \theta_{\tilde{k}}^j \right)^2$$

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

$$\lesssim \delta^2 \quad \text{for any } j, l \in M_1, j \neq l$$

where the last line follows from that $R_0 = \sqrt{\frac{\sigma}{g}}$ and $R_k = \sqrt{\sum_{k=0}^{\gamma} \frac{R_k}{k!}}$ for $k = 1, ..., \gamma$, in which case we have $\tilde{k} = 0$ and $\sum_{k=0}^{\gamma} \frac{R_k}{k!} = 1$. Recall that the lower bound $\log M \gtrsim \gamma + 1$ in Section A.1 holds for all $\delta$ such that $\frac{\sigma^2 (\gamma + 1)}{n} \gtrsim 2^{\gamma+1}$ and $\delta \left( \frac{k+1}{\gamma} \right) + \sum_{k=0}^{\gamma} \frac{R_k}{k!} \gtrsim \frac{R_k}{k!}$, which are reduced to $\delta \lesssim 2^{-(\gamma+1)}$ since $\tilde{k} = 0$ and $\sum_{k=0}^{\gamma} \frac{R_k}{k!} = 1$.

In terms of $M_2$, based on Section A.2, we can construct $M_2$ in the way such that each element in $M_2$ is $\delta$-apart, i.e.,

$$\left| f_{2,j} - f_{2,l} \right|^2_{2,p} = \delta^2 \quad \text{for any } j, l \in M_2, j \neq l$$

and $\log |M_2| \asymp \delta^{-\frac{1}{\gamma+3}}$.

Let us take $\delta^2 = c_1 \left( \frac{\sigma^2 (\gamma + 1)}{n} \right) \left( \frac{\sigma^2}{n} \right)^{\frac{2^{\gamma+3}}{\gamma+3}}$ for a sufficiently small universal constant $c_1 > 0$. Note that: (1) if $\frac{\sigma}{\sigma^2} \leq (\gamma + 1)^{2^{\gamma+3}}$, we have $\delta^2 = c_1 \frac{\sigma^2 (\gamma + 1)}{n}$; we also need the condition $2^{2^{\gamma+3}} (\gamma + 1) \gtrsim \frac{\sigma}{\sigma^2}$ to ensure $\delta \geq \sqrt{\frac{\sigma^2 (\gamma + 1)}{n}} \gtrsim 2^{-(\gamma+1)}$ so we can apply $\log |M_1| \asymp \gamma + 1$ below. (2) If $\frac{\sigma}{\sigma^2} \geq (\gamma + 1)^{2^{\gamma+3}}$, we have $\delta^2 = c_1 \left( \frac{\sigma^2}{n} \right)^{\frac{2^{\gamma+3}}{\gamma+3}}$.

In case (1),

$$\frac{1}{M^2} \sum_{j,l \in \{1, ..., M\}} D_{KL}(P_j \times P_X \parallel P_l \times P_X) \gtrsim \gamma + 1,$$

$$\log M = \log |M_1| + \log |M_2| \gtrsim \gamma + 1,$$

and therefore

$$\delta^2 \left( 1 - \frac{\log 2 + \frac{1}{M^2} \sum_{j,l \in \{1, ..., M\}} D_{KL}(P_j \times P_X \parallel P_l \times P_X)}{\log M} \right) \gtrsim \frac{\sigma^2 (\gamma + 1)}{n}.$$

In case (2),

$$\frac{1}{M^2} \sum_{j,l \in \{1, ..., M\}} D_{KL}(P_j \times P_X \parallel P_l \times P_X) \gtrsim \left( \frac{n}{\sigma^2} \right)^{\frac{1}{\gamma+3}},$$

$$\log M = \log |M_1| + \log |M_2| \gtrsim \left( \frac{n}{\sigma^2} \right)^{\frac{1}{\gamma+3}},$$
and therefore
\[ \delta^2 \left( 1 - \frac{\log 2 + \frac{1}{\sqrt{\pi}} \sum_{j,i \in \{1, \ldots, M\}} D_{KL}(P_j \times P_X \parallel P_l \times P_X)}{\log M} \right) \approx \left( \frac{\sigma^2}{n} \right)^{\frac{2+2}{2+3}}. \]

**Standard Hölder** $\mathcal{U}_{\gamma+1}$. We apply Lemma C.1(i) in Section C. The proof for the standard $\mathcal{U}_{\gamma+1}$ is nearly identical to the proof for $\mathcal{S}_{\gamma+1}$ shown previously. To construct $\mathcal{M}_1$, let us consider the $\delta$—packing set consisting of $M_0$ elements in the form (52) for $\mathcal{U}_{\gamma+1,1}$ with $R_k = \mathcal{C}$ for all $k = 0, \ldots, \gamma$. For $\mathcal{M}_2$, we can use the construction in Section A.3 to construct a $c_0\delta$—separated subset of $\mathcal{U}_{\gamma+1,2}$ with $R_k = \mathcal{C}$ for all $k = 0, \ldots, \gamma + 1$ in the way such that each element in this subset is $c_0\delta$—apart and $\log |\mathcal{M}_2| \approx \delta^{\frac{2}{\gamma+3}}$.

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

**Lemma B.1.** We have
\[ \log M_2 (\delta, \mathcal{S}_{\gamma+1}) \gtrsim \gamma + 1 + \frac{1}{\delta}\delta^{\frac{1}{\gamma+1}}, \forall \delta \gtrsim 2^{\gamma+1}, \]
\[ \log N_2 (\delta, \mathcal{S}_{\gamma+1}) \gtrsim (\gamma + 1) \log \frac{1}{\delta} + \delta^{\frac{1}{\gamma+1}}, \forall \delta \in (0, 1). \]

*If the density function $p(x)$ on $[0, 1]$ is bounded away from zero, i.e., $p(x) \geq c > 0$, then*
\[ \log M_{2,\mathcal{P}} (\delta, \mathcal{S}_{\gamma+1}) \gtrsim \gamma + 1 + \frac{1}{\delta}\delta^{\frac{1}{\gamma+1}}, \forall \delta \gtrsim 2^{\gamma+1}, \]
\[ \log N_{2,\mathcal{P}} (\delta, \mathcal{S}_{\gamma+1}) \gtrsim (\gamma + 1) \log \frac{1}{\delta} + \delta^{\frac{1}{\gamma+1}}, \forall \delta \in (0, 1). \]

**Proof.** To prove Lemma B.1, we use the bounds $\mathcal{B}_2 (\delta)$ and $\mathcal{B}_2$ in Lemma 3.1 (and Remark A at the end of Section A.3), as well as the bounds in Lemma 3.3. First, let us consider
\[ \mathcal{U}_{\gamma+1,1}^* = \left\{ f = \sum_{k=0}^{\gamma} \theta_k x^k : (\theta_k)_{k=0}^\gamma \in \mathcal{P}_\gamma, x \in [0, 1] \right\} \]
with the $(\gamma + 1)$—dimensional polyhedron
\[ \mathcal{P}_\gamma = \left\{ (\theta_k)_{k=0}^\gamma : \theta_0 \in \left[ -\sqrt{\frac{\mathcal{C}}{3}}, \sqrt{\frac{\mathcal{C}}{3}} \right], \theta_k \in \left[ -\sqrt{\frac{\mathcal{C}}{3\gamma k!}}, \sqrt{\frac{\mathcal{C}}{3\gamma k!}} \right], k = 1, \ldots, \gamma \right\} \]
as well as
\[ \mathcal{S}_{\gamma+1}^* = \left\{ f : [0, 1] \rightarrow \mathbb{R} | f is \gamma + 1 times differentiable a.e., \right. \]
\[ \left. for all \ k \leq \gamma, \ f^{(k)}(0) = 0, \right. \]
\[ f^{(\gamma)} \ is \ abs. \ cont. \ and \ \int_0^1 \left[ f^{(\gamma+1)}(t) \right]^2 dt \leq \frac{\mathcal{C}}{3}. \]

Note that
\[ \mathcal{U}_{\gamma+1,1}^* + \mathcal{S}_{\gamma+1}^* = \left\{ f_1 + f_2 : f_1 \in \mathcal{U}_{\gamma+1,1}^*, f_2 \in \mathcal{S}_{\gamma+1}^* \right\} \subset \mathcal{S}_{\gamma+1}. \]

As a result, we can apply (11) in Lemma 3.1 to show
\[ \log M_2 (\delta, \mathcal{U}_{\gamma+1,1}^*) \gtrsim \gamma + 1, \forall \delta \gtrsim 2^{\gamma+1}; \]
applying (16) in Lemma 3.3 and the sandwich result (4) yields
\[ \log M_2(\delta, S_{\gamma+1}^\ast) \gtrsim \delta^{-\gamma+1}. \]

The lower bounds above yield the part "\( \gtrsim \gamma + 1 + \delta^{-\gamma+1} \)" for \( \log M_2(\delta, S_{\gamma+1}) \) in Lemma B.1.

It remains to show the part "\( \lesssim (\gamma + 1) \log \frac{1}{\delta} + \delta^{-\gamma+1} \)" in Lemma B.1. Let us consider

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

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

\[ \mathcal{P}_\gamma^\dagger = \left\{ (\theta_k)_{k=0}^\gamma : \theta_k \in \left[ -\frac{C}{k!}, \frac{C}{k!} \right], k = 0, \ldots, \gamma \right\} \]

as well as

\[ S_{\gamma+1}^\dagger = \{ f : [0, 1] \to \mathbb{R} | f \text{ is } \gamma + 1 \text{ times differentiable a.e.,} \}
\]

\[ \text{for all } k \leq \gamma, f^{(k)}(0) = 0, \]

\[ f^{(\gamma)} \text{ is abs. cont. and } \int_0^1 \left[ f^{(\gamma+1)}(t) \right]^2 dt \leq C^2). \]

Note that

\[ U_{\gamma+1,1}^\dagger + S_{\gamma+1}^\dagger = \left\{ f_1 + f_2 : f_1 \in U_{\gamma+1,1}^\dagger, f_2 \in S_{\gamma+1}^\dagger \right\} \supseteq \mathcal{S}_{\gamma+1}. \]

As a result, we can apply (9) in Lemma 3.1 to show

\[ \log N_{\infty}(\delta, U_{\gamma+1,1}^\dagger) \lesssim (\gamma + 1) \log \frac{1}{\delta}, \forall \delta \in (0, 1). \]

Because \( \| \cdot \|_\infty \geq \frac{1}{2} \| \cdot \|_2 \), we also have

\[ \log N_2(\delta, U_{\gamma+1,1}^\dagger) \lesssim (\gamma + 1) \log \frac{1}{\delta}, \forall \delta \in (0, 1). \]

For \( S_{\gamma+1}^\dagger \), applying (15) in Lemma 3.3 yields

\[ \log N_2(\delta, S_{\gamma+1}^\dagger) \gtrsim \delta^{-\gamma+1}. \]

The upper bounds above yield the part "\( \lesssim (\gamma + 1) \log \frac{1}{\delta} + \delta^{-\gamma+1} \)" for \( \log N_2(\delta, \mathcal{S}_{\gamma+1}) \) in Lemma B.1.

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

\[ \log M_{2,F}(\delta, \mathcal{S}_{\gamma+1}) \asymp \log M_2(\delta, \mathcal{S}_{\gamma+1}), \]

\[ \log N_{2,F}(\delta, \mathcal{S}_{\gamma+1}) \asymp \log N_2(\delta, \mathcal{S}_{\gamma+1}). \]

Therefore we have (68) and (69).
B.3 Proof for Theorem 4.2

Step 1. We apply Lemma C.8 (in Section C) where \( \mathcal{W} \) corresponds to the Sobolev space containing \( \overline{\mathcal{F}}_{\gamma+1} \) and the kernel functions correspond to (18) and (19). Then solving (102) is reduced to solving
\[
\left( r \sqrt{\frac{(\gamma+1) \wedge n}{n}} \right) \left( \frac{1}{r} \sqrt{n^{2+1}} \right) = \frac{C r^2}{\sigma}.
\]
Under the condition \( n \geq \gamma+1, r = \overline{\delta}_1 = c_1 \left[ \sqrt{\frac{\sigma^2 (\gamma+1)}{n}} \right] \right) \right) \left( \frac{\sigma^2}{n} \right) \right), \]
solves the above. In a similar fashion, \( r = \overline{\delta}_2 = c_2 \left[ \sqrt{\frac{\sigma^2}{n}} \right] \left( \frac{\sigma^2}{n} \right) \right), \]
solves (103). Note that both \( \overline{\delta}_1 \) and \( \overline{\delta}_2 \) 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 \( \overline{\delta}_1 \), we apply Lemma C.6 to show that
\[
\left| \hat{f} - f \right|^2_n \lesssim t_1^2 \quad \text{for any } t_1 \geq \overline{\delta}_1
\]
with probability at least \( 1 - c' \exp \left(-c'' \frac{nt_1^2}{\sigma^2} \right) \), whenever \( \lambda \asymp t_1^2 \).

Step 3. Given \( \overline{\delta}_2 \), we now connect \( \left| \hat{f} - f \right|^2_n \) with \( \left| \hat{f} - f \right|^2_{2,P} \). We divide the argument into two cases depending on whether \( \overline{\delta}_2 \geq r^* \), the smallest positive solution to (89) with \( c = C \).

Case 1 (when \( \overline{\delta}_2 \leq r^* \)). Note that \( \overline{\delta}_2 \) is an upper bound for \( r^* \), the smallest positive solution to (91) with \( c_0 = C^{-1} \). For case 1, we can apply Lemma C.4 together with (73) to show that
\[
\left| \hat{f} - f \right|^2_{2,P} \lesssim t_1^2 + t_2^2 \quad \text{for any } t_1 \geq \overline{\delta}_1, t_2 \in [\overline{\delta}_2, r^*]
\]
with probability at least
\[
1 - c' \exp \left(-c'' \frac{nt_1^2}{\sigma^2} \right) - c_0 \exp \left(-c_0 nr^* \right),
\]
which is greater than
\[
1 - c' \exp \left(-c'' \frac{nt_1^2}{\sigma^2} \right) - c_0 \exp \left(-c_0 nt_2^2 \right). \quad (74)
\]

Case 2 (when \( \overline{\delta}_2 > r^* \)). In this case, we can apply Lemma C.2 (where we take \( r = r^* \)) together with (73) to show that
\[
\left| \hat{f} - f \right|^2_{2,P} \lesssim t_1^2 + t_2^2 \quad \text{for any } t_1 \geq \overline{\delta}_1, t_2 \geq \overline{\delta}_2
\]
with probability at least (74).

Applying Lemmas C.2 and C.4 requires the shifted class \( \overline{\mathcal{F}} \) associated with \( \mathcal{F} = \overline{\mathcal{F}}_{\gamma+1} \) 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 (18) and (19) and Lemma C.9.

Step 4. Integrating the tail probability in the form of (74) gives
\[
\mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,P} \right) \lesssim r^2 + \exp \left\{ -cnr^2 \right\},
\]
where
where $\tilde{r}^2 = \frac{\sigma^2(\gamma+1)}{n} \vee \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{\gamma+1+1}} \times \frac{\gamma+1}{n} \vee \left( \frac{\gamma+1}{n} \right)^{\frac{2(\gamma+1)}{\gamma+1+1}}$ since $\sigma \asymp 1$. Finally, we take sup and obtain
\[
\sup_{f \in \mathcal{F}_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,\mathbb{P}} \right) \preceq \tilde{r}^2 + \exp \left\{ -cn\tilde{r}^2 \right\}.
\]

Under (27), we have
\[
\sup_{f \in \mathcal{F}_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,\mathbb{P}} \right) \preceq r_1^2 + \exp \left\{ -cnr_1^2 \right\}
\]
where $r_1^2 = \frac{\sigma^2(\gamma+1)}{n}$. Under (28), we have
\[
\sup_{f \in \mathcal{F}_{\gamma+1}} \mathbb{E} \left( \left| \hat{f} - f \right|^2_{2,\mathbb{P}} \right) \preceq r_2^2 + \exp \left\{ -cnr_2^2 \right\},
\]
where $r_2^2 = \left( \frac{\sigma^2}{n} \right)^{\frac{2(\gamma+1)}{\gamma+1+1}}$.

**B.4 Proof for Theorem 4.3**

**Step 1.** We apply Lemma C.7 (in Section C) where $\mathcal{F}$ corresponds to the standard $\mathcal{U}_{\gamma+1}$. Taking $R_k = C$ for $k = 0, ..., \gamma + 1$ in (14) (the second bound) yields
\[
\log N_{\infty}(\delta, \mathcal{U}_{\gamma+1}) \preceq (\gamma + 1) \log \frac{1}{\delta} + \left( \frac{1}{\delta} \right)^{\gamma+1},
\]
where we have used the fact that $R^* \asymp 1$. Note that
\[
\sqrt{\frac{\gamma+1}{n}} \int_0^r \sqrt{\log N_{\infty}(\delta, \Omega(r; \mathcal{F}))} d\delta
\]
\[
\preceq r \sqrt{\gamma+1} \sqrt{\frac{1}{n} + \frac{1}{\sqrt{n}} \frac{2\gamma+1}{T(r)}},
\]
where the last line follows from (75). Setting $\sigma T(r) \asymp r^2$ yields $r = \bar{\delta}_1 = c_1 \left[ \sqrt{\frac{\sigma^2(\gamma+1)}{n}} \vee \left( \frac{\sigma^2}{n} \right)^{\frac{\gamma+1}{\gamma+1+1}} \right]$, which solves (100). In a similar fashion, $r = \bar{\delta}_2 = c_2 \left[ \sqrt{\frac{\gamma+1}{n}} \vee \left( \frac{1}{n} \right)^{\frac{\gamma+1}{\gamma+1+1}} \right]$ solves (101). 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 $\sigma \asymp 1$ (in Assumption 1) and $\bar{\delta}_1$, we apply Lemma C.5 to show that
\[
\left| \hat{f} - f \right|^2_{n} \preceq t_1^2 \text{ for any } t_1 \geq \bar{\delta}_1
\]
with probability at least $1 - c' \exp \left( -c'' \frac{n t_1^2}{\sigma^2} \right)$.

**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 $|g|_\infty \preceq 1$ for all $g \in \mathcal{F}$ associated with the standard $\mathcal{U}_{\gamma+1}$ 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 $F = \mathcal{H}_{\gamma+1}$ and the results in Lemma 3.3. By (85) 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 $\left( \frac{R_{\gamma+1} \sqrt{n}}{\sigma \epsilon} \right)^{\frac{1}{\gamma+1}} \asymp \epsilon^2$ yields $\epsilon^2 \asymp \left( \frac{R_{\gamma+1} \sqrt{n}}{\sigma^2} \right)^{\frac{1}{2(\gamma+1)+1}} =: \epsilon^*$. Observe that setting

$$\delta \asymp R_{\gamma+1}^{\frac{1}{2(\gamma+1)+1}} \left( \frac{\sigma^2}{n} \right) = R_{\gamma+1}^{\frac{1}{2(\gamma+1)+1}} \left( \frac{\sigma^2}{n} \right)$$

ensures

$$\left( R_{\gamma+1} \delta^{-1} \right)^{\frac{1}{\gamma+1}} \asymp \left( R_{\gamma+1} \delta^{-1} \right)^{\frac{1}{2(\gamma+1)+1}} \asymp \epsilon^*.$$

Consequently, we have

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

and

$$\inf_{\tilde{f}} \sup_{f \in \mathcal{H}_{\gamma+1}} \mathbb{E} \left( \left\| \tilde{f} - f \right\|_{2,p}^2 \right) \geq \frac{1}{2} \left( \frac{\sigma^2}{n} \right) \left( \frac{2}{\gamma+1} \right)^{\frac{2(\gamma+1)+1}{\gamma+1}} \left( \frac{2(\gamma+1)+1}{\gamma+1} \right)^{\frac{2(\gamma+1)+1}{\gamma+1}}.$$

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 $K(x, x') \lesssim 1$ for all $x, x' \in [0, 1]$. Moreover, $W$ contains $\mathcal{H}_{\gamma+1}$. Then solving (102) is reduced to

$$\frac{1}{\sqrt{n}} \sigma^{\frac{\gamma+1}{\gamma+2}} \asymp \frac{R_{\gamma+1} r^2}{\sigma}.$$

Note that $r = \bar{\delta}_1 = c_1 R_{\gamma+1}^{\frac{1}{2(\gamma+1)+1}} \left( \frac{\sigma^2}{n} \right)^{\frac{\gamma+1}{2(\gamma+1)+1}} \sigma^{\frac{\gamma+1}{\gamma+2}}$ solves the above. In a similar fashion, $r = \bar{\delta}_2 = c_2 R_{\gamma+1}^{\frac{1}{2(\gamma+1)+1}} \left( \frac{1}{n} \right)^{\frac{\gamma+1}{2(\gamma+1)+1}} \sigma^{\frac{\gamma+1}{\gamma+2}}$ solves (103). Note that both $\bar{\delta}_1$ and $\bar{\delta}_2$ are non-random and do not depend on the values of $\{x_i\}_{i=1}^n$.

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 $F = U_{\gamma+1,2}$ and the results in Lemma 3.2. By (85) and Lemma 3.2, we have

$$\log N_{KL}(\epsilon, Q) = \log N_{2,p} \left( \sqrt{\frac{2}{n}} \sigma \epsilon, U_{\gamma+1,2} \right) \lesssim \left( \frac{R^* \sqrt{n}}{\sigma \epsilon} \right)^{\frac{1}{\gamma+1}}.$$
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 $R^\ast$.

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

$$\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega(r; F))} d\delta \leq \frac{1}{\sqrt{n}} \int_0^r \log N_\infty(\delta, F) d\delta \lesssim \frac{1}{\sqrt{n}} \left( R^\ast \right)^{\frac{1}{2\gamma+2}} r^{\frac{2\gamma+1}{2\gamma+2}} T(r)$$

where the last line follows from Lemma 3.2.

Setting $\sigma T(r) \times r^2$ yields $r = \bar{\delta}_1 = c_1 (R^\ast)^{\frac{1}{2\gamma+1+\tau}} \left( \frac{a^2}{n} \right)^{\frac{\gamma+1}{2(\gamma+1)+1}}$, which solves (100). In a similar fashion, $r = \bar{\delta}_2 = c_2 (R^\ast)^{\frac{1}{2\gamma+1+\tau}} \left( \frac{b^2}{n} \right)^{\frac{\gamma+1}{2(\gamma+1)+1}}$ solves (101). Note that both $\bar{\delta}_1$ and $\bar{\delta}_2$ are non-random and do not depend on the values of $\{x_i\}_{i=1}^n$.

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.4. 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 $B_2$ 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. To construct $M_1$, let us consider the $\delta$–packing set consisting of $M_0$ elements in the form (52) for $\mathcal{U}_{\gamma+1}$ with $R_0 = \overline{C}$ and $R_k$ taking a value in $[\overline{C}, \overline{C} (k-1)!]$ for all $k = 1, \ldots, \gamma$. Let us choose $b = \gamma \lor 1$ in $\theta_{\gamma}^*$s of (52) for this construction. Recall that the lower bound $\log M_0 \gtrsim \gamma + 1$ in Section A.1 holds for all $\delta$ such that

$$\frac{R_k}{(k+1) ! \sqrt{\sum_{k=0}^{\gamma} R_k^2}} \gtrsim 2^{\gamma+1}$$

and $\delta \left( (k+1) ! \sqrt{\sum_{k=0}^{\gamma} \frac{R_k}{k!}} \right) \gtrsim \frac{R_k}{k!}$, which are reduced to

$$\frac{1}{\delta \left( 1 \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!} \right)} \gtrsim 2^{\gamma+1},$$

$$\delta \left( 1 \lor \sum_{k=0}^{\gamma} \frac{R_k}{k!} \right) \gtrsim 1,$$

since $\hat{k} = 0$.

For $M_2$, let us consider a $c_0 \delta$–separated subset of $\mathcal{U}_{\gamma+1,2}$ with $R_0 = \overline{C}$ and $R_k$ taking a value in $[\overline{C}, \overline{C} (k-1)!]$ for all $k = 1, \ldots, \gamma + 1$; in other words, each element in this subset is $c_0 \delta$–apart. In particular, we use the construction in Section A.3 where $R^\ast \frac{1}{\gamma+1} \asymp 1$. Therefore, $\log |M_2| \asymp \delta^{\frac{1}{\gamma+1}}$.

The rest of the arguments are identical to those in Section B.4.

**The upper bound.** Taking $R_0 = \overline{C}$ and $R_k = \overline{C} (k-1)!$ for $k = 1, \ldots, \gamma + 1$ in (14) (the
first bound) yields
\[ \log N_\infty (\delta, U_{\gamma+1}) \preceq (\gamma + 1) \log \frac{1}{\delta} + \left( \frac{1}{\delta} \right)^{\frac{1}{\gamma+1}}, \] (78)
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 \( B_U(\delta) \) in Lemma 3.1, as well as the bounds in Lemma 3.2. When \( R_k = \mathcal{C}k! \) for all \( k = 0, \ldots, \gamma+1, R^* \approx 1 \) and \( \log M_{2,P}(\delta, U_{\gamma+1,2}) \gtrsim \left( \frac{1}{\delta} \right)^{\frac{1}{\gamma+1}} \).

Moreover,
\[ \log N_\infty (\delta, U_{\gamma+1}) \preceq (\gamma + 1) \log \frac{1}{\delta} \] (79)
for \( \gamma > 1 \), we have
\[ \log M_{2,P}(\delta, U_{\gamma+1,1}) \geq c' \left[ (\gamma + 1) \log \frac{1}{\delta} - \gamma^2 \right] \]
\[ - (\gamma + 1) \log \gamma + (\gamma + 1) \log (\gamma - 1)! \]
\[ \approx \gamma \log \frac{1}{\delta} - \gamma^2; \] (80)
for \( \gamma \in \{0, 1\} \), we simply have
\[ \log M_{2,P}(\delta, U_{\gamma+1,1}) \gtrsim (\gamma + 1) \log \frac{1}{\delta} - 1. \] (81)

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

In terms of \( M_1 \), we use the results in Section A.4. In particular, we can construct \( M_1 \) such that each element in this subset is \( \delta \)-apart and by setting \( \delta \approx 2^{-(\gamma + 1)} \) in (80) and (81), we have
\[ \log |M_1| \gtrsim (\gamma + 1)^2. \]

Let us take \( \delta^2 = c_1 \left( \frac{\sigma^2 (\gamma + 1) \log (\gamma \vee 2)}{n} \right) \vee \left( \frac{\sigma^2}{n} \right)^{\frac{2\gamma + 3}{2\gamma + 3}} \) for a sufficiently small universal constant \( c_1 > 0 \).

Note that: (1) if \( \frac{n}{\sigma^2} \approx ((\gamma + 1) \log (\gamma \vee 2))^{2\gamma + 3} \), we have \( \delta^2 = c_1 \frac{\sigma^2 (\gamma + 1) \log (\gamma \vee 2)}{n} \); we also need the condition \( 4(\gamma + 1) \log (\gamma \vee 2) \approx \frac{n}{\sigma^2} \) to ensure \( \delta \approx \sqrt{\frac{\sigma^2 (\gamma + 1) \log (\gamma \vee 2)}{n}} \approx 2^{-(\gamma + 1)} \) so we can apply \( \log |M_1| \gtrsim (\gamma + 1)^2 \gtrsim (\gamma + 1) \log (\gamma \vee 2) \) below. (2) If \( \frac{n}{\sigma^2} \gtrsim ((\gamma + 1) \log (\gamma \vee 2))^{2\gamma + 3} \), we have \( \delta^2 = c_1 \left( \frac{\sigma^2}{n} \right)^{\frac{2\gamma + 3}{2\gamma + 3}} \).

In case (1),
\[ \log M = \log |M_1| + \log |M_2| \gtrsim (\gamma + 1) \log (\gamma \vee 2), \]
where we have used the fact that \( R^* \approx 1 \). The rest of the arguments are identical to those in Section B.4.
Lemma C.1 below provides two versions of Fano’s inequality. In most of our derivations of the minimax lower bounds, we apply the first version as it is more useful for showing the phase transition phenomenon. In a couple of cases, we apply the second version as it gives more insight about

\[ \delta^2 \left( 1 - \frac{\log 2 + \frac{1}{M^2} \sum_{j,l \in \{1, \ldots, M\}} D_{KL} (P_j \times P_X \parallel P_l \times P_X)}{\log M} \right) \gtrsim \frac{\sigma^2 (\gamma + 1) \log (\gamma \vee 2)}{n}. \]

In case (2),

\[ \frac{1}{M^2} \sum_{j,l \in \{1, \ldots, M\}} D_{KL} (P_j \times P_X \parallel P_l \times P_X) \lesssim \left( \frac{n}{\sigma^2} \right)^{\frac{1}{2 + \gamma}}, \]

and therefore

\[ \delta^2 \left( 1 - \frac{\log 2 + \frac{1}{M^2} \sum_{j,l \in \{1, \ldots, M\}} D_{KL} (P_j \times P_X \parallel P_l \times P_X)}{\log M} \right) \gtrsim \left( \frac{\sigma^2}{n} \right)^{\frac{2 + \gamma}{2 + \gamma / 3}}. \]

The upper bound. In this case, solving (100) yields \( r = \tilde{\delta}_1 = c_1 \left[ \sqrt{\frac{\sigma^2 (\gamma + 1) \log (\gamma \vee 2)}{n}} \vee \left( \frac{\sigma^2}{n} \right)^{\frac{\gamma + 1}{2 + \gamma / 3}} \right]. \)

In a similar fashion, solves (101) yields \( r = \tilde{\delta}_2 = c_2 \left[ \sqrt{\frac{\gamma + 1 \log (\gamma \vee 2)}{n}} \vee \left( \frac{1}{n} \right)^{\frac{\gamma + 1}{2 + \gamma / 3}} \right]. \) 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 3.4.

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 Mendelson (2002), Mendelson (2002), and Wainwright (2019). Recall (1) which satisfies Assumption 1. Suppose \( f \) belongs to the class \( F \).

Lemma C.1 below provides two versions of Fano’s inequality. In most of our derivations of the minimax lower bounds, we apply the first version as it is more useful for showing the phase transition phenomenon. In a couple of cases, we apply the second version as it gives more insight about where the rates are from.

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

\[ \inf \sup_{\tilde{f}} \mathbb{E} \left( \left\| \tilde{f} - f \right\|_{2,\mathbb{P}}^2 \right) \gtrsim \delta^2 \left( 1 - \frac{\log 2 + \frac{1}{M^2} \sum_{j,l \in \{1, \ldots, M\}} D_{KL} (P_j \times P_X \parallel P_l \times P_X)}{\log M} \right) \tag{82} \]

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

(ii) Let \( N_{KL} (\epsilon, Q) \) denote the \( \epsilon \)–covering number of \( F \) with respect to the square root of the \( KL \)–divergence, and \( M_{2,\mathbb{P}} (\delta, F) \) denote the \( \delta \)–packing number of \( F \) with respect to \( \left\| \cdot \right\|_{2,\mathbb{P}}. \) Then the Yang and Barron version of Fano’s inequality gives
\[
\inf \sup_{f \in F} \mathbb{E} \left( \left| f - f_{\cdot, p}^2 \right|^2 \right) \gtrsim \sup_{\delta, \epsilon} \delta^2 \left( 1 - \frac{\log 2 + \log N_{KL}(\epsilon, Q) + \epsilon^2}{\log M_{2,p}(\delta, F)} \right). \tag{83}
\]

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

\[
D_{KL}(P_j \times P_X \parallel P_l \times P_X) = \mathbb{E}_X \left[ D_{KL}(P_j \parallel P_l) \right] = \frac{n}{2\sigma^2} \left| f^j - f^l \right|_{2, P}^2, \tag{84}
\]

and

\[
\log N_{KL}(\epsilon, Q) = \log N_{2,p} \left( \sqrt{\frac{2}{n}} \sigma \epsilon, F \right). \tag{85}
\]

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

\[
\bar{F} := \{ g = g_1 - g_2 : g_1, g_2 \in F \}. \tag{86}
\]

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

\[
G_n(r; \bar{F}) := \mathbb{E}_{\tilde{\epsilon}} \left[ \sup_{g \in \Omega_n(r; \bar{F})} \left| \frac{1}{n} \sum_{i=1}^n \tilde{\epsilon}_i g(x_i) \right| \right], \tag{87}
\]

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

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

\[
\mathcal{R}(r; \bar{F}) := \mathbb{E}_{\tilde{\epsilon}, X} \left[ \sup_{g \in \Omega(r; \bar{F})} \left| \frac{1}{n} \sum_{i=1}^n \tilde{\epsilon}_i g(X_i) \right| \right], \tag{88}
\]

where \( \tilde{\epsilon} = \{ \tilde{\epsilon}_i \}_{i=1}^n \) 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

\[
\mathcal{R}(r; \bar{F}) \leq \frac{r^2}{c}. \tag{89}
\]

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

\[
\frac{1}{2} |g|_{2, p}^2 \leq |g|_n^2 + \frac{\delta^2}{2}. \tag{90}
\]
with probability at least $1 - c_1 \exp \left( -c_2 n \sigma^2 \right)$.

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

$$R_n(r; \bar{F}) \leq c_0 r^2$$  \hfill (91)

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

$$R(r; \bar{F}) \leq c_0 r^2$$  \hfill (92)

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 $\hat{r}^*$ be the smallest positive solution to (91) with $c_0 = c^{-1}$ and $r^*$ be the smallest positive solution to (92) with $c_0 = c^{-1}$. We have

$$|g|_{2,\bar{F}}^2 \lesssim |g|_n^2 + \hat{r}^{*2}$$  \hfill (93)

with probability at least

$$1 - c_1 \exp \left( -c_2 n \hat{r}^{*2} \right).$$  \hfill (94)

In the least squares problem (17), if we can bound $|\hat{f} - f|_n^2$ with high probability, then we can apply Lemmas C.2 or C.4 to bound $|\hat{f} - f|_{2,\bar{F}}^2$ 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 $\bar{\delta}$ be any positive solution to the critical inequality

$$G_n(r; \bar{F}) \leq \frac{r^2}{2\sigma}.$$  \hfill (95)

Then for any $\delta \geq \bar{\delta}$, we have

$$|\hat{f} - f|_n^2 \lesssim \delta \bar{\delta}$$  \hfill (96)

with probability at least $1 - c_1 \exp \left( -c_2 \frac{n \delta \bar{\delta}}{\sigma^2} \right)$.

The following lemma concerns the regularized least squares in the form

$$\hat{f} \in \arg\min_{f \in \mathcal{W}} \frac{1}{2n} \sum_{i=1}^n (y_i - \hat{f}(x_i))^2 + \lambda |\hat{f}|_H^2$$  \hfill (97)

where $\mathcal{W}$ is a space of real-valued functions with an associated semi-norm and contains $F$. When $\mathcal{W}$ is an RKHS with its RKHS norm $|\cdot|_H$, (97) is referred to as the Kernel Ridge Regression (KRR) estimators. In particular, as we discuss in Section 4, when $F = \mathcal{F}_{\gamma+1}$ in (17), we can transform (17) into the form (97), which is equivalent to solving (23) 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:
\[
\mathcal{G}_n(r; \bar{W}) := \mathbb{E}_\xi \left[ \sup_{g \in \Omega_n(r; \bar{W})} \left| \frac{1}{n} \sum_{i=1}^{n} \xi_i g(x_i) \right| \right],
\]
where

\[
\Omega_n(r; \bar{W}) = \{ g \in \bar{W} : |g|_n \leq r, |g|_H \leq 3 \}
\]
and

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

**Lemma C.6.** Suppose the class \( \mathcal{W}(\supseteq \mathcal{F}) \) is convex. Let \( \bar{\delta} \) be any positive solution to the critical inequality

\[
\mathcal{G}_n(r; \bar{W}) \leq \frac{Rr^2}{2\sigma} \tag{98}
\]
where \( R \) is a user defined radius. Then for any \( \delta \geq \bar{\delta} \), if (97) is solved with \( \lambda \geq 2\delta^2 \), we have

\[
\left| \hat{f} - f \right|_n^2 \lesssim R^2 \delta^2 + R^2 \lambda \tag{99}
\]
with probability at least \( 1 - c_1 \exp \left( -c_2 n R^2 R^2 \sigma^2 \right) \).

**Remark.** Concerning the problem in Section 4, \( \mathcal{W} \) corresponds to the Sobolev space, which is convex and contains \( \mathcal{F} \). Moreover, when \( \mathcal{F} = \mathcal{F}_{\gamma+1} \) in (17), we can take \( R = C \).

In order to make use of Lemmas C.5 and C.6 to establish sharp bounds on \( \left| \hat{f} - f \right|_n^2 \), we need good candidates for \( \bar{\delta} \) that solves (95) and (98), respectively. To make use of Lemmas C.2 and C.4 to connect \( \left| \hat{f} - f \right|_n^2 \) with \( \left| \hat{f} - f \right|_{2,\bar{s}}^2 \), we need a good candidate that solves (91). The following lemmas serve this purpose.

**Lemma C.7.** Suppose the class \( \bar{F} \) is star-shaped. Let \( N_n(\delta, \Omega_n(r; \bar{F})) \) be the \( \delta \)–covering number of the set \( \Omega_n(r; \bar{F}) \) in the \( | \cdot |_n \) norm.

(i) Any \( \delta \in (0, \sigma] \) that solves

\[
\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega_n(r; \bar{F}))} d\delta \asymp \frac{r^2}{\sigma} \tag{100}
\]
solves (95).

(ii) Suppose \( |g|_\infty \leq c \) for all \( g \in \bar{F} \). Then any \( \delta > 0 \) that solves

\[
\frac{1}{\sqrt{n}} \int_0^r \sqrt{\log N_n(\delta, \Omega_n(r; \bar{F}))} d\delta \asymp r^2 \tag{101}
\]
solves (91).

The following lemma concerns the KRR estimator (97) when \( \mathcal{W} \) in Lemma C.6 is an RKHS.

**Lemma C.8.** Suppose \( \mathcal{W} \) is a convex RKHS and the KRR estimator (97) is of interest. Let \( \tilde{\mu}_1 \geq \tilde{\mu}_2 \geq \ldots \geq \tilde{\mu}_n \geq 0 \) be the eigenvalues of the kernel matrix \( \mathbf{K} \in \mathbb{R}^{n \times n} \) consisting of entries

\[
\frac{1}{n} \mathbf{K}(x_i, x_j),
\]
where \( \mathbf{K} \) is the kernel function associated with \( \mathcal{W} \). Suppose \( \mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) is a positive semidefinite kernel function such that \( \mathcal{K}(x, x') \lesssim 1 \) for all \( x, x' \in \mathcal{X} \).
(i) Any $\delta > 0$ that solves
\[
\frac{1}{n} \sum_{i=1}^{n} \min \{ r^2, \tilde{\mu}_i \} \times \frac{R r^2}{\sigma}
\]
solves (98).

(ii) Any $\delta > 0$ that solves
\[
\frac{1}{n} \sum_{i=1}^{n} \min \{ r^2, \tilde{\mu}_i \} \times r^2
\]
solves (91) where $c_0 \approx 1$.

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

Lemma C.9. Let $K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a positive semidefinite kernel function such that $K(x, x') \lesssim 1$ for all $x, x' \in \mathcal{X}$. Then, $|f|_{\infty} \lesssim 1$ 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
\[
f(x + \Delta) = \sum_{k=0}^{\gamma} \sum_{p: P = k} \frac{\Delta^p D^p f(x)}{k!} + \sum_{p: P = \gamma} \left[ \frac{\Delta^p D^p f(z)}{\gamma!} - \frac{\Delta^p D^p f(x)}{\gamma!} \right]
\]
where $REM_0(x + \Delta)$

where $x, x + \Delta \in (-1, 1)^d$ and $z$ is some intermediate value. For a given $k \in \{0, ..., \gamma\}$, recall
\[
\text{card}(\{p: P = k\}) = \binom{d + k - 1}{d - 1} = D_k^*.
\]
Therefore, we have
\[
|REM_0(x + \Delta)| \leq \frac{D_k^* R_{\gamma+1} |\Delta|_{\infty}^{\gamma+1}}{\gamma!}.
\]
In a similar way, writing
\[
D^{\tilde{p}} f(x + \Delta) = \sum_{k=0}^{\gamma-\tilde{p}} \sum_{p: P = k} \frac{\Delta^p D^{p+\tilde{p}} f(x)}{k!} + \sum_{p: P = \gamma-\tilde{p}} \left[ \frac{\Delta^p D^{p+\tilde{p}} f(z)}{(\gamma - \tilde{p})!} - \frac{\Delta^p D^{p+\tilde{p}} f(x)}{(\gamma - \tilde{p})!} \right]
\]
\[
:= REM_{\tilde{p}}(x + \Delta)
\]
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

\[
|REM_{\tilde{P}}(x + \Delta)| \leq \frac{D^*_{\gamma-\tilde{P}} R_{\gamma-\tilde{P}+1} |\Delta|^{\gamma+1-\tilde{P}}}{(\gamma-\tilde{P})!}.
\] (105)

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 \(f, g \in U^d_{\gamma+1,2}\). Then we have

\[
|f(x + \Delta) - g(x + \Delta)| \leq \left| \sum_{k=0}^{\gamma} \sum_{p: P=k} \frac{\Delta^p}{k!} (D^p f(x) - D^p g(x)) \right| + 2D^*_{\gamma} R_{\gamma+1} |\Delta|^{\gamma+1}.
\]

Let \(\left(\max_{k\in\{1, \ldots, \gamma+1\}} \frac{D^*_{\gamma-1} R_k}{(k-1)!} \sqrt{1}\right) =: R^*\). Consider \(|\Delta|_\infty \leq d^{-1} (R^{*\delta_1}_* \frac{k!}{1})!\) and \(\delta_k = R^* \frac{1}{k!} \delta \frac{k!}{1}!\) for \(k = 0, \ldots, \gamma\). Then,

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

\[
\leq \delta \sum_{k=0}^{\gamma} \frac{1}{k!} + 2\delta \leq 5\delta
\] (106)

where we have used the fact that \(D^*_k \leq d^k\). On each dimension of \([-1, 1]^d\), we consider a \(d^{-1} (R^{*\delta_1}_* \frac{k!}{1})!\)-grid of points. The rest of the arguments follow closely those in Kolmogorov and Tikhomirov (1959).

### D.2 Proof for Lemma 6.2

For a given \(k \in \{0, \ldots, \gamma\}\), let \(\text{card} (\{p: P = k\}) = \binom{d+k-1}{d-1} = \binom{d+k-1}{k} = D^*_k\). Recall the definition of \(U^d_{\gamma+1,1}\):

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

with the \(\Gamma := \sum_{k=0}^{\gamma} D^*_k\)-dimensional polyhedron

\[
\mathcal{P}_\Gamma = \left\{ \theta_{(p,k)} : \{p: P = k\} \in \mathbb{R}^\Gamma : \text{for any given } k, \{\theta_{(p,k)}\}_p \in \left[ \frac{-R_k}{k!}, \frac{R_k}{k!} \right] \right\}
\]

where \(\theta = \{\theta_{(p,k)}\}_{(p,k)}\) denotes the collection of \(\theta_{(p,k)}\) over all \((p, k)\) configurations and \(\{\theta_{(p,k)}\}_p\) denotes the collection of \(\theta_{(p,k)}\) over all \(p\) configurations for a given \(k \in \{0, \ldots, \gamma\}\).
To bound \( \log N_\infty (\delta, \mathcal{U}_{\gamma+1,1}^d) \) from above, note that for \( f, f' \in \mathcal{U}_{\gamma+1,1}^d \), we have

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

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

To cover \( \mathcal{P}_\Gamma \) within \( \delta \)-precision, using arguments similar to those in Section A.1, we find a smallest \( \frac{\delta}{(\gamma+1)D_k^*} \)–cover of \( \left[ -\frac{R_k}{k!}, \frac{R_k}{k!} \right] \) for each \( k = 0, \ldots, \gamma \), \( \{ \theta_1^k, \ldots, \theta_{N_k}^k \} \), such that for any \( \theta \in \mathcal{P}_\Gamma \), there exists some \( i_{(p,k)} \in \{ 1, \ldots, N_k \} \) with

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

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

\[
\log N_2, p (\delta, \mathcal{U}_{\gamma+1,1}^d) \leq \log N_\infty (\delta, \mathcal{U}_{\gamma+1,1}^d) \leq \sum_{k=0}^{\gamma} D_k^* \log \frac{4(\gamma + 1)D_k^* R_k}{\delta k!}.
\]

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

\[
\log N_2, p (\delta, \mathcal{U}_{\gamma+1,1}^d) \leq \log N_\infty (\delta, \mathcal{U}_{\gamma+1,1}^d) \lesssim \left( \sum_{k=0}^{\gamma} D_k^* \right) \log \frac{1}{\delta} + \sum_{k=0}^{\gamma} D_k^* \log R_k.
\]

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