Stratified incomplete local simplex tests for curvature of nonparametric multiple regression

YANGLEI SONG 1, XIAOHUI CHEN 2 and KENGO KATO 3

1 Department of Mathematics and Statistics, Queen’s University, Jeffery Hall, Kingston, ON, Canada, K7L 3N6, E-mail: yanglei.song@queensu.ca
2 Department of Statistics, University of Illinois at Urbana-Champaign, 725 S. Wright Street, Champaign, IL 61820, E-mail: xhchen@illinois.edu
3 Department of Statistics and Data Science, Cornell University, 1194 Comstock Hall, Ithaca, NY 14853, E-mail: kk976@cornell.edu

Principled nonparametric tests for regression curvature in \( \mathbb{R}^d \) are often statistically and computationally challenging. This paper introduces the stratified incomplete local simplex (SILS) tests for joint concavity of nonparametric multiple regression. The SILS tests with suitable bootstrap calibration are shown to achieve simultaneous guarantees on dimension-free computational complexity, polynomial decay of the uniform error-in-size, and power consistency for general (global and local) alternatives. To establish these results, we develop a general theory for incomplete \( U \)-processes with stratified random sparse weights. Novel technical ingredients include maximal inequalities for the supremum of multiple incomplete \( U \)-processes.

Keywords: Nonparametric regression; Curvature testing; Incomplete \( U \)-processes; Stratification

1. Introduction

This paper concerns the hypothesis testing problem for curvature (i.e., concavity, convexity, or linearity) of a nonparametric multiple regression function. Testing the validity of such geometric hypothesis is important for performing high-quality subsequent shape-constrained statistical analysis. For instance, there has been considerable effort in nonparametric estimation of a convex (concave) regression function, partly because estimation under convexity constraint requires no tuning parameter as opposed to e.g. standard kernel estimation whose performance depends critically on a user-chosen bandwidth parameter [41, 40, 54, 32, 60, 53, 11, 10, 33, 15, 12, 38, 47]. In empirical studies such as economics and finance, convex (concave) regressions have wide applications in modeling the relationship between wages and education [57], between firm value and product price [6], and between mutual fund return and multiple risk factors [26, 1].

Consider the nonparametric multiple regression model

\[ Y = f(V) + \varepsilon, \]

where \( Y \) is a scalar response variable, \( V \) is a \( d \)-dimensional covariate vector, \( \varepsilon \) is a random error term such that \( \mathbb{E}[\varepsilon | V] = 0 \) and \( \text{Var}(\varepsilon) > 0 \), and \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) is the conditional mean (i.e., regression) function. Let \( P \) be the joint distribution of \( X = (V, Y) \in \mathbb{R}^{d+1} \) and \( X_i := (V_i, Y_i), i \in [n] := \{1, \ldots, n\} \) be a sample of independent random vectors with common distribution \( P \). For a given convex, compact subset \( \mathcal{V} \subset \mathbb{R}^d \), based on the observations \( \{X_i\}_{i=1}^n \), we aim to test the following hypothesis:

\[ H_0 : f \text{ is concave on } \mathcal{V}, \]
against some (globally or locally) non-concave alternatives. In this work, we directly leverage the simplex characterization of concave functions, i.e., $f$ is concave on $\mathcal{V}$ if and only if
\begin{equation}
 a_1 f(v_1) + \cdots + a_{d+1} f(v_{d+1}) \leq f(a_1 v_1 + \cdots + a_{d+1} v_{d+1}),
\end{equation}
for any $v_1, \ldots, v_{d+1} \in \mathcal{V}$ and nonnegative reals $a_1, \ldots, a_{d+1}$ such that $a_1 + \cdots + a_{d+1} = 1$. Working with this definition allows us to circumvent the need to estimate the regression function $f$, and thus the resulting tests would be robust to model misspecification. Further, the concavity hypothesis can be quantitatively evaluated on the observed data, which is the idea behind the simplex statistic in [1].

Specifically, $d + 1$ covariate vectors in $\mathbb{R}^d$ form a simplex. Consider $r := d + 1$ data points $x_1 := (v_1, y_1), \ldots, x_r := (v_r, y_r) \in \mathbb{R}^{d+1}$ generated from the model (1). If for all $j \in [r]$, $v_j$ is not in the simplex spanned by $\{v_i : i \neq j\}$, for example the vectors $\{v_1, v_2, v_3\}$ in Figure 1, then we set $w(x_1, \ldots, x_r) = 0$. Otherwise, there exists a unique $j$ such that $v_j$ can be written as a convex combination of other covariate vectors, i.e., $v_j = \sum_{i \neq j} a_i v_i$ for some $a_i \geq 0$, $\sum_{i \neq j} a_i = 1$; in this case, we compare the response $y_j$ with the same combination of others, $\{y_i : i \neq j\}$, i.e., setting
\[ w(x_1, \ldots, x_r) = \sum_{i \neq j} a_i y_i - y_j. \]
For example, in Figure 1, $v_4$ is in the simplex spanned by $\{v_1, v_2, v_3\}$. We note that the index $j$ and the coefficients $\{a_i : i \neq j\}$ are functions of $\{v_i : i \in [r]\}$, and defer the precise definitions to Section 3.

If $f$ is indeed concave (i.e., $H_0$ is true) and $\varepsilon$ is symmetric about zero, then $\mathbb{E}\left[\text{sign}(w(X_1, \ldots, X_r))\right] \leq 0$ due to (3), where $\text{sign}(t) := 1(t > 0) - 1(t < 0)$ is the sign function. Thus [1] proposes to use the following global $U$-statistic of all $r$-tuples from $\{X_i : i \in [n]\}$ and reject the null if the statistic is large:
\begin{equation}
|I_{n,r}|^{-1} \sum_{i \in I_{n,r}} \text{sign}(w(X_i)), \text{ with } X_i = (X_{i_1}, \ldots, X_{i_r}),
\end{equation}
where $I_{n,r} := \{i = (i_1, \ldots, i_r) : 1 \leq i_1 < \ldots < i_r \leq n\}$, and $\cdot$ denotes the set cardinality.

1.1. Local simplex statistics

Since the global $U$-statistic in (4) is not consistent against general alternatives, e.g., when $f$ is only non-concave in a small region, [1] also proposes the localized simplex statistics. Specifically, let $L : \mathbb{R}^d \to \mathbb{R}$ be a function such that $L(z) = 0$ if $\|z\|_\infty := \max_{j \in [d]} |z_j| > 1/2$, and $L_b(\cdot) := b^{-d} L(\cdot/b)$ for $b > 0$. For $x_i := (v_i, y_i) \in \mathbb{R}^{d+1}, i \in [r]$, and a bandwidth parameter $b_n > 0$, define
\begin{equation}
h^{\text{gs}}(x_1, \ldots, x_r) := \text{sign}(w(x_1, \ldots, x_r)) b_n^{d/2} \prod_{k=1}^r L_{b_n}(v - v_k), \quad v \in \mathcal{V}.
\end{equation}
Thus for each $v \in \mathcal{V}$, only nearby data points are utilized in constructing a local statistic. Note that $h^{\text{gs}}_v$ depends on $b_n$, which we omit in most places for simplicity of notations.

Given a finite collection of query (or design) points $\mathcal{V}_n \subset \mathcal{V}$, [1] proposes to reject the null if
\begin{equation}
\sup_{v \in \mathcal{V}_n} U_n(h^{\text{gs}}_v) \text{ is large, where } U_n(h^{\text{gs}}_v) := |I_{n,r}|^{-1} \sum_{i \in I_{n,r}} h^{\text{gs}}_v(X_i).
\end{equation}
Testing for regression curvature

Figure 1: Each circle represents a two-dimensional feature vector (i.e., $d = 2$). For each query point $v \in \mathcal{V}$, a sampling plan is a collection of Bernoulli random variables $\{Z_\iota(v) : \iota \in I_{n,r}\}$, one for each subset of $r = d + 2$ data points. If $Z_\iota(v) = 1$, then $h^{sg}_v(X_\iota)$ contributes to the average in (6).

The space $\mathcal{V}$ is stratified into disjoint regions (e.g., 1-by-1 squares above). The query points in each region share the same sampling plan (e.g., $\{Z_\iota(m)\}$ for the dotted region $\mathcal{V}_m$), while different regions have independent sampling plans. For example, the indicator for $\iota = (v_1, v_2, v_3, v_4)$ may be one for $\mathcal{V}_m$, but zero for the dashed region.

Due to the localizing kernel (5), for each query point $v \in \mathcal{V}$, it suffices to consider data points that are within $b/2$ distance to $v$ in each coordinate. Thus for $\mathcal{V}_m$ above, e.g., it suffices to consider data points within the dotted square ($b = 8$). The key idea is that query points in a small region share similar nearby data points, and the region-specific sampling plan allows us to allocate the “limited resources” only in “important areas”.

In [1], it requires the query points in $\mathcal{V}_n$ to be well separately, i.e., $\|v - v'\|_\infty > b_n$ for each pair of distinct $v, v' \in \mathcal{V}_n$, which is restrictive when $d \geq 2$ and $b_n$ cannot be too small. Such a requirement is imposed since [1] uses extreme value theory to obtain the asymptotic distribution of the supremum, for which the convergence of approximation error is known to be logarithmically slow [37].

In [14], a valid jackknife multiplier bootstrap (JMB) is proposed to calibrate the distribution of the supremum of the (local) $U$-process, $\sup_{v \in \mathcal{V}} U_n(h^{sg}_v)$. Even though JMB tailored to the concavity test problem is statistically consistent, it requires tremendous, if not prohibitive, resources to compute $\sup_{v \in \mathcal{V}} U_n(h^{sg}_v)$, as well as calibrating its distribution via bootstrap, for $d \geq 2$. For instance, suppose that $\mathcal{V}$ has a Lebesgue density that is bounded away from zero on $\mathcal{V}$. Then the number of data points within the $b_n$-neighbourhood of $v \in \mathcal{V}$ is on average $O(nb_n^d)$. Thus to compute $U_n(h^{sg}_v)$ for a fixed $v \in \mathcal{V}$, the required number of evaluations of $w(\cdot)$ is on average $O((nb_n^d)^r)$, which is computationally intensive, if $d \geq 2$ (thus $r = 4$), and the bandwidth $b_n$ is not too small. In fact, in the numerical study (Section 5), we estimate that for $d = 3, n = 1000, b_n = 0.6 (b_n/2$ is the half width), it would take more than 7 days to use bootstrap for calibration even with 40 computer cores.
It is tempting to break the computational bottleneck by using the incomplete version of the $U$-process \( \{U_n(h_{\|X\|}^\delta) : v \in V \} \), which has been studied for high-dimensional $U$-statistics [13]. Specifically, we may associate each subset of $r$ data points, $i \in I_{n,r}$, with an independent Bernoulli random variable $Z_i$, and only include $h_{\|X\|}^\delta(X_i)$ in the average in (6) if $Z_i = 1$. Note that this is a centralized sampling plan, in the sense that \( \{Z_i : i \in I_{n,r}\} \) is shared by each $v \in V$. Here, we explain intuitively why such a plan does not solve the computational challenge, and postpone the detailed discussion until Section 4. First, for each $i = (i_1, \ldots, i_r) \in I_{n,r}$, if $\|v_{i_j} - v_{i_k}\|_\infty > b_n$ for some $j, k \in [r]$ (e.g., $v_5, v_6$ in Figure 1), then $h_{\|X\|}^\delta(X_i) = 0$ for each $v \in V$. As a result, with a very high probability, a randomly selected $r$-tuples $X_i$ is “wasted”. Second, if two query points $v, v'$ are not close, in the sense that $\|v - v'\|_\infty > b_n$ (e.g. $v_5, v_6$ in Figure 1 if they are used as query points), then they share no nearby data points as defined by the localizing kernel in (5), which is a property ignored by the centralized sampling.

1.2. Our contributions

In this paper, we introduce the stratified incomplete local simplex (SILS) statistics for testing the concavity assumption in nonparametric multiple regression. We show that SILS tests have simultaneous guarantees on dimension-free computational complexity, polynomial decay of the uniform error-in-size, and power consistency against general alternatives. We elaborate below our contributions, and also refer readers to Figure 1 for a pictorial illustration of key ideas.

Computational contributions. The SILS test is proposed to address the computational issue with the test statistic (6), as well as calibrating its distribution. Specifically, we first partition the space $V$ into disjoint regions \( \{V_m : m \in [M]\} \) for some integer $M \geq 1$. Let $N := n^{\kappa} b_n^{-d}$ be a computational parameter for some $\kappa > 0$, and for each $m \in [M]$, let \( \{Z_{i,m} : i \in I_{n,r}\} \) be a collection of independent Bernoulli random variables with success probability $p_m := N/|I_{n,r}|$, which is called a sampling plan. For different regions, the sampling plans are independent. Then we consider the stratified, incomplete version of (6) as our statistic for testing the hypothesis (2):

\[
\sup_{m \in [M]} \sup_{v \in V_m} \left( \sum_{i \in I_{n,r}} Z_{i,m} h_{\|X\|}^\delta(X_i) \right) / \left( \sum_{i \in I_{n,r}} Z_{i,m} \right)
\]

Similar idea is applied to bootstrap calibration (see Subsection 2.2), which involves another computational parameter $N_2 := n^{\kappa'} b_n^{-d}$ for some $\kappa' > 0$. Due to the localization by the kernel (5) and the stratification (see Figure 1), we show in Section 4.2 that the overall computational cost is $O(M n^{1+\kappa} b_n^{-d} \log(n) + B M n^{1+\kappa} b_n^{-d} \log(n))$, where $B$ is the number of bootstrap iterations. Our theory allows $\kappa, \kappa'$ to be arbitrarily small, but due to power analysis, we recommend $\kappa = \kappa' = 1$. In addition, $M$ is usually chosen so that $M = O(b_n^{-d})$, and to ensure a non-vanishing number of local data points, we must have $b_n^{-d} = O(n)$; thus the cost is independent of the dimension $d$.

Further, to alleviate the burden of selecting a single bandwidth, we propose to use the supremum of the statistics in (7) associated with multiple $b_n$ (Subsection 3.3). Finally, we conduct extensive simulations to demonstrate the computational feasibility of the proposed method, and to corroborate our theory.\footnote{The implementation can be found on the github (https://github.com/ysong44/Stratified-incomplete-local-simplex-tests).}
Statistical contributions. In addition to the function class $\mathcal{H}_{\text{sg}} := \{h^{\text{sg}}_v\}$, which uses the sign of simplex statistics, we also consider another class of functions $\mathcal{H}_{\text{id}} := \{h^{\text{id}}_v\}$, where $h^{\text{id}}_v$ uses $w(\cdot)$ instead of its sign (see (20)); note that $h^{\text{id}}_v$ is unbounded unless $\varepsilon$ has bounded support. On one hand, $\mathcal{H}_{\text{sg}}$ requires the observation noise $\varepsilon$ to be conditionally symmetric about zero [1], but otherwise is robust to heavy tailed $\varepsilon$. On the other hand, $\mathcal{H}_{\text{id}}$ requires $\varepsilon$ to have a light tail, but otherwise imposes no restrictions [14]. For both classes of functions, we establish the size validity, as well as power consistency against general alternatives, for the proposed procedure, under no smoothness assumption on the regression function.

In fact, under fairly general moment assumptions, we derive a unified Gaussian approximation and bootstrap theory for stratified, incomplete $U$-processes (Section 2 and 6), associated with a general function class $\mathcal{H}$, where the SILS test for regression concavity is an application of the general results.

Technical contributions. The analysis of the stratified, incomplete $U$-processes requires a strategy different from the coupling approach used for complete $U$-processes [14]: (i) we establish corresponding results for high dimensional stratified, incomplete $U$-statistics (Appendix B); (ii) we show that the supremum of the process is well approximated by the supremum over a finite, but diverging, collection of $v \in V$. The main novelty are local and non-local maximal inequalities to bound the supremum difference between a complete $U$-process and its stratified, incomplete version (Section 7 and Appendix A.3), which can also be useful for other applications involving sampling, such as estimating the density of functions of several random variables [30].

We note that the developed maximal inequalities are novel compared to [14] and [13]. First, [14] studies complete $U$-processes, and neither stratification nor sampling is involved. Second, [13] establishes inequalities for incomplete high dimensional $U$-vectors, whose proofs are fundamentally different from those for processes, and which does not have the stratification component. See also Remark 3.3 for technical challenges associated with local $U$-processes.

1.3. Related work

Regression under concave/convex restrictions has a long and rich history dating back to [41]. Traditionally, the literature focused on the univariate ($d = 1$) case [40, 54, 32, 10, 33, 15], but there is a significant recent theoretical progress in the multivariate case [60, 53, 38, 47]; see also [55, 46, 39, 56]. We refer readers to [20, 35] for a review on estimation and inference under shape constraints including concave/convexity constraints.

The literature on testing the hypotheses of regression concavity is relatively scarce, especially for multiple regression, i.e., $d \geq 2$. Simplex statistic and its local version are introduced in [1], and the bootstrap calibration (without computational concerns) is investigated in [14]. Several testing procedures based on splines [22, 65, 45] have been proposed, which, however, are only proven to work for the univariate case since they are essentially second-derivative tests at the spline knots. Thus such methods can only test marginal concavity in the presence of multiple covariates, and multi-dimensional spline interpolation is much less understood in the nonparametric regression setting. Further, in the univariate case with a white-noise model, multi-scale testing for qualitative hypotheses is considered in [24], and minimax risks for estimating the $L^q$ distance ($1 \leq q < \infty$) between an unknown signal and the cones of positive/monotone/convex functions are established in [44].

A very recent work by [27] proposes a projection framework for testing shape restrictions including concavity, which we call “FS” test. Specifically, the FS test [27] first estimates the regression function $f$ using unconstrained, nonparametric methods (e.g. by sieved splines), and then evaluate and calibrate the $L^2$ distance between the estimator and the space of concave functions. As discussed in
Appendix E.4, the FS test is expected to achieve descent power, but fails to control the size properly when \( f \) is not smooth; this is because if \( f \) is not smooth enough, there is no choice of tuning parameter (e.g., the number of terms in sieved B-splines) that can meet its two requirements simultaneously: under-smoothing and strong approximation (see Appendix E.4). In simulation studies (Section 5), we observe that the FS test rejects \( H_0 \) with a very large probability when \( f \) is concave, piecewise affine. In contrast, for our procedure, the probability of rejecting the null attains the maximum when \( f \) is an affine function, as the equality in (3) is achieved if and only if \( f \) is affine; thus, the size validity requires no additional assumption on \( f \) (see Subsection 3.2.1). Finally, we show in Section 5 that the proposed method achieves a comparable power to the FS test.

We postpone the discussion of related work on the distribution approximation and bootstrap for \( U \)-processes until Subsection 6.3.

### 1.4. Organization of the paper

In Section 2, we introduce stratified, incomplete \( U \)-processes, as well as bootstrap calibration, for a general function class \( \mathcal{H} \). In Section 3, we apply the general theory to the concavity test application, and establish its size validity and power consistency. In Section 4, we discuss the computational complexity of the proposed procedure as well as its implementation. In Section 5, we present simulation results for \( d = 2 \), with the cases of \( d = 3, 4 \) presented in Appendix D. In Section 6, we establish the validity of Gaussian approximation and bootstrap for stratified, incomplete \( U \)-processes. In Section 7, we highlight a local maximal inequality for multiple incomplete \( U \)-processes, which is one of the main technical contributions. The additional results, proofs, and discussions are presented in Appendix.

### 1.5. Notation

We denote \( X_1, \ldots, X_d \) by \( X_i^d \) for \( i \leq i' \). For any integer \( n \), we denote by \( [n] \) the set \{1, 2, \ldots, \( n \)\}. For \( a, b \in \mathbb{R} \), let \( [a] \) denote the largest integer that does not exceed \( a \), \( a \lor b = \max\{a, b\} \) and \( a \land b = \min\{a, b\} \). For \( a \in \mathbb{R}^d \) and \( q \in [1, \infty) \), denote \( \|a\|_q = \left( \sum_{i=1}^{d} |a_i|^q \right)^{1/q} \), and \( \|a\|_\infty = \max_{i \in [d]} |a_i| \).

For \( a, b \in \mathbb{R}^d \), we write \( a \leq b \) if \( a_j \leq b_j \) for \( 1 \leq j \leq d \), and write \([a, b]\) for the hyperrectangle \( \prod_{j=1}^{d} [a_j, b_j] \) if \( a \leq b \). For \( \beta > 0 \), let \( \psi_\beta : [0, \infty) \to \mathbb{R} \) be a function defined by \( \psi_\beta(x) = e^{x^\beta} - 1 \), and for any real-valued random variable \( \xi \), define \( \|\xi\|_{\psi_\beta} = \inf\{C > 0 : \mathbb{E}[\psi_\beta(|\xi|/C)] \leq 1\} \). Denote by \( I_{n, r} := \{t = (i_1, \ldots, i_r) : 1 \leq i_1 < \ldots < i_r \leq n\} \) the set of all ordered \( r \)-tuples of \([n]\) and denote by \( |\cdot| \) the set cardinality.

For a nonempty set \( T \), denote \( \ell^\infty(T) \) the Banach space of real-valued functions \( f : T \to \mathbb{R} \) equipped with the sup norm \( \|f\|_T := \sup_{t \in T} |f(t)| \). For a semi-metric space \((T, d)\), denote by \( N(T, d, \epsilon) \) its \( \epsilon \)-covering number, i.e., the minimum number of closed \( \epsilon \)-balls with radius \( \epsilon \) that cover \( T \); see [64, Section 2.1]. For a probability space \((T, \mathcal{T}, Q)\) and a measurable function \( f : T \to \mathbb{R} \), denote \( Qf = f dQ \) whenever it is well defined. For \( q \in [1, \infty] \), denote by \( \|\cdot\|_{Q, q} \) the \( L^q(Q) \)-seminorm, i.e., \( \|f\|_{Q, q} = (Q|f|^q)^{1/q} \) for \( q < \infty \) and \( \|f\|_{Q, \infty} \) for the essential supremum.

For \( k = 0, 1, \ldots, r \) and a measurable function \( f : (S^r, \mathcal{S}^r) \to (\mathbb{R}, \mathcal{B}(\mathbb{R})) \), let \( P^{r-k} f \) denote the function on \( S^k \) such that

\[
P^{r-k} f(x_1, \ldots, x_k) = \mathbb{E}[f(x_1, \ldots, x_k, X_{k+1}, \ldots, X_r)],
\]
whenever it is well defined. For a generic random variable $Y$, let $P_{|Y}(\cdot)$ and $E_{|Y}[\cdot]$ denote the conditional probability and expectation given $Y$, respectively. Throughout the paper, we assume that

$$r \geq 2, \quad d \geq 3, \quad n \geq 4, \quad N \geq 4, \quad p_n := N/|I_{n,r}| \leq 1/2, \quad N \geq n/r \geq 1. \quad (8)$$

Also, we assume the probability space is rich enough in the sense that there exists a random variable that has the uniform distribution on $(0,1)$ and is independent of all other random variables.

2. Stratified incomplete $U$-processes

In this section, we introduce stratified, incomplete $U$-processes, as well as bootstrap calibration, for a general function class $\mathcal{H}$. For intuitions, it may help to think of $\mathcal{H}$ as the collection of functions $h_{n,r}^\mathcal{Y}$ in (5) indexed by $v \in \mathcal{Y}$, and refer to Figure 1.

Thus, let $X_{1}^{n} := \{X_{1}, \ldots, X_{n}\}$ be independent and identically distributed (i.i.d.) random variables taking value in a measurable space $(S,S)$ with common distribution $P$. Fix $r \geq 2$, and let $\mathcal{H}$ be a collection of symmetric, measurable functions $h : (S^n, S^n) \to (\mathbb{R}, B(\mathbb{R}))$. Define the $U$-process and its standardized version as follows: for $h \in \mathcal{H}$,

$$U_{n}(h) := \frac{1}{|I_{n,r}|} \sum_{i \in I_{n,r}} h(X_{i_{1}}, \ldots, X_{i_{r}}), \quad U_{n}(h) := \frac{1}{|I_{n,r}|} \sum_{i \in I_{n,r}} h(X_{i}),$$

$$\mathbb{U}_{n}(h) := \sqrt{n} \left( U_{n}(h) - \mathbb{E}[U_{n}(h)] \right). \quad (9)$$

The summation in the above complete $U$-process involves $\sim n^r$ terms, and thus is computationally expensive even for a moderate $r$ (say $\geq 3$), which motivates its stratified incomplete version.

2.1. Test statistics

Let $\{H_{m} : m \in [M]\}$ be a partition of $\mathcal{H}$, i.e., $H_{m_{1}} \cap H_{m_{2}} = \emptyset$ for $m_{1} \neq m_{2}$, and $\bigcup_{m=1}^{M} H_{m} = \mathcal{H}$. The partition, and thus $M$, may depend on the sample size $n$. Given a positive integer $N$, which represents a computational parameter, define

$$\{Z_{i}^{(m)} : m \in [M], \quad i \in I_{n,r}\} \overset{i.i.d.}{\sim} \text{Bernoulli}(p_n), \quad \text{with } p_n := N/|I_{n,r}|,$$

which are independent of the data $X_{1}^{n}$. For $m \in [M]$, denote by $\tilde{N}^{(m)} := \sum_{i \in I_{n,r}} Z_{i}^{(m)}$ the total number of sampled $r$-tuples for the subclass $H_{m}$. Further, define a function $\sigma : \mathcal{H} \to \{1, \ldots, M\}$ that maps $h \in \mathcal{H}$ to the index of the partition $h$ belongs:

$$\sigma(h) = m \iff h \in H_{m}.$$ 

Finally, we define the stratified, incomplete $U$-process and its standardized version: for $h \in \mathcal{H}$,

$$U'_{n,N}(h) := \frac{1}{N(\sigma(h))} \sum_{i \in I_{n,r}} Z_{i}^{(\sigma(h))} h(X_{i}),$$

$$\mathbb{U}'_{n,N}(h) := \sqrt{n} \left( U'_{n,N}(h) - \mathbb{E}[U'_{n,N}(h)] \right). \quad (10)$$
An important goal of the paper is to develop bootstrap methods to calibrate the distribution of the supremum of the stratified incomplete $U$-process:

$$M_n := \sup_{h \in \mathcal{H}} U'_{n,N}(h). \quad (11)$$

**Statistical tests.** We will use $\sqrt{n} \sup_{h \in \mathcal{H}} U'_{n,N}(h)$ as the *test statistic*, which can be evaluated given the data $X_1^n$ and sampling plans $\{Z^{(m)}_i\}$. If under the null, $P^r h \leq 0$ for each $h \in \mathcal{H}$, then

$$\sqrt{n} \sup_{h \in \mathcal{H}} U'_{n,N}(h) \leq \sup_{h \in \mathcal{H}} U'_{n,N}(h) = M_n.$$ 

Thus a test based on the $\alpha$-th upper quantile of $M_n$ controls the size below $\alpha$. If, in addition, under certain configuration in the null, $P^r h = 0$ for each $h \in \mathcal{H}$, then the test is *non-conservative*, i.e., controlling the size at $\alpha$.

**Remark 2.1.** A stratification of $\mathcal{H} = \{h^{(v)}_k : v \in \mathcal{V}\}$ is equivalent to partitioning $\mathcal{V}$ into sub-regions $\{\mathcal{V}_m : m \in [M]\}$ and letting $\mathcal{H}_m = \{h^{(v)}_k : v \in \mathcal{V}_m\}$ (see Figure 1). Query points in $\mathcal{V}_m$ share the same sampling plan $\{Z^{(m)}_i \cdot : i \in [n,r]\}$.

As we shall see in Section 4, it is computationally important to partition the function class $\mathcal{H}$ so that each partition has its individual sampling plan. Our analysis is non-asymptotic, so no stratification ($M = 1$) is also allowed.

### 2.2. Bootstrap calibration

To operationalize the above test, we use multiplier bootstrap to calibrate the distribution of $M_n$. To gain intuition, assume for a moment $P^r h = 0$ for $h \in \mathcal{H}$, and observe that

$$(\hat{\sigma}^2(h) N^{-1}) U'_{n,N}(h) = U_n(h) + \sqrt{n} N^{-1} \sum_{i \in I_{n,r}} (Z^{(\hat{\sigma}(h))}_i - p_n) h(X_i). \quad (12)$$

The first term on the right is a complete $U$-statistic, and thus is approximated by its Hájek projection $\tau_n \sum_{k \in [r]} P^{r-1} h(X_k)$. The second term is due to stratified sampling: *conditional* on data $X^n_1$, it is a sum of independent centered Bernoulli random variables, with variance approximately given by $nN^{-1} U_n(h^2)$. We will handle these two sources of variation.

The Hájek projection part requires additional notations. Let $\mathcal{D}_n := X_1^n \cup \{Z^{(m)}_i \cdot : i \in I_{n,r}, m \in [M]\}$ be the data involved in the definition of $U'_{n,N}$ in (10). For each $k \in [n]$, denote by

$$I^{(k)}_{n-1,r-1} := \{(i_1, \ldots, i_{r-1}) : 1 \leq i_1 < \cdots < i_{r-1} \leq n, \ i_j \neq k \ \text{for} \ 1 \leq j \leq r - 1 \},$$

the collection of all ordered $r - 1$ tuples in the set $\{1, \ldots, n\} \setminus \{k\}$. Let $N_2$ be another computational budget, and define

$$\left\{ Z^{(k,m)}_i : k \in [n], m \in [M], i \in I^{(k)}_{n-1,r-1} \right\} \stackrel{i.i.d.}{\sim} \text{Bernoulli}(q_n), \ q_n := N_2 / |I_{n-1,r-1}|,$$

that are independent of $\mathcal{D}_n$. For $\mathcal{H} = \{h^{(v)}_k : v \in \mathcal{V}\}$, each pair of data point $X_k$ and region $\mathcal{V}_m$ is associated with an independent sampling plan $\{Z^{(k,m)}_i \cdot : i \in I_{n,r}\}$; see Figure 1.
Further, denote $\widehat{N}^{(k,m)}_2 := \sum_{i \in I^{(k)}_{n-1,r-1}} Z^{(k,m)}_i$ for $k \in [n]$ and $m \in [M]$, and define for $k \in [n]$, $h \in \mathcal{H}$, and $m = \sigma(h)$,

$$
\mathbb{G}^{(k)}(h) := \frac{1}{\widehat{N}^{(k,m)}_2} \sum_{i \in I^{(k)}_{n-1,r-1}} Z^{(k,m)}_i h(X_i), \quad \mathbb{G}(h) := \frac{1}{n} \sum_{k=1}^n \mathbb{G}^{(k)}(h),
$$

where $\iota^{(k)} := \{k\} \cup \iota$. Here, $\mathbb{G}^{(k)}(h)$ is intended as an estimator for the $k^{th}$ term in the Hájek projection, since by definition $E[h(X_{\iota^{(k)}})] = D^{r-1} h(X_k)$.

**Multiplier bootstrap.** Now let $\{\xi_k, \xi^{(m)}_i : k \in [n], m \in [M], i \in I_{n,r}\} \sim N(0,1)$ be independent standard Gaussian multipliers, independent from the data $X^n_1$ and the sampling plans, i.e.,

$$
D'_n := D_n \cup \{Z^{(k,m)}_i : k \in [n], m \in [M], i \in I^{(k)}_{n-1,r-1}\}.
$$

Define for $h \in \mathcal{H}$ and $m = \sigma(h)$,

$$
U^\#_{n,A}(h) := \frac{1}{\sqrt{M}} \sum_{k=1}^n \xi_k \left( \mathbb{G}^{(k)}(h) - \mathbb{G}(h) \right),
$$

$$
U^\#_{n,B}(h) := \frac{1}{\sqrt{M(n)}} \sum_{i \in I_{n,r}} \xi^{(m)}_i \sqrt{Z^{(m)}_i} \left( h(X_i) - U^r_{n,N}(h) \right),
$$

where 0/0 is interpreted as 0. Note that the multipliers $\{\xi_k\}$ are shared across regions, while $\{\xi^{(m)}_i\}$ are region-specific. In view of (12) (and also (32)), we combine these two processes and define $\alpha_n := n/N$,

$$
U^\#_{n,s}(h) := r U^\#_{n,A}(h) + \alpha_n^{1/2} U^\#_{n,B}(h) \quad \text{for } h \in \mathcal{H}, \quad M^\#_n := \sup_{h \in \mathcal{H}} U^\#_{n,s}(h).
$$

Finally, we estimate the conditional (on $D'_n$) distribution of $M^\#_n$ by bootstrap, i.e., by repeatedly generating independent realizations of the multipliers $\{\xi_k, \xi^{(m)}_i\}$ with the data $X^n_1$ and the sampling plans $\{Z^{(m)}_i, Z^{(k,m)}_i\}$ fixed, and obtain the critical value for the previous test statistic from the conditional distribution of $M^\#_n$.

### 2.3. A simplified version of approximation results

To justify the bootstrap procedure, we need to show that conditional on $D'_n$, the distribution of $M^\#_n$ is close to that of $M_n$, which is the main result in Section 6. Here we state a simplified version of the approximation results for a uniformly bounded function class $\mathcal{H}$. Note that the bound on $\mathcal{H}$ is allowed to vary with $n$.

**Definition 2.2** (VC type function class [14, 18]). A collection, $\mathcal{H}$, of functions on $S'$ with a measurable envelope function $H$ (i.e. $H \geq \sup_{h \in \mathcal{H}} |h|$ pointwise) is said to be VC type with characteristics $(A, \nu)$ if $\sup_{Q} N(\mathcal{H}, \| \cdot \|_{H}, Q) \leq (A/\nu)^\nu$ for any $\nu \in (0,1)$, where $\sup_{Q}$ is taken over all finitely discrete probability measures on $S'$.
We work with the following assumptions.

(PM). $\mathcal{H}$ is pointwise measurable in the sense that for any $n \in \mathbb{N}$, there exists a countable subset $\mathcal{H}'_n \subset \mathcal{H}$ such that, almost surely, for every $h \in \mathcal{H}$, there exists a sequence $\{h_m\} \subset \mathcal{H}'_n$ with $\lim_m h_m(X_i) = h(X_i)$ for $i \in [n]$.

(VC). $\mathcal{H}$ is VC type with envelope $H$ and characteristics $A \geq e \vee (e^{2(r-1)/16})$ and $\nu \geq 1$. Denote $K_n := \nu \log(A \vee n)$.

(MB). For some absolute constant $C_0 > 0$, $\log(M) \leq C_0 \log(n)$.

(MT-$\infty$). There exist absolute constants $\sigma > 0$, $c_0 \in (0, 1)$, and a sequence of reals $D_n \geq 1$ such that for each $0 \leq \ell \leq r$ and $1 \leq s \leq 4$,

$$\begin{align*}
\text{Var} \left( P^{r-\ell} h(X_1) \right) &\geq \sigma^2, & \text{Var} (h(X_1^r)) &\geq c_0 D_n^{2r-2}, \\
\|P^{r-\ell} h^s\|_{P^r,\tilde{q}} &\leq D_n^{2r(s-1)+2\ell-s-2\ell/q}, & \text{for } &\tilde{q} \in \{2, 3, 4\}, h \in \mathcal{H}, \\
\|P^{r-\ell} H^s\|_{P^r,\tilde{q}} &\leq D_n^{2r(s-1)+2\ell-s-(2\ell-2)/q}, & \text{for } &\tilde{q} \in \{2, \infty\}, & \| (P^{r-2} H)^{\circ 2} \|_{P^2,\infty} &\leq D_n^4,
\end{align*}$$

where for a function $f : S^2 \to \mathbb{R}$, define $f^{\circ 2}(x_1, x_2) := \int f(x_1, x) f(x_2, x) dP(x)$.

**Theorem 2.3.** Assume the conditions (PM), (VC), (MB) and (MT-$\infty$). Then there exists a constant $C$, depending only on constants $r, \sigma, c_0, C_0$, such that with probability at least $1 - C g_n^0$,

$$\sup_{t \in \mathbb{R}} \left| \mathbb{P}(M_n \leq t) - \mathbb{P}(M_n^\# \leq t) \right| \leq C g_n^0,$$

where $g_n^0 := \left( \frac{D_n^{2r} N^2}{N+N_2} \right)^{1/8} + \left( \frac{D_n^{2r} N^2}{n} \right)^{1/8} + \left( \frac{D_n^{2r} N^2}{n} \right)^{2/7}$.

**Proof.** It follows from Theorem 6.1 and Theorem 6.2. Specifically, (MT-$\infty$) verifies (MT) with $q = \infty$ and $B_n = D_n^{r-2}$. Further, we may without loss of generality assume that $\eta_n^{(1)}, \eta_n^{(2)}$ and $\rho_n$, in Theorem 6.1 and 6.2, are bounded by 1, and then it is clear that $\eta_n^{(1)} + \eta_n^{(2)} + \rho_n \leq C g_n^0$.

**Remark 2.4.** The condition (MB) requires $\log(M) \leq C_0 \log(n)$, and the impact of $M$ has been absorbed into $K_n$, since $K_n \geq \log(n)$.

The condition (MT-$\infty$) is motivated by the application of testing the concavity of a regression function in Section 3. It holds if we use (i), the sign kernel $\{h^{s,g}_v : v \in \mathcal{V}\}$ in (5) or (ii), the identity kernel $\{h^{s,g}_v : v \in \mathcal{V}\}$ in (20) under the additional assumption that the observation noise $\varepsilon$ in (1) is bounded. The more general results in Section 6 are required to remove this assumption.

3. Stratified incomplete local simplex tests: statistical guarantees

In this section, we apply the general theory in Section 2 to the concavity test of a regression function, i.e., $H_0$ in (2), formally introduce stratified incomplete local simplex tests, and establish the size validity and power consistency. Finally, we propose a test that combines multiple bandwidths.
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We first recall the simplex statistics proposed in [1]. For \( v_1, \ldots, v_{d+1} \in \mathbb{R}^d \), denote by

\[
\Delta^0(v_1, \ldots, v_{d+1}) := \left\{ \sum_{i=1}^{d+1} a_i v_i : \sum a_i = 1, \ a_i > 0 \text{ for } i \in [d+1] \right\}
\]

the interior of the simplex spanned by \( v_1, \ldots, v_{d+1} \), and define \( S := \bigcup_{j=1}^{r} S_j \), where \( r := d + 2 \) and

\[
S_j = \left\{ (v_1, \ldots, v_r) \in \mathbb{R}^{d \times r} : v_1, \ldots, v_{j-1}, v_{j+1}, \ldots, v_r \text{ are affinely independent and } v_j \in \Delta^0(v_1, \ldots, v_{j-1}, v_{j+1}, \ldots, v_r) \right\}.
\]

Clearly, \( S_1, \ldots, S_r \) are disjoint. To illustrate, in Figure 1, \( (v_1, v_2, v_3, v_4) \in S_4 \), but \( (v_1, v_2, v_3, v_5) \not\in S \). For \( j \in [r] \), there exists a unique collection of functions \( \{ \tau_{k}^{(j)} : S_j \to (0, 1) : i \in [r] \setminus \{j\} \} \) such that for any \( v_1^i := (v_1, \ldots, v_r) \in S_j \),

\[
v_j = \sum_{i \in [r] \setminus \{j\}} \tau_{i}^{(j)}(v_1^i) v_i, \quad \sum_{i \in [r] \setminus \{j\}} \tau_{i}^{(j)}(v_1^i) = 1.
\]

Now define \( w : \mathbb{R}^{(d+1) \times r} \to \mathbb{R} \) as follows: for \( x_i := (v_i, y_i) \in \mathbb{R}^{d+1} \), \( i \in [r] \),

\[
w(x_1, \ldots, x_r) := \sum_{j=1}^{r} \left( \sum_{i \in [r] \setminus \{j\}} \tau_{i}^{(j)}(v_1^i) y_i - y_j \right) \mathbb{1} \{ v_1^i \in S_j \}.
\]

It is clear that \( S \) is permutation invariant for \( v_1, \ldots, v_r \), and that \( w(\cdot) \) is symmetric in its arguments. Key observations are that if the regression function \( f \) is concave (i.e. \( H_0 \) holds), then \( P^r w \leq 0 \), and that if \( f \) is an affine function, \( P^r w = 0 \), where recall that \( P \) is the distribution of \( X := (V, Y) \).

Let \( L(\cdot) \) be a kernel function and \( b_n > 0 \) be a bandwidth parameter. Define for \( x_i := (v_i, y_i) \in \mathbb{R}^{d+1} \), \( i \in [r] \),

\[
h^{id}_{v}(x_1, \ldots, x_r) := w(x_1, \ldots, x_r) b_n^{d/2} \prod_{k=1}^{r} L_{b_n}(v - v_k), \quad v \in \mathcal{V},
\]

where recall \( L_b(\cdot) := b^{-d} L(\cdot / b) \) for \( b > 0 \).

Now let \( \mathcal{H}^{id} := \{ h^{id}_{v} : v \in \mathcal{V} \} \), and \( \{ \mathcal{V}_m : m \in [M] \} \) be a partition of \( \mathcal{V} \); see Figure 1. Then \( \mathcal{H}^{id}_m := \{ h^{id}_{v} : v \in \mathcal{V}_m \} : m \in [M] \} \) is a partition of \( \mathcal{H}^{id} \). Recall the definitions of \( U^r_{n,N}(\cdot) \) in (10), \( D^r_{n} \) in (14), and \( M_{n}^{\#} \) in (16). For \( \alpha \in (0,1) \), denote by \( q_{\alpha}^{\#} \) the \( (1 - \alpha)^{th} \) quantile of \( M_{n}^{\#} \) conditional on \( D^r_{n} \). We propose to reject the null in (2) if and only if

\[
\sup_{v \in \mathcal{V}} \sqrt{n} U^r_{n,N}(h^{id}_{v}) \geq q_{\alpha}^{\#}.
\]

**Sign function.** We also consider the function class \( \mathcal{H}^{sg} := \{ h^{sg}_{v} : v \in \mathcal{V} \} \), where \( h^{sg}_{v} \) is defined in (5).

As we shall see, \( \{ h^{sg}_{v} : v \in \mathcal{V} \} \) has the advantage of being bounded, but it requires that the conditional distribution of \( \varepsilon \) given \( V \) is symmetric about zero. On the other hand, \( \{ h^{id}_{v} : v \in \mathcal{V} \} \) imposes no assumption on the shape of the conditional distribution, but requires \( \varepsilon \) to have a light tail; in this Section, we assume \( \varepsilon \) to be bounded for \( \{ h^{id}_{v} : v \in \mathcal{V} \} \) so that we can apply Theorem 2.3, and relax this assumption in Appendix.
3.1. Assumptions for concavity tests

We assume the distribution of \((V, \varepsilon)\) in (1) to be fixed, but allow \(f\) to depend on the sample size \(n\), which permits the study of local alternatives. We make the following assumptions: for some absolute constant \(C_0 > 1\),

(C1). The kernel \(L : \mathbb{R}^d \to \mathbb{R}\) is continuous, of bounded variation, and has support \([-1/2, 1/2]^d\). Or \(L(\cdot)\) is the uniform kernel on \([-1/2, 1/2]^d\), i.e., \(L(v) = \mathbb{1}\{v \in (-1/2, 1/2)^d\}\) for \(v \in \mathbb{R}^d\).

(C2). The number of partitions, \(M\), grows at most polynomially in \(n\), i.e., \(\log(M) \leq C_0 \log(n)\).

(C3). The bandwidth \(b_n\) does not vanish too fast in \(n\), i.e., \(1 \leq b_n^{-3d/2} \leq C_0 n^{1-1/C_0}\).

(C4). \(V\) has a Lebesgue density \(p\) such that \(C_0^{-1} \leq p(v) \leq C_0\) for \(v \in V^{2b_n}\), where \(V^b := \{v' \in \mathbb{R}^d : \inf_{v'' \in V} \|v' - v''\|_\infty \leq b\}\) is the \(b\)-enlargement of \(V\).

(C5). Assume for \(* = \text{id} or \text{sg}\) and \(n \geq C_0\), \(\inf_{v \in V} \text{Var}(P^{r-1}h_v^*(X_1)) \geq C_0^{-1}\).

(C6-id') Assume that \(\sup_{v \in V^{b_n}} |f(v)| \leq C_0\) and that \(\varepsilon\) is bounded by \(C_0\) almost surely.

(C6-sg') Assume that \(\sup_{v \in V^{b_n}} |f(v)| \leq C_0\), and that \(\varepsilon\) is independent of \(V\), symmetric about zero, i.e., \(\mathbb{P}(\varepsilon > t) = \mathbb{P}(\varepsilon < t)\) for any \(t > 0\), and \(\mathbb{P}(\varepsilon > 2C_0) > 0\).

Some comments are in order. (C1) is a standard assumption on the kernel \(L\), which is satisfied by many commonly used kernels. Recall that \(V\) is compact, so (C2) is satisfied if we partition each coordinate into segments of length \(\eta b_n\) for some small \(\eta \in (0, 1)\). (C3) imposes the same condition on the bandwidth \(b_n\) as for the procedure using the complete \(U\)-process [14, (T5) in Section 4], which holds as long as \(n^{-2/(3d+3)} \leq b_n\) for arbitrarily small \(\eta \in (0, 1)\); in comparison, [1] has a (slightly) milder condition on the bandwidth, \(n^{-1/d} \eta \leq b_n\) for the discretized \(U\)-statistics. (C4) is necessary that for each \(v \in V\), there are enough data points in the \(b_n\)-neighbourhood of \(v\). The condition (C6-id') is assumed for the class \(\mathcal{H}^{ld}\), while (C6-sg') for \(\mathcal{H}^{sg}\).

Now we focus on (C5) with the function class \(\mathcal{H}^{ld}\), as the discussion for \(\mathcal{H}^{sg}\) is similar. For simplicity, assume \(\varepsilon = 0\) and \(V \in (1)\) are independent. By a change-of-variable and due to the fact that \(\tau_i^{(j)}(v - b_n u_1, \ldots, v - b_n u_r) = \tau_i^{(j)}(u_1, \ldots, u_r)\),

\[
\mathbb{E}
\left[
\text{Var}
\left(P^{r-1}h_v^*(V_1, Y_1)|V_1\right)
\right] = \text{Var}(\varepsilon) \int p(v - b_n u_1) L^2(u_1) T_v(u_1) du_1,
\]

where

\[
T_v(u_1) = \int \left( \mathbb{1}\{u_1^r \in S_1\} - \sum_{j=2}^r \tau_i^{(j)}(u_1^r) \mathbb{1}\{u_1^r \in S_j\} \right) \prod_{i=2}^r L(u_i) p(v - b_n u_i) du_i.
\]

The key observation is that \(\text{Var}(P^{r-1}h_v^*(X_1))\) does not vanish as \(b_n \to 0\). Then we can find more primitive conditions for (C5). For example, (C5) holds if \(L(\cdot) = \mathbb{1}\{\cdot \in (-1/2, 1/2)^d\}\), \(p\) is continuous on \(V\), and \(\lim_{n \to \infty} b_n = 0\).

**Remark 3.1.** In Appendix E.1, we relax the condition (C6-id'), requiring \(\varepsilon\) to have a light tail, instead of being bounded; see (C6-id). Further, in Appendix E.2, we relax the condition (C6-sg'), allowing \(\varepsilon\) and \(V\) to be dependent, and \(\varepsilon\) to have limited support; see (C6-sg).
3.2. Size validity and power consistency

The following is the master theorem for the statistical guarantees for the stratified incomplete local simplex tests.

**Theorem 3.2.** Consider the function class \( \mathcal{H}^{id} \) or \( \mathcal{H}^{sg} \). Assume that (C1)-(C5) hold and that (C6-id') (resp. (C6-sg')) holds for \( \mathcal{H}^{id} \) (resp. \( \mathcal{H}^{sg} \)). Further, for some \( \kappa, \kappa' > 0 \),

\[
N := n^{\kappa} b_n^{-d r}, \quad N_2 := n^{\kappa'} b_n^{-dr}.
\]  
(22)

Then there exists a constant \( C \), depending only on \( C_0, d, \kappa, \kappa' \), such that with probability at least \( 1 - C n^{-1/C} \),

\[
\sup_{t \in \mathbb{R}} \left| \mathbb{P}(M_n \leq t) - \mathbb{P}_{D_n}(M_n^\# \leq t) \right| \leq C n^{-1/C}.
\]

**Proof.** In Appendix E.1 and E.2, we show that (PM) and (VC) is implied by (C1), where the latter is due to [31, Proposition 3.6.12]. (MB) is the same as (C2). Further, we verify that (MT-\( \infty \)) holds with \( D_n = C b_n^{-d/2} \). Then the proof is complete by Theorem 2.3 and due to the requirement on the bandwidth, i.e., (C3).

**Remark 3.3.** The main challenge in working with \( \{ h_v^{id} : v \in V \} \) (and also with \( \mathcal{H}^{id} \)) is that the size of the projections of the kernels, \( \{ \text{Pr} h_v^{id} : \ell = 0, 1, \ldots, r \} \) has different orders of magnitude due to localization. The same is true for the absolute moments of \( \{|h_v^{sg}|^s\} \) for \( s \geq 1 \). Specifically, in Appendix E.2, we verify (17) holds for any \( \bar{q} \geq 1 \). Thus for a fixed \( s \), projections onto consecutive levels differ by a factor of \( b_n^{-d(1-1/\bar{q})} \). On the other hand, for a fixed \( \ell \), the second moment \((s = 2)\) is greater than the first moment \((s = 1)\) by a factor \( b_n^{-d(r-1/2)} \).

The next Corollary establishes the size validity of the proposed procedure. Among all concave functions, affine functions have the largest rejection probabilities, which attain the nominal levels uniformly over \((0, 1)\) for large \( n \).

**Corollary 3.4 (Size validity).** Consider the procedure (21) for testing the hypothesis (2) with \( \mathcal{H}^* \) for \( * = id \) or sg. Assume the conditions in Theorem 3.2 hold. If the regression function \( f \) is concave, i.e., \( H_0 \) holds, then for some constant \( C \), depending only on \( C_0, d, \kappa, \kappa' \),

\[
\mathbb{P} \left( \sup_{v \in V} \sqrt{n} U_{n,N}^\ell(h_v^*) \geq q_\alpha^\# \right) \leq \alpha + C n^{-1/C}, \text{ for any } \alpha \in (0,1).
\]

Further, if \( f \) is an affine function, then

\[
\sup_{\alpha \in (0,1)} \left| \mathbb{P} \left( \sup_{v \in V} \sqrt{n} U_{n,N}^\ell(h_v^*) \geq q_\alpha^\# \right) - \alpha \right| \leq C n^{-1/C}.
\]

**Proof.** If \( f \) is concave, then \( P^\ell h_v^* \leq 0 \) for \( v \in V \). Further, if \( f \) is linear, then \( P^\ell h_v^* = 0 \) for \( v \in V \). Then the results follows from Theorem 3.2.

The next Corollaries concern the power of the proposed procedure. The proofs can be found in Appendix E.3.
Corollary 3.5 (Power). Consider the setup as in Corollary 3.4. If in addition
\[ \sqrt{n} P_n^r h_{v_n}^* \geq (C_0)^{-1} n^{\kappa''}, \text{ for some } v_n \in V, \quad \kappa'' > \max \{(1 - \kappa)/2, 0\}, \]  \tag{23}
then for some constant $C$, depending only on $C_0, d, \kappa, \kappa', \kappa''$, 
\[ \mathbb{P} \left( \sup_{v \in V} \sqrt{n} U_{n,N}^r(h_{v_n}^*) \geq q_{\alpha} \right) \geq 1 - C n^{-1/C}, \text{ for any } \alpha \in (0, 1). \]

Remark 3.6. The condition (23) ensures that the bias $\sqrt{n} P_n^r h_{v_n}^*$ is significantly larger than the standard deviation of $U_{n,N}^r(h_{v_n}^*)$. If $\kappa \geq 1$, then $\kappa''$ in (23) can be arbitrarily small. Note that due to (C2), the impact of $M$ is absorbed into the constant $C$.

Next we provide examples for which (23) holds, and focus on the class $H_{id}$. The discussion for $H_{*g}$ is similar.

Corollary 3.7 (Power - smooth $f$). Consider the setup as in Corollary 3.4. Assume that $f$ is fixed and twice continuously differentiable at some $v_0 \in V$ with a positive definite Hessian matrix at $v_0$, and that $\lim_{n \to \infty} b_n = 0$. Then $\liminf_{n \to \infty} P_n^r h_{v_0}^* \left( b_n^{2+d/2} \right) > 0$. Thus if $b_n^{(d+4)} \leq C_0 n^{1-2\kappa''}$ for some $\kappa'' > \max \{(1 - \kappa)/2, 0\}$, then for any $\alpha \in (0, 1)$, the power converges to one as $n \to \infty$.

Remark 3.8. Note that Theorem 7 in [1] establishes the consistency of their test using $H_{*g}$ (discrete, complete version) under the condition that $n b_n^{d+4} / \log(n) \to \infty$, which is in the same spirit as the requirement on $b_n$ in Corollary 3.7.

Corollary 3.9 (Power - piecewise affine $f$). Consider the setup as in Corollary 3.4. For $j \in \{1, 2\}$, let $\theta_{n,j} \in \mathbb{R}^d$ and $\omega_{n,j} \in \mathbb{R}$ such that $\theta_{n,1} \neq \theta_{n,2}$. Let 
\[ f(v) = f_n(v) := \max \{ f_{n,1}(v), f_{n,2}(v) \}, \quad \text{where} \quad f_{n,j}(v) := \theta_{n,j}^T v + \omega_{n,j} \text{ for } j = 1, 2. \]

If there exists $v_n \in V$ such that $f_{n,1}(v_n) = f_{n,2}(v_n)$ for each $n$, then
\[ \liminf_{n \to \infty} P_n^r h_{v_n}^* \left( b_n^{1+d/2} \|\theta_{n,1} - \theta_{n,2}\|_2 \right) > 0. \]

Thus if $b_n^{(d+2)} \leq C_0 n^{1-2\kappa''} \|\theta_{n,1} - \theta_{n,2}\|_2^2$ for some $\kappa'' > \max \{(1 - \kappa)/2, 0\}$, then for any $\alpha \in (0, 1)$, the power converges to one as $n \to \infty$.

Remark 3.10. If $f$ does not depend on $n$, in particular $\theta_{n,j} = \theta_j$ for each $n$, then the requirement on $b_n$ becomes $b_n^{-(d+2)} \leq C_0 n^{1-2\kappa''}$, which is weaker than that for smooth functions $f$ in Corollary 3.7.

On the other hand, if we choose $b_n = b > 0$ for each $n$, then to achieve power consistency, we require $\|\theta_{n,1} - \theta_{n,2}\|_2 \geq C^{-1} n^{-1/2 + \kappa''}$. Observe that $f_n$ is convex if $\theta_{n,1} \neq \theta_{n,2}$, and affine if $\theta_{n,1} = \theta_{n,2}$. Thus this allows "local alternatives" that approach the null at the rate of $n^{-1/2 + \kappa''}$.

3.2.1. Discussions

The stratified incomplete local simplex test (SILS) is a least favorable configuration test, with affine functions being least favorable. Specifically, for any regression functions $f_1, f_2$, if for any $j \in [r]$ and
\( \sum_{i \in [r] \setminus \{j\}} \tau_i^{(j)}(v_i^*) f_1(v_i) - f_1(v_j) \leq \sum_{i \in [r] \setminus \{j\}} \tau_i^{(j)}(v_i^*) f_2(v_i) - f_2(v_j), \) \tag{24}

then the test statistic \( \sup_{v \in V} \sqrt{n}U_{n,N}(h_v^*) \) for \( f_1 \) is stochastically smaller than for \( f_2 \). In particular, for a concave function \( f \) (i.e., in \( H_0 \)), we have \( \sum_{i \in [r] \setminus \{j\}} \tau_i^{(j)}(v_i^*) f(v_i) - f(v_j) \leq 0 \), with equality for affine functions.

**Remark 3.11.** The least favourable configuration type test was first proposed for testing the monotonicity of a (univariate) regression function by [29], and then extended to test the (multi-variate, coordinate-wise) stochastic monotonicity by [49], and to test the (multi-variate) convexity by [1]. See also [14] for the distribution approximation of these test statistics. It is not clear how to extend this idea to test other shape constraints, such as quasi-convexity [45], because it is not easy to identify the least favourable configuration, or to compute the expectation of test statistics under it.

From Corollary 3.4, the SILS test is asymptotically non-conservative; however, it is non-similar [50], in the sense that for strictly concave functions, the probability of rejection is strictly less than the nominal level \( \alpha \). Being non-similar alone is not evidence against the SILS test (e.g., Z-test for normal means is optimal despite being non-similar), but a least favorable configuration test may be less powerful than alternative tests. The condition (23) requires “local convex curvature” of \( f \), but a least favorable configuration test may be less powerful than alternative tests. The condition (23) requires “local convex curvature” of \( f \), but a least favorable configuration test may be less powerful than alternative tests. The question of how (23) is related to the local L2 separation rate (see Appendix E.4) is left for future research.

In Appendix E.4, we discuss the \( L_2 \) minimax separation rate for concavity test, and an alternative test (“FS” test) [27], which (almost) achieves the minimax rate for smooth functions for \( d = 1 \) and may do so for \( d \geq 2 \); thus the FS test is expected to have decent power. We note that the validity of our SILS test does not require \( f \) being smooth, and that in simulation studies (Section 5) it achieves comparable power to the FS test. In contrast, the FS test fails to control the size properly when \( f \) is not smooth (e.g., piecewise affine); this is observed in Section 5, and we also provide a detailed explanation in Appendix E.4 (e.g., if \( d = 2 \), it requires \( f \) to be Hölder continuous with smoothness parameter \( s > 4 \)).

**3.3. Combining multiple bandwidths**

The theory in Subsection 3.2 does not suggest a particular choice for the bandwidth \( b_n \). Since the size validity holds for a wide range of \( b_n \), its selection depends on the targeted alternatives. If the targets are “globally” convex, then \( b_n \) should be large in order for the bias, \( \sqrt{n}P h_v^* : v \in V \), to be large. On the other hand, if the targets are only convex in a small region, then \( b_n \) should be able to localize those convex regions. See Subsection 5.4 for concrete examples.

One possible remedy is to use multiple bandwidths. Let \( B_n \subset (0, \infty) \) be a finite collection of bandwidths. For each \( b \in B_n \), we denote the function \( h_v^{id} \) in (20) (resp. \( h_v^{id} \) in (5)) by \( h_{v,b}^{id} \) (resp. \( h_{v,b}^{id} \)) to emphasize the dependence on the bandwidth, and \( H_b = \{ h_{v,b}^*: v \in V \} \) for \( * = id \text{ or } sg \). Further, for each \( b \in B_n \), let \( N_b \) and \( N_{2,b} \) be two computational parameters, and consider two independent collections of Bernoulli random variables

\[
S_b := \left\{ Z_{i}^{(m,b)} : m \in [M], i \in I_{n,r} \right\} \overset{i.i.d.}{\sim} \text{Bernoulli}(p_{n,b}),
\]

\[
S'_b := \left\{ Z_{i}^{(k,m,b)} : k \in [n], m \in [M], i \in I_{n-1,r-1}^{(k)} \right\} \overset{i.i.d.}{\sim} \text{Bernoulli}(q_{n,b}),
\]

for \( \forall b \in B_n \).
where \( p_{n,b} := N_b / |I_{n,r}| \), \( q_{n,b} := N_{2,b} / |I_{n-1,r-1}| \), and they are independent of \( X^n \). In other words, the sampling plan is independent for each \( b \in B_n \).

Then for each \( b \in B_n \), we denote \( U'_{n,N,b}(h) \) in (10) by \( U'_{n,N,b}(h) \) with the sampling plan given by \( S_b \) in (25). Similarly, we denote \( \mathbb{G}^{(k)}(h) \) and \( \mathbb{G}(h) \) in (13) by \( \mathbb{G}^{(k,b)}(h) \) and \( \mathbb{G}^{(b)}(h) \) respectively with the sampling plan given by \( S'_b \) in (25).

Now let \( \mathcal{D}'_n := X^n \cup \{ S_b, S'_b : b \in B_n \} \), and denote Gaussian multipliers by

\[
\{ \xi_k : k \in [n] \}, \quad \{ \xi^{(m,b)}_i : m \in [M], \ i \in I_{n,r}, b \in B_n \} \quad \text{i.i.d.} \quad N(0,1),
\]

independent of \( \mathcal{D}'_n \). Define for \( b \in B_n \) and \( v \in \mathcal{V}_m \),

\[
\mathcal{U}^\#_{n,v,b}(h_{v,b}^*) := \frac{r}{\sqrt{n}} \sum_{k=1}^{n} \xi_k \left( \mathbb{G}^{(k,b)}(h_{v,b}^*) - \mathbb{G}^{(b)}(h_{v,b}^*) \right) + \alpha_{n,b}^{1/2} \frac{1}{\sqrt{M(b,m)}} \sum_{i \in I_{n,r}} \xi^{(m,b)}_i \sqrt{Z_{i}^{(m,b)}} \left( h_{v,b}^*(X_i) - U'_{n,N,b}(h_{v,b}^*) \right),
\]

where \( \alpha_{n,b} := n / N_b \) and \( \tilde{N}(m,b) := \sum_{i \in I_{n,r}} Z_{i}^{(m,b)} \) for \( m \in [M] \).

Finally, for each \( \alpha \in (0,1) \), denote \( q^\#_{1/\alpha} \) the \((1 - \alpha)^{\text{th}}\) quantile of \( \sup_{b \in B_n,v \in \mathcal{V}} \mathcal{U}^\#_{n,v,b}(h_{v,b}^*) \), conditional on \( \mathcal{D}'_n \). Then we propose to reject the null in (2) if

\[
\sup_{b \in B_n,v \in \mathcal{V}} \sqrt{n} U'_{n,N,b}(h_{v,b}^*) \geq q^\#_{1/\alpha}.
\]

**Remark 3.12.** It is possible to allow \( B_n \) to be uncountable, for example, \( B_n := (\ell_n, u_n) \), which corresponds to the uniform in bandwidth results \([25, 14]\). However, we choose to present the results for finite \( B_n \) for simplicity, since otherwise we need to also stratify \( B_n \). This is in some sense similar to the Dümbgen and Spokoiny’s multi-scale testing of qualitative hypotheses \([24]\). To establish the size validity and analyze the power of the test (26) (SILS), we need a more general theory than those in Section 2 for a function class \( \{ h_{v,b} : v \in \mathcal{V}, b \in B_n \} \), where \( \mathcal{V} \) is an index set. The key difference is that for each \( b \in B_n \), the computational parameters \( N_b \) and \( N_{2,b} \) may be of a different order (see, e.g., (22)). The rigorous statements for \( \{ h_{v,b} : v \in \mathcal{V}, b \in B_n \} \), which follow from similar arguments as those in Section 6, are not included for simplicity of the presentation. In Subsection 5.4, we conduct a simulation study to investigate the empirical performance of the SILS test with multiple bandwidths.

### 4. Stratified incomplete local simplex tests: computation

In this section, we discuss the computational complexity and implementation for the stratified incomplete local simplex tests. We focus on \( \mathcal{H}^{id} \) in our discussion and omit the superscript for simplicity. Assume that (C1)-(C6-id) hold, and that the computational parameters \( N, N_2 \) are given in (22). Further, as \( \mathcal{V} \) is compact, we assume \( \mathcal{V} \subset [0,1]^d \) without loss of generality.

For some small \( \eta \in (0, 1/2) \), let \( t := [1/(\eta b_n)] \), and \( v_i = i \eta b_n \) for \( i = 0, 1, \ldots, t \) and \( v_t = 1 \). Now we partition each coordinate into segments of length \( \eta b_n \) (except for the rightmost one), i.e., each \( \mathcal{V}_m \) is of the form \( \mathcal{V} \cap [v_{i_1}^{(1)}, v_{i_2}^{(1)}] \times \cdots \times [v_{i_d}^{(1)}, v_{i_d}^{(1)}] \), where \( 0 \leq i_j^{(1)} < i_j^{(2)} \leq t + 1 \) for \( j \in [d] \). Then the number of partitions \( M \leq (1 + \eta^{-1} b_n^{-1})^d \).
For any \( v \in \mathbb{R}^d \) and \( A \subset \mathbb{R}^d \), we denote the \( b_n \)-neighbourhood by
\[
\mathcal{N}(v, b_n) := \{ v' \in \mathbb{R}^d : \| v - v' \|_\infty \leq b_n/2 \}, \quad \mathcal{N}(A, b_n) := \bigcup_{v \in A} \mathcal{N}(v, b_n).\]

Denote by \( \text{ND}(v, b_n) := \{ i \in [n] : V_i \in \mathcal{N}(v, b_n) \} \) and \( \text{ND}(A, b_n) := \bigcup_{v \in A} \text{ND}(v, b_n) \) the indices for data points within \( b_n \)-neighbourhood of \( v \) and \( A \) respectively.

As an illustration, in Figure 1 (where \( b = 8, \eta = 1/8 \)), \( V \) is partitioned into small squares of size 1. For the dotted region \( \mathcal{V}_m \), \( \mathcal{N}(\mathcal{V}_m, b_n) \) is area encompassed by the big dotted square, so \( v_4 \in \mathcal{N}(\mathcal{V}_m, b_n) \), but \( v_5 \notin \mathcal{N}(\mathcal{V}_m, b_n) \). Further, \( \text{ND}(\mathcal{V}_m, b_n) \) are indices for data points within the dotted square.

### 4.1. Stratified sampling

For \( m \in [M] \), let \( \mathcal{A}(\mathcal{V}_m) := \{ \iota = (i_1, \ldots, i_r) \in I_{n,r} : i_j \in \text{ND}(\mathcal{V}_m, b_n) \text{ for } j \in [r] \} \) be the collection of \( r \)-tuples whose members are all within \( b_n \)-neighbourhood of \( \mathcal{V}_m \). For example, in Figure 1, \((v_1, v_2, v_3, v_4) \in \mathcal{A}(\mathcal{V}_m) \), but \((v_1, v_2, v_3, v_5) \notin \mathcal{A}(\mathcal{V}_m) \). Due to the localization by \( L(\cdot) \) (cf. (C1)),
\[
h_u(x_i) = 0, \text{ for any } v \in \mathcal{V}_m \text{ and } \iota \in [I_{n,r}] \setminus \mathcal{A}(\mathcal{V}_m).\]

As a result, the individual values of \( \{ Z_i^{(m)} : \iota \in [I_{n,r}] \setminus \mathcal{A}(\mathcal{V}_m) \} \) are irrelevant, except for their sum, which is a part of \( \tilde{N}^{(m)} \). Thus, we generate a Binomial\(|[I_{n,r}] \setminus \mathcal{A}(\mathcal{V}_m)|, p_n \) random variable, that accounts for \( \sum_{\iota \in [I_{n,r}] \setminus \mathcal{A}(\mathcal{V}_m)} Z_i^{(m)} \).

On the other hand, the number of selected \( r \)-tuples in \( \mathcal{A}(\mathcal{V}_m) \) is on average
\[
\mathbb{E} \left[ \sum_{\iota \in \mathcal{A}(\mathcal{V}_m)} Z_i^{(m)} \right] \lesssim \left( n \left( 1 + \frac{1}{d} \right)^d b_n^d \frac{n^\kappa b_n^{-dr}}{|I_{n,r}|} \right) \lesssim (1 + \eta)^d r n^\kappa,
\]
since the \( \| \cdot \|_\infty \)-diameter of \( \mathcal{V}_m \) is \( \eta b_n \), and the density of \( V \) is bounded (see (C4)). Thus to compute \( \sup_{v \in \mathcal{V}_m} \sqrt{n} U^t_{n,N}(h_v) \), the number of evaluations of \( w(\cdot) \) is on average \( \lesssim n^\kappa \), and the computational complexity can be made independent of the dimension \( d \) (as \( \eta \) can be chosen to be small).

**Remark 4.1.** Above calculation of complexity does not include the cost of maximizing over \( \mathcal{V}_m \). In practice, we select a finite number of query points as in the Subsection 4.2. The discussion for the bootstrap part is similar, and we analyze below the complexity of its actual implementation.

**Why stratification?** Without stratifying \( V \), each \( v \in V \) share the same sampling plan \( \{ Z_i : \iota \in I_{n,r} \} \).

However, we cannot afford to generate all \( \{ Z_i : \iota \in I_{n,r} \} \), as on average there are \( N = n^\kappa b_n^{dr} \) non-zero terms. We may attempt to use the above short-cut. For \( v_1, v_2 \in V \), to compute \( U^t_{n,N}(h_{v_1}) \) (for \( i = 1, 2 \)), we only generate \( \{ Z_i : \iota \in \mathcal{A}(\{v_1\}) \} \), and the individual values of \( \{ Z_i : \iota \in I_{n,r} \setminus \mathcal{A}(\{v_1\}) \} \) are not explicitly generated.

However, the issue is to ensure consistency. (i) In computing \( U^t_{n,N}(h_{v_1}) \), although the individual values of \( \{ Z_i : \iota \in I_{n,r} \setminus \mathcal{A}(\{v_1\}) \} \) are irrelevant, we still need to generate a Binomial random variable to account for their sum. However, \( (I_{n,r} \setminus \mathcal{A}(\{v_1\})) \cap \mathcal{A}(\{v_2\}) \) in many cases is non-empty, and thus \( \sum_{\iota \in (I_{n,r} \setminus \mathcal{A}(\{v_1\})) \cap \mathcal{A}(\{v_2\})} Z_i^{(m)} \) and \( \{ Z_i : \iota \in \mathcal{A}(\{v_2\}) \} \) are not independent. (ii) In many cases, \( \mathcal{A}(\{v_1\}) \cap \mathcal{A}(\{v_2\}) \) is non-empty, so we cannot independently generate \( \{ Z_i : \iota \in \mathcal{A}(\{v_1\}) \} \) and \( \{ Z_i : \iota \in \mathcal{A}(\{v_2\}) \} \). Note also that the calculation is needed for multiple \( v \in V \) instead of only \( v_1, v_2 \).
Remark 4.2. In Appendix E.5, we present an algorithm without stratification that addresses the above consistency issue. Its computational complexity is \( \lesssim 2^{dr} n^d b_n^{-d} \) evaluations of \( w(\cdot) \). If \( d \) is fixed, it only loses a \( b_n^{-d} \) factor in theory, but \( 2^{dr} \) can be very large in practice, and thus it is not computationally feasible (e.g., \( 2^{dr} = 32768 \) if \( d = 3 \)).

4.2. Implementation of SILS

In practice, instead of taking the supremum over \( \mathcal{V} \), we choose a (finite) collection of query points, \( \mathcal{V}_n \), one from each partition \( \{ \mathcal{V}_m : m \in [M] \} \), and approximate the supremum over \( \mathcal{V} \) by that over \( \mathcal{V}_n \). As a result, each \( v \in \mathcal{V}_n \) has its individual sampling plan (\( \{Z_{\tau}^{(m)} : \tau \in I_{n,r} \} \) if \( v \in \mathcal{V}_m \)), which can be generated independently for different query points. Further, the test still takes the form of (21) with a finite function class \( \mathcal{H} = \{ h_v : v \in \mathcal{V}_n \} \).

Remark 4.3. It is without loss of generality to pick one query point from each region, since we could always decrease \( \eta \), i.e., making each region smaller. Further, since only one element is picked, if \( v \in \mathcal{V}_m \), instead of considering \( ND(\mathcal{V}_m, b_m) \), we can focus on \( ND(\{v\}, b_n) \).

Remark 4.4. In establishing the bootstrap validity for stratified, incomplete \( U \)-processes, we first consider the corresponding results for high-dimensional \( U \)-statistics (Appendix B), and then approximate the supremum of a \( U \)-process by that of its discretized version. Thus the above procedure, which can be viewed as a practical implementation of approximating the supremum of a process, can also be directly justified by Theorem B.2 and B.3.

Computing the test statistic. In Algorithm 1, we show the pseudo-code to compute, for each \( v \in \mathcal{V}_n \), the statistic \( U_{n,N}^{\prime}(h_v) \), and at the same time the conditional (on \( D_{n}^{\prime} \)) variance \( \hat{\gamma}_B(h_v) \) (in (32)) of \( U_{n,B}^{\#}(h_v) \) (in (10)). It is well known that sampling \( T \) items without replacement from \( S \) elements \( (S \gg T) \) can be done in \( O(T \log(T)) \) time [36]. Then based on the discussions in the previous subsection, the computational complexity for Algorithm 1 is \( O(M n^{d} \log(n)) \).

Bootstrap. For a fixed \( k \in [n] \), notice that \( \{G^{(k)}(h_v) : v \in \mathcal{V}_n \} \) in (13) takes the same form of stratified, incomplete \( U \)-processes as the test statistics, and thus we can apply Algorithm 1, with appropriate inputs, to compute it. Since we need to compute \( G^{(k)} \) for each \( k \in [n] \), the complexity is

\[
n \times M \times \left( \frac{(n - 1)b_n^d}{r - 1} \right)^{d} n^{r - d} \log(n) \lesssim M n^{1 + r - d} \log(n).
\]

Further, as we pick one element from each \( \mathcal{V}_m \), conditional on \( D_{n}^{\prime} \), \( \{U_{n,B}^{\#}(h_v) : v \in \mathcal{V}_n \} \) are conditionally independently, with conditional variances \( \{\hat{\gamma}_B(h_v) : v \in \mathcal{V}_n \} \) computed in Algorithm 1, and we no longer need to generate Gaussian multipliers \( \{\xi^{(m)}(\tau) : \tau \in [I_{n,1} \cup \cdots \cup I_{n,R}] \} \) for each summand indexed by \( \tau \) in (15).

Finally, for independent standard Gaussian multipliers \( \{\xi_k, \xi^{(m)} : k \in [n], m \in [M] \} \), we compute for each \( v \in \mathcal{V}_n \),

\[
\frac{1}{\sqrt{n}} \sum_{k=1}^{n} \xi_k \left( G^{(k)}(h_v) - \hat{\mathbb{E}}(h_v) \right) + \xi^{(\sigma(h_v))} \sqrt{\hat{\gamma}_B(h_v)}.
\]
We use the uniform localization kernel \( U \). Parameters related to the computational budget, we set algorithms can be implemented in a parallel manner using clusters; in particular, \( O \) is the computational bottleneck. In the simulation studies, we consider setups where the regression function \( f \) is defined on \((0,1)^d\), and the covariates \( V = (V_1, \ldots, V_d) \) have a uniform distribution on \((0,1)^d\), for \( d = 2, 3, 4 \). In this section, the error term \( \varepsilon \) in (1) has a Gaussian distribution with zero mean and variance \( \sigma^2 \).

**Remark 4.5.** The computational bottleneck is in computing \( \{G(k) : k \in [n]\} \), which, however, is outside the bootstrap iterations. Thus we can afford large \( B \) in the bootstrap calibration. The above algorithms can be implemented in a parallel manner using clusters; in particular, \( G(k) \) can be computed separately for each \( k \in [n] \). As a result, the efficiency scales linearly in the number of computing cores.

---

**Algorithm 1:** compute \( U_{n,N}' \) and \( \hat{\gamma}_B \) over \( \mathcal{V}_n \) for the concavity test.

```
Input: Observations \( \{X_i = (V_i, Y_i) \in \mathbb{R}^{d+1} : i \in [n]\} \), budget \( N \), kernel \( L(\cdot) \), bandwidth \( b_n \), query points \( \mathcal{V}_n \) (size \( M \)).

Output: \( U_{n,N}' \), \( \hat{\gamma}_B \): two vectors of length \( M \)

Initialization: \( p_n = N/\binom{n}{b} \), \( U_{n,N}' \), \( \hat{\gamma}_B \) both set zero;

for \( m \leftarrow 1 \) to \( M \) do
  \( v = \mathcal{V}_n[m] \);
  Generate \( T_1 \sim \text{Binom}(\binom{\binom{\text{IB}(v,b_n)}{r}}{p_n}) \), \( T_2 \sim \text{Binom}(\binom{\text{IB}(v,b_n)}{p_n}) \);
  \( \hat{N} \leftarrow T_1 + T_2 \);
  Sample without replacement \( T_1 \) terms, \( \{s : 1 \leq s \leq T_1 \} \), from \( A\{v\} \);
  for \( \ell \leftarrow 1 \) to \( T_1 \) do
    \( U_{n,N}[m] \leftarrow U_{n,N}'[m] + h_v(X_{s,\ell}) \);
    \( \hat{\gamma}_B[m] \leftarrow \hat{\gamma}_B[m] + (h_v(X_{s,\ell}))^2 \);
  end
  \( U_{n,N}'[m] \leftarrow U_{n,N}'[m]/\hat{N} \); \( \hat{\gamma}_B[m] \leftarrow \hat{\gamma}_B[m]/\hat{N} - (U_{n,N}'[m])^2 \);
end
```

5. Simulation results

In the simulation studies, we consider setups where the regression function \( f \) in (1) is defined on \((0,1)^d\), and the covariates \( V = (V_1, \ldots, V_d) \) have a uniform distribution on \((0,1)^d\), for \( d = 2, 3, 4 \). In this section, the error term \( \varepsilon \) in (1) has a Gaussian distribution with zero mean and variance \( \sigma^2 \).

**Remark 5.1.** The results for \( d = 3 \) and \( 4 \) are qualitatively similar, and presented mostly in Appendix D, where we also study asymmetric or heavy tailed distributions for the noise \( \varepsilon \) (Appendix D.2).

We compare our proposed procedure with the method in [27], denoted by “FS”.

**Proposed procedure.** We use the uniform localization kernel \( L(\cdot) = 1\{\cdot \in (-1/2, 1/2)^d\} \). The query points are \( \mathcal{V}_n := \{0.3, 0.4, 0.5, 0.6, 0.7\}^2 \) for \( d = 2 \), and \( \mathcal{V}_n := \{0.3, 0.5, 0.7\}^d \) for \( d = 3, 4 \). For parameters related to the computational budget, we set \( N = 10 \times 25 \times n \times b_n^{d \times r} \) for \( d = 2, 3, 4 \), \( N_2 = 10^4 \times b_n^{d \times r} \) for \( d = 2, 3 \) and \( N_2 = 2 \times 10^4 \times b_n^{d \times r} \) for \( d = 4 \), and the Bootstrap iterations \( B = 1500 \). The \( N \) is selected so that \( \alpha_n := n/N \) is very small, and further increasing it will not improve the power of the test. The estimation of \( \{H_n(k^*) : k \in [n], v \in \mathcal{V}_n\} \) is the computational bottleneck,
and empirically we find that further increasing the selected value for $N_2$ does not improve the accuracy in terms of the size of the proposed procedure. We consider two types of kernels, $H_{id}$ and $H_{sg}$, and use below “ID” for the former and “SG” for later. For each parameter configuration below, we independently generate (at least) 1,000 datasets, apply our procedure, and estimate the rejection probability.

**FS method [27]**. We use the implementation provided by the authors\(^2\), where either quadratic or cube splines with $j$ knots in each coordinate are used in constructing an initial estimator for the regression function; we denote the former by FS-Q$^j$ and later by FS-C$^j$. We set the tuning parameter $\gamma_n = 0.01/\log(n)$ and the Bootstrap iteration $B = 200$ as recommended by [27]. Below, the rejection probabilities are estimated based on 1,500 independently generated datasets.

### 5.1. Running times

The computational savings compared to using the complete $U$-process, $p_n := N/\binom{n}{r}$ and $q_n = N_2/\binom{n-1}{r-1}$, are listed in Table 2 for several typical configurations. It is clear that for a moderate size dataset (say $n \sim 1000$), using the complete $U$-process has a very high, if not prohibitive, computational cost (see Table 1 for the running time using the stratified, incomplete $U$-process). For example, for $d = 3, n = 1000, b_n = 0.6$, it takes on average 5.26 minutes to run our procedure with 40 cores, which implies that with the complete version it would take at least 7.2 days ($= 5.26 \text{ mins} / q_n$).

In contrast, the FS method [27] has a much shorter running time. For example, with $d = 2, n = 1000$, it takes less than 20 seconds with 4 cores (see Table E4 in [27]). For $d \geq 3$, it could be challenging to apply the FS method due to the accuracy of estimating the regression function, the projection onto a function space, and the numerical integration needed to compute the distance etc.

| $d = 2, b_n = 0.5$ | $d = 3, b_n = 0.6, |V_n| = 27$ | $d = 4, b_n = 0.7$ |
|---------------------|-----------------|------------------|
| $n = 1000, |V_n| = 25$ | $n = 500$ | $n = 1000$ | $n = 1500$ |
| 5.06 mins | 1.31 mins | 5.26 mins | 9.12 mins |
| 33.4 mins |

**Table 1.** Running time of the proposed procedure in minutes using 40 computer cores, where $N$ and $N_2$ are described in the introduction of Section 5.

<table>
<thead>
<tr>
<th>$d = 2, b_n = 0.5$</th>
<th>$d = 3, b_n = 0.6$</th>
<th>$d = 4, b_n = 0.7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n = 500$ $p_n$</td>
<td>$n = 1000$ $p_n$</td>
<td>$n = 1500$ $p_n$</td>
</tr>
<tr>
<td>1.2E-2</td>
<td>1.5E-3</td>
<td>4.5E-4</td>
</tr>
<tr>
<td>$n = 500$ $q_n$</td>
<td>$n = 1000$ $q_n$</td>
<td>$n = 1500$ $q_n$</td>
</tr>
<tr>
<td>1.2E-1</td>
<td>1.5E-2</td>
<td>4.6E-3</td>
</tr>
</tbody>
</table>

**Table 2.** Computational efficiency for typical configurations, where $N$ and $N_2$ are described in the introduction of Section 5. For $d = 4, b_n = 0.7, n = 2000$, we have $p_n = 5.9E-8, q_n = 3.9E-7$. Here, sE-t = s$x10^{-t}$.

**Remark 5.2.** For $d \geq 5$, although the proposed method is still computationally feasible, the statistical power becomes very small, due to the curse of dimensionality, as well as the fact that the probability of one point in the simplex of other $(r - 1)$ points is small. To wit, recall the set $S$ in Section 3. If $V$ has a uniform distribution over $(0, 1)^d$, then $P((V_1, \ldots, V_r) \in S)$ is approximately 0.31 for $d = 2, 6.9E-2$ for $d = 3, 1.3E-2$ for $d = 4, and 2.0E-3 for d = 5$.

5.2. Size validity

We start with our proposed procedure, and consider *concave* functions given by

$$f(v) = v_1^{\kappa_0} + \ldots + v_d^{\kappa_0}, \quad \text{for } v := (v_1, \ldots, v_d) \in (0, 1)^d,$$

(27)

for $0 < \kappa_0 \leq 1$. As discussed in Subsection 3.2.1, affine functions (e.g., $f$ in (27) with $\kappa_0 = 1$) are the least favourable configuration in the null, and for smaller $0 < \kappa_0 < 1$, $f$ is “deeper” in $H_0$ in the ordering of (24). Thus as far as the size, which is the largest rejection probability under $H_0$, is concerned, it suffices to consider $f$ in (27) with $\kappa_0 = 1$.

For each query point, the average number of data points within its $b_n$-neighbourhood is $n \times b_n^{-d}$. Since a decent size of local points is necessary for the validity of Gaussian approximation, we select $b_n$ so that locally there are at least 150 data points. As we shall see in Subsection 5.3, smaller $b_n$ has a better localization power, while larger $b_n$ is suitable if the targeted alternatives are globally convex.

In Table 3, we list the size for different bandwidth $b_n$ and error variance $\sigma^2$ at levels 5% and 10% for $f$ in (27) with $\kappa_0 = 1$. From the Table 3, it is clear that the proposed procedure is consistently on the conservative side. We note that the conservativeness is not due to the stratified sampling. For $d = 1$, we were able to implement the complete version, and observed a similar phenomenon. Further, [14] uses complete $U$-processes to test regression monotonicity, which are also conservative (see Table 1 therein). Further, in Table 4, we list the rejection probabilities for $f \in H_0$ in (27) with $\kappa_0 \leq 1$. As expected, the rejection probabilities becomes smaller as $\kappa_0$ decreases and $f$ becomes more “concave”.

**FS method [27].** In Table E2 of [27], we can observe the slight inflation of the empirical size of the FS method when the function is linear. Here, we consider the following *concave*, piecewise affine regression function:

$$f(v_1, v_2) = -|v_1 - 0.8| - |v_2 - 0.8|, \quad \text{for } v_1, v_2 \in (0, 1).$$

(28)

The rejection probabilities of the FS method [27] at the nominal level 5% are listed in Table 5. Recall that FS-Q$_j$ (resp. FS-C$_j$) is for using quadratic (resp. cubic) splines with $j$ knots in each coordinate as the initial estimator for the regression function. Except for the global test FS-Q0, which places no interior knots, these probabilities far exceed the nominal level. We provide explanations for the significant size inflation of the FS method [27] in Appendix E.4.

5.3. Power comparison

We study two types of alternatives for the regression function.

**Polynomial functions.** In the first, we consider $f$ in (27) for $\kappa_0 \in \{1, 2, 1.5\}$.

**Locally convex functions.** For the second, we consider regression functions that are mostly concave over $(0, 1)^d$, but convex in a small region. Specifically, consider the function $\varphi: \mathbb{R}^d \to \mathbb{R}$ defined via $\varphi(v) := \exp(-||v||^2/2)$; clearly $\varphi$ is concave on the region $\{v \in \mathbb{R}^d : ||v||_\infty < 1\}$. Then for $c_1, c_2, \omega_1, \omega_2 > 0$ and $\mu_1, \mu_2 \in \mathbb{R}^d$, we consider

$$f(v) = c_1 \varphi((v - \mu_1)/\omega_1) - c_2 \varphi((v - \mu_2)/\omega_2), \quad \text{for } v \in (0, 1)^d.$$

(29)

We let $c_1 = 1$, $\omega_1 = 1.5$, and $\mu_1 = (0.75, \ldots, 0.75)$ so that without the second term, $f$ would be concave in the entire region $(0, 1)^d$. We let $\mu_2 = (0.25, \ldots, 0.25)$, and set $c_2$ and $\omega_2$ to be small so that $f$
$n = 500$ $n = 1000$

<table>
<thead>
<tr>
<th>$d = 2$, Level = 5%</th>
<th>$b_n = 0.6$</th>
<th>$b_n = 0.55$</th>
<th>$b_n = 0.5$</th>
<th>$b_n = 0.5$</th>
<th>$b_n = 0.45$</th>
<th>$b_n = 0.4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ID, $\sigma = 0.1$</td>
<td>3.1</td>
<td>2.9</td>
<td>2.8</td>
<td>4.1</td>
<td>2.6</td>
<td>3.4</td>
</tr>
<tr>
<td>SG, $\sigma = 0.1$</td>
<td>3.1</td>
<td>4.1</td>
<td>2.8</td>
<td>3.0</td>
<td>3.8</td>
<td>2.7</td>
</tr>
<tr>
<td>ID, $\sigma = 0.2$</td>
<td>3.2</td>
<td>3.7</td>
<td>3.0</td>
<td>2.9</td>
<td>3.1</td>
<td>2.4</td>
</tr>
<tr>
<td>SG, $\sigma = 0.2$</td>
<td>3.6</td>
<td>3.3</td>
<td>2.9</td>
<td>3.6</td>
<td>3.1</td>
<td>2.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$d = 2$, Level = 10%</th>
<th>$b_n = 0.6$</th>
<th>$b_n = 0.55$</th>
<th>$b_n = 0.5$</th>
<th>$b_n = 0.5$</th>
<th>$b_n = 0.45$</th>
<th>$b_n = 0.4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ID, $\sigma = 0.1$</td>
<td>8.3</td>
<td>6.8</td>
<td>6.7</td>
<td>8.1</td>
<td>7.5</td>
<td>7.7</td>
</tr>
<tr>
<td>SG, $\sigma = 0.1$</td>
<td>7.4</td>
<td>8.0</td>
<td>6.6</td>
<td>8.1</td>
<td>7.7</td>
<td>6.1</td>
</tr>
<tr>
<td>ID, $\sigma = 0.2$</td>
<td>7.8</td>
<td>8.0</td>
<td>6.2</td>
<td>7.6</td>
<td>7.8</td>
<td>6.0</td>
</tr>
<tr>
<td>SG, $\sigma = 0.2$</td>
<td>8.7</td>
<td>7.1</td>
<td>7.0</td>
<td>8.6</td>
<td>7.0</td>
<td>6.7</td>
</tr>
</tbody>
</table>

Table 3. Size validity of the proposed procedure for $d = 2$. The sizes, i.e., the probability of rejection under the linear regression function, are in the unit of percentage.

\[ \kappa_0 = 1 \quad \text{(size)} \quad 0.95 \quad 0.90 \quad 0.85 \quad 0.80 \quad 0.75 \quad 0.70 \]

<table>
<thead>
<tr>
<th>ID</th>
<th>7.6</th>
<th>6.5</th>
<th>4.6</th>
<th>3.9</th>
<th>3.0</th>
<th>1.9</th>
<th>1.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>SG</td>
<td>8.6</td>
<td>6.0</td>
<td>5.0</td>
<td>3.4</td>
<td>2.9</td>
<td>2.1</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Table 4. The rejection probabilities (in percentage) of the proposed procedure for concave functions $f \in H_0$ in (27) with varying $\kappa_0$ at level 10% for $n = 1000$, $b_n = 0.5$, $\sigma = 0.2$.

<table>
<thead>
<tr>
<th>Knots $j$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>FS-Q</td>
<td>99.5</td>
<td>46.5</td>
<td>9.2</td>
<td>23.6</td>
<td>33.9</td>
<td>16.0</td>
<td>16.0</td>
<td>23.1</td>
<td>20.3</td>
<td>20.3</td>
</tr>
<tr>
<td>FS-C</td>
<td>97.1</td>
<td>50.7</td>
<td>15.3</td>
<td>32.8</td>
<td>23.9</td>
<td>13.6</td>
<td>17.7</td>
<td>21.0</td>
<td>19.9</td>
<td>22.2</td>
</tr>
</tbody>
</table>

Table 5. The rejection probabilities (in percentage) for FS-Q$^j$ and FS-C$^j$ [27] at level 5% for the concave (i.e. $H_0$ holds) function in (28), where $n = 1000$ and $\sigma = 0.1$.

\[ \kappa_0 = 1 \quad \text{(size)} \quad 0.95 \quad 0.90 \quad 0.85 \quad 0.80 \quad 0.75 \quad 0.70 \]

<table>
<thead>
<tr>
<th>ID</th>
<th>8.4</th>
<th>7.6</th>
<th>6.1</th>
<th>4.7</th>
<th>3.8</th>
<th>2.4</th>
<th>2.2</th>
</tr>
</thead>
</table>

Table 6. The rejection probabilities (in percentage) of the proposed procedure with multiple bandwidth, $\mathcal{H}_b^{id}$, for concave functions $f \in H_0$ in (27) with varying $\kappa_0$ at level 10% with $n = 1000$, $\sigma = 0.5$.

is mostly concave and locally convex in a small neighbourhood of $\mu_2$. (In Figure 2 in Appendix D.1, we plot the regression function $f$ together with one realization of dataset.)

In Table 7 (a) and (b), for the two types of alternatives, we list the power of $\mathcal{H}_b^{id}$ with different bandwidth parameters $b_n$, and the FS method [27] using either quadratic (Q) or cubic (C) splines with $j = 0, 1, 2, 5$ knots in each coordinate.$^3$

For our proposed method, if $f$ is a polynomial function (27), the power increases as $b_n$ increases, as $f$ is globally convex. However, for the locally convex function $f$ (29), the power initially increases as $b_n$ increases.

$^3$ $j = 0, 1$ is used in [27]
Testing for regression curvature

$b_{n_1}$ increases, but later drops significantly, as $f$ is only locally convex, but “globally concave”. Thus the choice of bandwidth depends on the targeted alternatives. Similar statements can be made about the FS method [27]. Adding knots decreases its power for (27), while a “global” test such as FS-Q0 has little power against (29).

In summary, the proposed procedure has a comparable power to the FS method [27], which however fails to control the size in general. Further, we show next that the issue with selecting $b_{n_1}$ can be partly solved by combining multiple bandwidths.

<table>
<thead>
<tr>
<th>Rej. Prob.</th>
<th>$\mathcal{H}<em>{id}$ with single $b</em>{n_1}$</th>
<th>FS method [27]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$b_{n_1} = 0.6$</td>
<td>$b_{n_1} = 0.8$</td>
</tr>
<tr>
<td>Level 5%</td>
<td>25.6</td>
<td>69.1</td>
</tr>
<tr>
<td></td>
<td>93.8</td>
<td>81.6</td>
</tr>
</tbody>
</table>

(a) Polynomial $f$ (27) with $\kappa_0 = 1.5$

<table>
<thead>
<tr>
<th>Rej. Prob.</th>
<th>$\mathcal{H}<em>{id}$ with single $b</em>{n_1}$</th>
<th>FS method [27]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$b_{n_1} = 0.5$</td>
<td>$b_{n_1} = 0.6$</td>
</tr>
<tr>
<td>Level 10%</td>
<td>20.3</td>
<td>40.3</td>
</tr>
<tr>
<td></td>
<td>7.1</td>
<td>49.7</td>
</tr>
</tbody>
</table>

(b) Locally convex $f$ (29) with $\omega_2 = 0.15, c_2 = 0.3$

<table>
<thead>
<tr>
<th>Polynomial $f$ (27) with $\kappa_0 = 1.5$ at 5%</th>
<th>Locally convex $f$ (29) with $\omega_2 = 0.15, c_2 = 0.3$ at 10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rej. Prob.</td>
<td>71.7</td>
</tr>
</tbody>
</table>

Table 7. The rejection probabilities (in percentage) of the proposed method $\mathcal{H}_{id}$, the FS method [27], and the proposed method with multiple bandwidth $\mathcal{H}_{id}^{\{b\}} : b \in \{0.6, 0.8, 1\}$ for $d = 2$, $n = 1000$, $\sigma = 0.5$.

5.4. Combining multiple bandwidths

We consider the procedure (26) in Subsection 3.3 that combines multiple bandwidths, $\mathcal{H}_{id}^{\{b\}} : b \in \mathcal{B}_n$ with $\mathcal{B}_n = \{0.6, 0.8, 1\}$. In Table 6, we list the rejection probabilities for $f$ in (27) with $\kappa_0 \leq 1$. In Table 7 (c), we present its power against the two alternatives.

With a range of bandwidths, $\mathcal{H}_{id}^{\{b\}} : b \in \mathcal{B}_n$ achieves a reasonable power, and is adaptive to the properties of the regression function $f$. As expected, it is not as powerful as the best performance achieved by $\mathcal{H}_{id}^{\{b\}}$ with a single $b_{n_1}$. Further, its computational cost is linear in $|\mathcal{B}_n|$.

In practice, we would recommend the procedure (26) with multiple bandwidths $\mathcal{B}_n$. In choosing $\mathcal{B}_n$, one approach is to first decide reasonable lower and upper bounds, $b_{\text{min}}$ and $b_{\text{max}}$, for the bandwidth, and then based on available computational resource, select a few bandwidths in $[b_{\text{min}}, b_{\text{max}}]$ (say equally spaced) to form $\mathcal{B}_n$. As a rule of thumb, one may choose $b_{\text{min}}$ so that there are enough data points in the $b_{n_1}$ neighbourhood of each query point (say $\geq 120$). On the other, $b_{\text{max}}$ could be decided based on the diameter of the region of interest, $\mathcal{V}$.

Remark 5.3. The procedure (26) is asymptotically non-conservative. Another way to combine multiple bandwidths is to use multiple testing techniques, which however are conservative. In Appendix D.5, we present preliminary simulation results using Bonferroni correction.
6. Gaussian approximation and bootstrap for stratified, incomplete $U$-processes

In this section, we consider a general function class $\mathcal{H}$, and establish Gaussian approximation and bootstrap results for its associated stratified, incomplete $U$-processes in Section 2, under the more general moment assumptions (MT) instead of (MT-$U$)-processes. There exist absolute constants $\bar{\gamma}, \tilde{\gamma}$ for its associated stratified, incomplete $U$-processes. In particular, the condition (MT) does not require the envelope function $H$ in (VC) to be bounded.

(MT). There exist absolute constants $\sigma > 0, c_0 \in (0, 1), q \in [4, \infty]$, and $B_n \geq D_n \geq 1$ such that

\[
\var(\sup_{h \in \mathcal{H}} |P_{r-1}h(X_1)|) \geq \sigma^2, \quad \text{for } h \in \mathcal{H},
\]

\[
\sup_{h \in \mathcal{H}} \mathbb{E} \left| P_{r-1}h(X_1) - P_{r}h \right|^{2+k} \leq D_n^k \quad \text{for } k = 1, 2, \quad \|P_{r-1}H\|_{p,q} \leq D_n,
\]

\[
\|P_{r-1}H^s\|_{p^r,q} \leq B_n^{2-2}D_n^{s+1-s}, \quad \text{for } \ell \geq 2, s = 1, 2, 3, 4,
\]

\[
\|P_{r-1}H^s\|_{p^r,q} \leq B_n^{2-2}D_n^{(2/3)-2/q}, \quad \text{for } \ell = 1, 2, s = 2, 3, 4,
\]

\[
\|P_{r-1}H^s\|_{p^r,q} \leq B_n^{2-2}D_n^{s-2/q}, \quad \text{for } \ell = 0, 1, 2, s \in \{4\} \text{ with } \ell + s > 2, h \in \mathcal{H},
\]

\[
\|H\|_{p^r,q} \leq B_n^{2-2/q}D_n^{q-1}, \quad \|H\|_{p^r,2} \leq B_n^2,
\]

\[
c_0B_n^2D_n^{-2} \leq \var(h(X_1^1)) \leq \min\{D_n^{2(r-1)}, B_n^2D_n^{-2}\}, \quad \text{for } h \in \mathcal{H},
\]

\[
\sup_{h \in \mathcal{H}} \|P_{r-1}H^2\|_{p^r,4} \leq D_n^2, \quad \|P_{r-1}H^2\|_{p^r,4} \leq D_n^4/q,
\]

where $1/q = 0$ if $q = \infty$, and recall that for a measurable function $f : S^2 \to \mathbb{R}$, define $f^{\bigcirc 2}$ to be a function on $S^2$ such that $f^{\bigcirc 2}(x_1, x_2) := \int f(x_1, x)f(x_2, x)dP(x)$.

6.1. Gaussian approximation

We first approximate the supremum of the stratified, incomplete $U$-process (10) by that of an appropriate Gaussian process. Specifically, denote $P_{r-1}h$ the function on $S$ such that $P_{r-1}f(x_1) := \mathbb{E}[h(X_1), \ldots, X_r)]$, and $(\ell^\infty(\mathcal{H}), \| \cdot \|_\infty)$ the space of bounded functions indexed by $\mathcal{H}$ equipped with the supremum norm. Assume there exists a tight Gaussian random variable $W_P$ in $\ell^\infty(\mathcal{H})$ with zero mean and covariance function $\gamma_s(h, h') := \text{Cov}(W_P(h), W_P(h')) = r^2\gamma_A(h, h') + \alpha_n\gamma_B(h, h')$ for $h, h' \in \mathcal{H}$ where

\[
\gamma_A(h, h') := \text{Cov}\left(P_{r-1}h(X_1), P_{r-1}h'(X_1)\right), \quad \alpha_n := n/N,
\]

\[
\gamma_B(h, h') := \text{Cov}\left(h(X_1^1), h'(X_1^1)\right) 1\{\sigma(h) = \sigma(h')\}.
\]

Note that $\gamma_B(h, h') = 0$ if $\sigma(h) \neq \sigma(h')$, which is due to the stratification. The existence of $W_P$ is implied by (VC) and (MT) (see [18][Lemma 2.1]). If $h = h'$, we write $\gamma_s(h)$ for $\gamma_s(h, h)$, and the same applies to $\gamma_A$ and $\gamma_B$. Further, denote $M_n := \sup_{h \in \mathcal{H}} W_P(h)$. We will bound the Kolmogorov
distance between the two suprema

\[ \rho(M_n, \tilde{M}_n) := \sup_{t \in \mathbb{R}} \left| \mathbb{P}(M_n \leq t) - \mathbb{P}(\tilde{M}_n \leq t) \right|. \]  

(31)

**Theorem 6.1.** Assume the conditions (PM), (VC), (MB), and (MT-0)-(MT-4). Then there exists a constant \( C \), depending only on \( r, q, \bar{\sigma}, c_0, C_0 \), such that

\[ \rho(M_n, \tilde{M}_n) \leq C \eta_n^{(1)} + C \eta_n^{(2)}, \]

with

\[ \eta_n^{(1)} := \left( \frac{D_n^2 K_n^7}{n} \right)^{1/8} + \left( \frac{D_n^2 K_n^4}{n^{1-2/q}} \right)^{1/4} + \left( \frac{D_n^2 K_n^5}{n^{1-1/q}} \right)^{1/2}, \]

\[ \eta_n^{(2)} := \left( \frac{B_n^2 K_n^7}{N} \right)^{1/8} + \left( \frac{n^{4r/q} K_n^5 B_n^{2-8/q} D_n^{8/q}}{N} \right)^{1/4} + \left( \frac{M^{2/q} B_n^{2-4/q} D_n^{4/q} K_n^5}{N^{1-2/q}} \right)^{1/4}, \]

where \( 1/q = 0 \) if \( q = \infty \).

**Proof.** The strategy is to first establish Gaussian approximation results for a finite, yet “dense”, subset \( \mathcal{H}' \) of \( \mathcal{H} \) (Appendix B), and then approximate the supremum over \( \mathcal{H} \) by that over \( \mathcal{H}' \), which requires the local maximal inequalities developed in Section 7. See details in Section C.2. \( \blacksquare \)

### 6.2. Bootstrap validity

The next Theorem shows that conditional on \( D_n' \), the maximum of the bootstrap process, \( M_n'^{\#} \) in (16), is well approximated by the maximum of \( W_p, \tilde{M}_n \), in distribution.

**Theorem 6.2.** Assume the conditions (PM), (VC), (MB), and (MT-0)-(MT-5). Let

\[ q_n := \left( \frac{M^{2/q} B_n^{2-4/q} D_n^{4/q} K_n^5}{N \wedge N_2^{1-2/q}} \right)^{1/4} + \left( \frac{B_n^2 K_n^7}{N \wedge N_2} \right)^{1/8} + \left( \frac{D_n^2 K_n^7}{n^{1-2/q}} \right)^{1/8} + \left( \frac{D_n^2 K_n^4}{n^{1-1/q}} \right)^{1/4} + \left( \frac{M^{8/q} K_n^{15}}{n^{3-4/q}} \right)^{1/14} + \left( \frac{D_n^{3-2/q} K_n^4}{n^{1-1/q}} \right)^{2/7}. \]

Then there exists a constant \( C \) depending only on \( r, q, \bar{\sigma}, c_0, C_0 \) such that with probability at least \( 1 - C q_n \),

\[ \sup_{t \in \mathbb{R}} \left| \mathbb{P}_{D_n'}(M_n'^{\#} \leq t) - \mathbb{P}(\tilde{M}_n \leq t) \right| \leq C q_n. \]
Proof. Note that conditional on $D_n$, $U_{n,A}^\#$, $U_{n,B}^\#$, and $U_{n,*}^\#$ are centered Gaussian processes with the following covariance functions: for $h, h' \in H$,

\begin{align*}
\hat{\gamma}_A(h, h') &:= n^{-1}\sum_{k=1}^{n} \left( G^{(k)}(h) - \overline{G}(h) \right) \left( G^{(k)}(h') - \overline{G}(h') \right), \\
\hat{\gamma}_B(h, h') &:= \frac{1}{N(\sigma(h))} \sum_{i \in I_{n,r}} Z_i^{(\sigma(h))} \left( h(X_i) - U_{n,N}(h) \right) \left( h'(X_i) - U_{n,N}'(h') \right) 1\{ \sigma(h) = \sigma(h') \}, \\
\hat{\gamma}_*(h, h') &:= r^2 \hat{\gamma}_A(h, h') + \alpha_n \hat{\gamma}_B(h, h').
\end{align*}

(32)

The key steps are to show that $\hat{\gamma}_A(\cdot, \cdot)$ and $\hat{\gamma}_B(\cdot, \cdot)$ are good estimators for $\gamma_A(\cdot, \cdot)$ and $\gamma_B(\cdot, \cdot)$ in (30). See details in Appendix C.4. ■

6.3. Related work

$U$-processes offer a general framework for many statistical applications such as testing for qualitative features (e.g., monotonicity, curvature) of regression functions [29, 8, 1], testing for stochastic monotonicity [49], nonparametric density estimation [58, 28, 30], and establishing limiting distributions of $M$-estimators [2, 61]. When indexing function classes are fixed, it is known that the Uniform Central Limit Theorems (UCLTs) [59, 2, 21, 7], as well as limit theorems for bootstrap [3, 66], hold for $U$-processes under metric (or bracketing) entropy conditions. These references [59, 2, 21, 7, 3, 66] cover both non-degenerate and degenerate $U$-processes where limiting processes of the latter are Gaussian chaoses rather than Gaussian processes. When the UCLTs do not hold for a possibly changing (in $n$) indexing function class (i.e., the function class cannot be embedded in any fixed Donsker class), [14] develops a general non-asymptotic theory for approximating the suprema of $U$-processes, extending the earlier work by [18] on empirical processes. Incomplete $U$-statistics for a fixed dimension are first considered in [5], and the asymptotic distributions are studied in [9, 43]. In high dimensions, non-asymptotic Gaussian approximation and bootstrap results for randomized incomplete $U$-statistics are established in [13] for a fixed order and in [62] for diverging orders. The current work considers randomized incomplete (local) $U$-processes with stratification.

7. A local maximal inequality for multiple incomplete $U$-processes

In this section, we highlight a local maximal inequality in Theorem 7.1 for multiple incomplete $U$-processes. Thus, let $\mathcal{F}$ be a collection of symmetric, measurable functions $f : (S^r, S^r) \to (\mathbb{R}, B(\mathbb{R}))$ with a measurable envelope function $F : S^r \to [0, \infty)$ such that $0 < P^\tau F^2 < \infty$. For $\tau > 0$, define the uniform entropy integral

\begin{equation}
\bar{J}(\tau) := \bar{J}(\tau, \mathcal{F}, F) := \int_0^\tau \sqrt{1 + \sup_Q \log N(\mathcal{F}, || \cdot ||_{Q,2}, \epsilon, ||F||_{Q,2})} \, d\epsilon,
\end{equation}

where the $\sup_Q$ is taken over all finitely supported probability measures on $S^r$. An important observation is that it is equivalent to take the supremum over all finitely support measures $Q$ with $Q(S^r) < \infty$. 

Let $M \geq 1$ be an integer, and $\{Z^{(m)}_t : t \in I_{n,r}, m \in [M]\}$ be a collection of i.i.d. Bernoulli random variables with success probability $p_n = N/|I_{n,r}|$ for some integer $0 < N \leq |I_{n,r}|$, which are independent of the data $X^n$. For $m \in [M]$, let

$$D_n^{(m)}(f) := \frac{1}{\sqrt{N}} \sum_{t \in I_{n,r}} (Z^{(m)}_t - p_n) f(X_t), \quad \text{for } f \in \mathcal{F}. \quad (34)$$

**Theorem 7.1.** Let $\sigma_r > 0$ be such that $\sup_{f \in \mathcal{F}} \|f\|_{P^r,2} \leq \sigma_r \leq \|F\|_{P^r,2}$. Then for some absolute constant $C > 0$, $C^{-1} \mathbb{E} \left[ \max_{m \in [M]} \|D_n^{(m)}(f)\|_F \right]$ is upper bounded by

$$\sqrt{M \log(2M) J(\delta_r)} \|F\|_{P^r,2} + \frac{\log(2M) \|\bar{T}\|_{P^2} f^2(\delta_r)}{\sqrt{N}} + \sqrt{\Delta \log(2M) J(\delta_r)},$$

where we define

$$\delta_r := \frac{\sigma_r}{\sqrt{M} \|F\|_{P^r,2}}, \quad \Delta := \mathbb{E} \left[ \sup_{f \in \mathcal{F}} \left| I_{n,r} \right|^{-1} \sum_{t \in I_{n,r}} f^2(X_t) \right], \quad \bar{T} := \max_{t \in I_{n,r}, m \in [M]} Z^{(m)}_t F(X_t).$$

Further, $\|\bar{T}\|_{P,2} \leq M^{1/q} N^{1/q} \|F\|_{P,q}$, for any $q \in [2, \infty]$, with the understanding that $1/q = 0$ if $q = \infty$. In addition, if $\mathcal{F}$ is VC type class with characteristics $(A, \nu)$, $J(\tau) \leq C \tau \sqrt{\nu \log(A/\tau)}$ for $\tau \in (0, 1)$.

**Proof.** See Appendix A.1. 

**Remark 7.2.** For a VC-type class, the upper bound depends on $M$ only via $\log^2(2M)$ if we use $\|F\|_{P^r,\infty}$ to bound $\|\bar{T}\|_{P,2}$. To further bound $\Delta$, which is the expectation of the supremum of a complete $U$-process, we use the multi-level local maximal inequalities developed in [14], which are summarized in Appendix A.5 for convenience.

**Remark 7.3.** There are two difficulties in the proof. First, $p_n := N/|I_{n,r}|$ is very small (in most cases, asymptotically vanishing), which prevents us from directly applying sub-Gaussian inequality to $D_n^{(m)}(\cdot)$. One possible approach is to use Bernstein’s inequality, which however involves the infinity norm, $\max_{t \in I_{n,r}} F(X_t)$ (in comparison to $\bar{T}$ in the above Lemma), and leads to sub-optimal rate. Second, we hope to achieve logarithmic dependence on $M$, so that the number of partitions will only impose a mild requirement on the sample size $n$ and computational budget $N$.

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References


Appendix A: Maximal inequalities

A.1. Proof of Theorem 7.1

The idea of the current proof is in similar spirit as the proof for [18, Theorem 5.2] and [14, Theorem 5.1]. That is, we try to bound second moment by a concave function of first moment (see Step 3 in the
Proof of Theorem 7.1 below), which, in [18, Theorem 5.2] and [14, Theorem 5.1], was achieved by the contraction principle ([18, Lemma A.5]) and Hoffman-Jørgensen inequality([18, Theorem A.1]).

However, in the presence of sampling (\{Z_\ell^{(m)}\}), these tools cannot be applied easily, and we need the following generalization of the contraction principle.

**Lemma A.1** (Contraction principle). Let $M, L \geq 1$ be integers, $\Theta \subset \mathbb{R}^L$ and $\{\epsilon_\ell^{(m)} : \ell \in [L], m \in [M]\}$ be a collection of independent Rademacher variables. Then

$$
E \left[ \sup_{m \in [M], \theta \in \Theta} \left| \sum_{\ell \in [L]} \epsilon_\ell^{(m)} \theta_{\ell}^2 \right| \right] \leq 4T E \left[ \sup_{m \in [M], \theta \in \Theta} \left| \sum_{\ell \in [L]} \epsilon_\ell^{(m)} \theta_{\ell} \right| \right],
$$

where $T := \sup_{\theta \in \Theta, \ell \in [L]} |\theta_{\ell}|$.

**Proof.** Define $\mathcal{A} := \bigcup_{m \in [M]} \mathcal{A}_m$, where

$$
\mathcal{A}_m := \bigcup_{\theta \in \Theta} \{ \alpha \in \mathbb{R}^{L \times M} : \alpha_{\ell,j} = \theta_{\ell} \mathbbm{1}\{j = m\} \text{ for } \ell \in [L], j \in [M]\},
$$

It is clear that $E \left[ \sup_{m \in [M], \theta \in \Theta} \left| \sum_{\ell \in [L]} \epsilon_\ell^{(m)} \theta_{\ell} \right| \right] = E \left[ \sup_{\alpha \in \mathcal{A}} \left| \sum_{\ell \in [L], j \in [M]} \epsilon_\ell^{(j)} (\alpha_{\ell,j})^2 \right| \right]$ and $E \left[ \sup_{m \in [M], \theta \in \Theta} \left| \sum_{\ell \in [L]} \epsilon_\ell^{(m)} \theta_{\ell}^2 \right| \right] = E \left[ \sup_{\alpha \in \mathcal{A}} \left| \sum_{\ell \in [L], j \in [M]} \epsilon_\ell^{(j)} (\alpha_{\ell,j})^2 \right| \right]$. Then the proof is complete by the usual contraction principle[48, Theorem 4.12].

**Proof of Theorem 7.1.** First, define a collection of random measures (not necessarily probability measures) on $(S^r, \mathcal{S}^r)$ that play important roles:

$$
\tilde{Q}_m := N^{-1} \sum_{\ell \in I_{n,r}} Z_\ell^{(m)} \delta_{X_\ell} \text{ for } m \in [M], \quad \tilde{Q} := \sum_{m=1}^M \tilde{Q}_m,
$$

where $\delta_{(x_1, \ldots, x_r)}$ is the Dirac measure such that $\delta_{(x_1, \ldots, x_r)}(A) = \mathbbm{1}\{(x_1, \ldots, x_r) \in A\}$ for any $A \in \mathcal{S}^r$. Further, define

$$
\hat{V}_n := \max_{m \in [M]} \sup_{f \in \mathcal{F}} \|f\| \tilde{Q}_{m,2} = \max_{m \in [M]} \sup_{f \in \mathcal{F}} \sqrt{N^{-1} \sum_{\ell \in I_{n,r}, m \in [M]} Z_\ell^{(m)} f^2(X_\ell)},
$$

$$
z^* := \sqrt{M^{-1} E[\hat{V}_n^2] / \|F\|^2_{\mathcal{P}_{2r,2}}}. \quad \quad (36)
$$

Finally, let $\{\epsilon_\ell^{(m)} : \ell \in I_{n,r}, m \in [M]\}$ be a collection of independent Rademacher random variables that are independent of $D_n := \{Z_\ell^{(m)} : \ell \in I_{n,r}, m \in [M]\} \cup \mathcal{X}_n^\theta$. Define for $f \in \mathcal{F}$,

$$
\hat{\mathcal{D}}_n^{(m)}(f) := N^{-1/2} \sum_{\ell \in I_{n,r}} \epsilon_\ell^{(m)} Z_\ell^{(m)} f(X_\ell) \text{ for } m \in [M], \quad \hat{\mathcal{D}}_n(f) := \max_{m \in [M]} |\hat{\mathcal{D}}_n^{(m)}(f)|,
$$

$$
\tilde{\mathcal{D}}_n(f) := \max_{m \in [M]} \left| N^{-1/2} \sum_{\ell \in I_{n,r}} \epsilon_\ell^{(m)} Z_\ell^{(m)} f^2(X_\ell) \right|.
$$
Step 1. bound $E\left[\max_{m \in [M]} \|D_n^{(m)}\|_F\right]$. Since $\{Z_i^{(m)} : i \in I_{n,r}, m \in [M]\}$ is independent of $X^n_1$, by first conditioning on $X^n_1$ and then applying symmetrization inequality,

$$E\left[\max_{m \in [M]} \|D_n^{(m)}(f)\|_F\right] = E\left[ E\left[ \max_{m \in [M]} \|D_n^{(m)}(f)\|_F \mid X^n_1\right]\right] \leq E\left[ E\left[ \max_{m \in [M]} \|\hat{D}_n^{(m)}(f)\|_F \mid X^n_1\right]\right]$$

$$= E\left[ \max_{m \in [M]} \|\hat{D}_n^{(m)}(f)\|_F\right] = E\left[ \|\hat{D}_n(f)\|_F\right].$$

Then we apply the standard entropy integral bound conditioning on $D_n$. Specifically, for $m \in [M]$ and $f_1, f_2 \in \mathcal{F}$, by Hoeffding’s inequality [64, Lemma 2.2.7],

$$\|\hat{D}_n^{(m)}(f_1) - \hat{D}_n^{(m)}(f_2)\|_{\psi_2 | D_n} \lesssim \sqrt{1 \over N} \sum_{i \in I_{n,r}} (Z_i^{(m)})^2(f_1(X_i) - f_2(X_i))^2 = \|f_1 - f_2\|_{\tilde{Q}_{m,2}},$$

where note that $Z^2 = Z$ for any Bernoulli random variable $Z$. Now we use $\hat{V}_n$ as the diameter for $\mathcal{F}$ under $\| \cdot, \tilde{Q}_{m,2}$, and by the entropy integral bound [64, Corollary 2.2.5],

$$\|\|\hat{D}_n^{(m)}(f)\|_F\|_{\psi_2 | D_n} \lesssim \int_0^{\hat{V}_n} \sqrt{1 + \log N(\mathcal{F}, \| \cdot, \tilde{Q}_{m,2}, \epsilon) \mid f} \, \rho \leq \int_0^{\hat{V}_n} \sqrt{1 + \log N(\mathcal{F}, \| \cdot, \tilde{Q}_{m,2}, \epsilon) \mid f} \, \rho \leq \|f\|_{\tilde{Q}_{m,2}} \hat{J}(\hat{V}_n/\|f\|_{\tilde{Q}_{m,2}}),$$

where in the second inequality we used the fact that $\tilde{Q}$ dominates $\hat{Q}_m$, and in the third we used change-of-variable technique and the definition of $\hat{J}(\cdot)$ (recall again $\hat{Q}$ may not be a probability measure). Then by maximal inequality [64, Lemma 2.2.2],

$$E\left[ \max_{m \in [M]} \|\hat{D}_n^{(m)}(f)\|_F \mid D_n\right] \lesssim \sqrt{\log(2M)}\|f\|_{\tilde{Q}_{m,2}} \hat{J}(\hat{V}_n/\|f\|_{\tilde{Q}_{m,2}}) \tag{37}$$

Since $(x, y) \mapsto \hat{J}(\sqrt{x/y})\sqrt{y}$ is jointly concave (see [18, Lemma A.2]), by Jensen’s inequality,

$$E\left[ \max_{m \in [M]} \|\hat{D}_n^{(m)}(f)\|_F \right] \lesssim \sqrt{\log(2M)} \sqrt{E\left[ \|f\|_{\tilde{Q}_{m,2}}^2 \right]} \hat{J}(\sqrt{E[\tilde{V}_n^2]/E\left[ \|f\|_{\tilde{Q}_{m,2}}^2 \right]} \tag{38}$$

$$= \sqrt{M\log(2M)}\|f\|_{\tilde{Q}_{m,2}} \hat{J}(z^*),$$

where for the equality, we use the fact that

$$E\left[ \|f\|_{\tilde{Q}_{m,2}}^2 \right] = E\left[ N^{-1} \sum_{m \in [M]} \sum_{i \in I_{n,r}} Z_i^{(m)} F^2(X_i) \right] = M\|f\|_{\tilde{Q}_{m,2}}^2.$$
Step 2. bound $\mathbb{E}[\hat{V}_n^2]$. Observe that

$$
\mathbb{E}[\hat{V}_n^2] \leq \frac{1}{N} \mathbb{E} \left[ \max_{m \in [M]} \sup_{f \in \mathcal{F}, i \in I_{n,r}} \left( Z_i^{(m)} - p_n \right)^2 \right] + \mathbb{E} \left[ \sup_{f \in \mathcal{F}} |I_{n,r}|^{-1} \sum_{i \in I_{n,r}} f^2(X_i) \right]
$$

where in the last inequality we again first condition on $X_1^n$ and then apply symmetrization inequality. For the first term, conditional on $\mathcal{D}_n$, by Lemma A.1 (contraction principle) and (37),

$$
\mathbb{E} \left[ \left\| \hat{D}_n(f) \right\|_{\mathcal{F}} \right|_{\mathcal{D}_n} \leq \bar{T} \mathbb{E} \left[ \left\| \hat{D}_n(f) \right\|_{\mathcal{F}} \right|_{\mathcal{D}_n} \leq \sqrt{\log(2M)} \bar{T} \|F\|_{\bar{Q},2} \hat{J} \left( \left\| \hat{V}_n \right\|_{\mathcal{F}} \right).
$$

Denote $\xi := \bar{T} \|F\|_{\bar{Q},2}$. Since $(x, y) \mapsto \hat{J}(x/y)y$ is jointly concave (see [18, Lemma A.3]), by Jensen’s inequality and Cauchy-Schwarz inequality,

$$
\mathbb{E} \left[ \left\| \hat{D}_n(f) \right\|_{\mathcal{F}} \right] \leq \sqrt{\log(2M)} \mathbb{E} \left[ \left\| \hat{D}_n(f) \right\|_{\mathcal{F}} \right] \leq \sqrt{\log(2M)} \mathbb{E} \left[ \left\| \hat{D}_n(f) \right\|_{\mathcal{F}} \right] \leq \sqrt{\log(2M)} \mathbb{E} [\xi] \hat{J} \left( \frac{\mathbb{E} [\hat{V}_n]}{\xi} \right).
$$

Since $\hat{J}(\cdot)$ is non-decreasing in $[0, \infty)$ and for $c \geq 1$, $\hat{J}(ct) \leq c \hat{J}(t)$ (see [18, Lemma A.2]) and by definition of $z^*$, we have

$$
\mathbb{E} \left[ \left\| \hat{D}_n(f) \right\|_{\mathcal{F}} \right] \leq \sqrt{\log(2M)} \mathbb{E} [\xi] \hat{J} \left( \left( \mathbb{E} [\xi]^{-1} \left\| \bar{T} \right\|_{p,2} \sqrt{M} \|F\|_{p,2} \vee 1 \right) z^* \right)
$$

$$
\leq \sqrt{\log(2M)} \left( \sqrt{M} \left\| \bar{T} \right\|_{p,2} \|F\|_{p,2} + \mathbb{E} [\xi] \right) \hat{J}(z^*)
$$

$$
\leq 2 \sqrt{M} \log(2M) \left\| \bar{T} \right\|_{p,2} \|F\|_{p,2} \hat{J}(z^*),
$$

where in the last inequality we applied Cauchy-Schwarz inequality.

Step 3. bound $(z^*)^2$ by $\hat{J}(z^*)$. Applying (40) to the first term in (39), we have

$$
(z^*)^2 = M^{-1} \mathbb{E} \left[ \hat{V}_n^2 \right] / \|F\|_{p,2}^2 \leq \frac{\Delta}{M \|F\|_{p,2}^2} + \frac{\sqrt{\log(2M)} \left\| \bar{T} \right\|_{p,2} \hat{J}(z^*)}{M \|F\|_{p,2} \sqrt{MN}}.
$$

Now define

$$
\Delta' := \max \left\{ \delta_r, \sqrt{M^{-1} \Delta} / \|F\|_{p,2} \right\} \geq \delta_r.
$$

Applying [63, Lemma 2.1], we have

$$
\hat{J}(z^*) \leq \hat{J}(\Delta') + \frac{\sqrt{\log(2M)}}{M \|F\|_{p,2} \sqrt{MN}} \frac{\hat{J}^2(\Delta')}{\Delta'^2}.
$$
Now we apply the above result to (38):

\[
\mathbb{E} \left[ \max_{m \in [M]} \| D_n^{(m)}(f) \|_F \right] \lesssim \sqrt{M \log(2M)} \left( \hat{J} (\Delta') \| F \|_{p^r, 2} + \frac{\sqrt{\log(2M)} \| \hat{T} \|_{p^r, 2} J^2 (\Delta')} {\sqrt{MN} (\Delta')^2} \right).
\]

Since \( J(\tau) / \tau \) is non-increasing (see [18, Lemma 5.2]), we have

\[
\hat{J}(\Delta') \lesssim \frac{\sqrt{\Delta \hat{J}(\delta_r)}} {\delta_r} = \max \left\{ \hat{J}(\delta_r), \frac{\sqrt{\Delta \hat{J}(\delta_r)}} {\sqrt{M} \| F \|_{p^r, 2} \delta_r} \right\},
\]

which completes the proof of the first inequality.

\[\text{Remark A.2. } \text{In Appendix A.3, we also establish a non-local maximal inequality for the supremum of multiple } U\text{-processes, which is simpler, and will be used to bound the second moment of the supremum.}\]

**A.2. A Corollary to Theorem 7.1**

The following Corollary is needed in establishing the validity of bootstrap, which has essentially been established in the proof of Theorem 7.1.

**Corollary A.3.** Assume the conditions and notations in Theorem 7.1. Recall the definitions of \( \hat{Q} \) in (35) and \( \hat{V}_n \) in (36). Then for some absolute constant \( C > 0 \),

\[
C^{-1} \sqrt{\log(2M)} \mathbb{E} \left[ \| F \|_{\hat{Q}, 2} \hat{J}(\hat{V}_n / \| F \|_{\hat{Q}, 2}) \right] \leq
\]

\[
\sqrt{M \log(2M)} \hat{J}(\delta_r) \| F \|_{p^r, 2} + \frac{\log(2M) \| \hat{T} \|_{p^r, 2} J^2 (\delta_r)} {\sqrt{N}} + \frac{\sqrt{\log(2M)} \hat{J}(\delta_r)} {\delta_r},
\]

\[
\mathbb{E} \left[ \hat{V}_n^2 \right] \lesssim \Delta + \sigma_r^2 + \frac{\log(2M) \| \hat{T} \|_{p^r, 2} J^2 (\delta_r)} {N \delta_r^2},
\]

where recall that \( \Delta := \mathbb{E} \left[ \sup_{f \in F} | I_{n, r} |^{-1} \sum_{i \in I_{n, r}} f^2 (X_i) \right] \).

**Proof.** In the Step 1 of proving Theorem 7.1, we bound \( \mathbb{E} \left[ \max_{m \in [M]} \| D_n^{(m)}(f) \|_F \right] \) through an upper bound on \( \sqrt{\log(2M)} \mathbb{E} \left[ \| F \|_{\hat{Q}, 2} \hat{J}(\hat{V}_n / \| F \|_{\hat{Q}, 2}) \right] \) (see (37)). Thus the first inequality has been established.

For the second inequality, in the Step 3 of proving Theorem 7.1, we showed that

\[
\mathbb{E} \left[ \hat{V}_n^2 \right] \lesssim \Delta + \frac{\| \hat{T} \|_{p^r, 2}} {\sqrt{N}} \sqrt{M \log(2M)} \| F \|_{p^r, 2} \hat{J}(z^*),
\]

\[
\sqrt{M \log(2M)} \| F \|_{p^r, 2} \hat{J}(z^*) \lesssim
\]

\[
\sqrt{M \log(2M)} \| F \|_{p^r, 2} + \frac{\log(2M) \| \hat{T} \|_{p^r, 2} J^2 (\delta_r)} {\sqrt{N} \delta_r^2} + \frac{\sqrt{\log(2M)} \hat{J}(\delta_r)} {\delta_r}.
\]
As a result,

\[
\mathbb{E} \left[ \hat{V}_n^2 \right] \lesssim \Delta + \frac{\log(2M)\|\hat{T}\|_{\mathbb{P}, 2}^2}{N\delta^2} J_\epsilon + \frac{M \log(2M) \|\hat{T}\|_{\mathbb{P}, 2} \|F\|_{P^r, 2} J_\epsilon}{\sqrt{N}} + \frac{\sqrt{\log(2M) \Delta} \|\hat{T}\|_{\mathbb{P}, 2} J_\epsilon}{\sqrt{N}\delta}.
\]

Then the results follow by Cauchy-Schwarz inequality and due to the definition that \( \sigma_r := \sqrt{M}\delta_r \|F\|_{P^r, 2} \).

\[\Box\]

A.3. Non-local maximal inequalities for multiple incomplete \( U \)-processes

In this subsection, we establish an upper bound for the second moment of the supremum over multiple incomplete \( U \)-processes, as defined in Section 7, which however is non-local. Recall the notations in Section 7.

**Lemma A.4.** Denote \( z := \mathbb{E} \left[ \max_{m \in [M]} N^{-1} \sum_{i \in I_{n, r}} Z_i^{(m)} F^2(X_i) \right] \), and recall the definition of \( \hat{T} \) in Theorem 7.1. Then for some absolute constant \( C > 0 \),

\[ z \leq C \left( \|F\|_{P^r, 2}^2 + \frac{\log(2M) \|\hat{T}\|_{\mathbb{P}, 2}^2}{N} \right). \]

**Proof.** Observe that \( z \leq \mathbb{E} \left[ \max_{m \in [M]} N^{-1} \sum_{i \in I_{n, r}} (Z_i^{(m)} - p_n) F^2(X_i) \right] + \|F\|_{P^r, 2}^2 \). Let \( \{\epsilon_i^{(m)} : i \in I_{n, r}, m \in [M]\} \) be a collection of independent Rademacher random variables that are independent of \( D_n := \{Z_i^{(m)} : i \in I_{n, r}, m \in [M]\} \cup X_1^n \). By the symmetrization inequality (conditional on \( X_1^n \)), the contraction principle (Lemma A.1, conditional on \( D_n \)), and Cauchy-Schwarz inequality,

\[
\begin{align*}
  z & \lesssim \mathbb{E} \left[ \max_{m \in [M]} \left| N^{-1} \sum_{i \in I_{n, r}} \epsilon_i^{(m)} Z_i^{(m)} F^2(X_i) \right| + \|F\|_{P^r, 2}^2 \right] \\
  & \lesssim \mathbb{E} \left[ \hat{T} \max_{m \in [M]} \left| N^{-1} \sum_{i \in I_{n, r}} \epsilon_i^{(m)} Z_i^{(m)} F(X_i) \right| + \|F\|_{P^r, 2}^2 \right] \\
  & \lesssim \|\hat{T}\|_{\mathbb{P}, 2} \left( \mathbb{E} \left[ \max_{m \in [M]} \left| N^{-1} \sum_{i \in I_{n, r}} \epsilon_i^{(m)} Z_i^{(m)} F(X_i) \right|^{2^*} \right] \right)^{1/2} + \|F\|_{P^r, 2}^2.
\end{align*}
\]

By Hoeffding’s inequality [64, Lemma 2.2.7], for \( m \in [M] \),

\[
\left\| N^{-1} \sum_{i \in I_{n, r}} \epsilon_i^{(m)} Z_i^{(m)} F(X_i) \right\|_{\psi_2 | D_n} \lesssim \sqrt{N^{-2} \sum_{i \in I_{n, r}} Z_i^{(m)} F^2(X_i)}.
\]
Thus by maximal inequality [64, Lemma 2.2.2],

\[
\mathbb{E} \left[ \max_{m \in [M]} \left| N^{-1} \sum_{i \in I_{n,r}} \epsilon_i^{(m)} Z_i^{(m)} F(X_i) \right|^2 \right] \leq \mathbb{E} \left[ \log(2M) \max_{m \in [M]} N^{-2} \sum_{i \in I_{n,r}} Z_i^{(m)} F^2(X_i) \right] \leq \log(2M) z/N.
\]

Thus we have \( z \lesssim \|\mathcal{T}\|_{p,2}^2 \sqrt{\log(2M)} \sqrt{z} + \|F\|_{p,2}^2 \), which implies the conclusion. 

Recall the definition of \( \hat{\delta}_n^{(m)} \) in (34).

**Lemma A.5.** Recall the definition of \( \hat{T} \) in Theorem 7.1. Then for some absolute constant \( C > 0 \),

\[
\mathbb{E} \left[ \max_{m \in [M]} \|D_n^{(m)}(f)\|_{\mathcal{F}}^2 \right] \leq C \mathcal{J}^2(1) \left( \log(2M)\|F\|_{p,2}^2 + \frac{\log^2(2M)\|\mathcal{T}\|_{p,2}^2}{N} \right).
\]

**Proof.** Recall the definitions of \( \hat{\delta}_n^{(m)} \), \( \hat{Q}_m \), and \( D_n \) in the proof for Theorem 7.1. Define for \( m \in [M] \),

\[
\hat{V}_n^{(m)} := \sup_{f \in \mathcal{F}} \|f\|_{\hat{Q}_m,2}.
\]

By the same argument leading to (37) as in the proof for Theorem 7.1, we have

\[
\mathbb{E} \left[ \max_{m \in [M]} \|D_n^{(m)}(f)\|_{\mathcal{F}}^2 \mid X_1^n \right] \leq \mathbb{E} \left[ \max_{m \in [M]} \|\hat{\delta}_n^{(m)}(f)\|_{\mathcal{F}}^2 \mid X_1^n \right]
\]

\[
\mathbb{E} \left[ \max_{m \in [M]} \|\hat{\delta}_n^{(m)}(f)\|_{\mathcal{F}}^2 \mid D_n \right] \leq \log(2M) \max_{m \in [M]} \left( \int_0^{\hat{V}_n^{(m)}} \sqrt{1 + \log N(\mathcal{F}, \|\cdot\|_{\hat{Q}_m,2}, \epsilon)} \, d\epsilon \right)^2 \leq \log(2M) \max_{m \in [M]} \|F\|_{\hat{Q}_m,2}^2 \mathcal{J}^2(1),
\]

where we used change-of-variable, and the fact that \( \hat{V}_n^{(m)} \leq \|F\|_{\hat{Q}_m,2} \). Then the proof is complete by taking expectation on both sides, and applying the Lemma A.4. 

**A.4. A discretization lemma**

Theorem 7.1 will usually be applied after discretization. The following lemma is useful for discretizing a VC-type class, as defined in (2.2), so that the difference class has the desired property.

**Lemma A.6.** Assume \((\mathcal{F}, F)\) is a VC-type class with characteristics \((A, \nu)\) and \(P^n F^4 < \infty\). For any \( \epsilon \in (0, 1) \), there exists a finite collection \( \{f_j : 1 \leq j \leq d\} \subset \mathcal{F} \) such that the following two conditions hold: (i). \( d \leq (4A/\epsilon)^\nu \); (ii). for any \( f \in \mathcal{F} \), there exists \( 1 \leq j^* \leq d \) such that

\[
\max \left\{ \|f - f_{j^*}\|_{p^*,2}, \|f - f_{j^*}\|_{p^*,4}^2 \right\} \leq \epsilon \|1 + F^2\|_{p^*,2}.
\]
Further, define
\[ \mathcal{F}_\epsilon := \{ f - f' : \max \{|f - f'|_{P^r,2}, |f - f'|_{P^{r,4}}^2 \} \leq \epsilon \}, \]

Then \((\mathcal{F}_\epsilon, 2F)\) is a VC-type class with characteristics \((A, 2\nu)\).

**Proof.** We start with the first claim. Define a measure \(Q^*\) (not probability) on \((S^r, S^r)\) as follows:
\[ Q^*(A) := \int_A (1 + F^2) dP^r, \text{ for any } A \in S^r. \]

Since \(P^r F^4 < \infty\), \(Q^*\) is a finite measure and \(Q^* F^2 < \infty\). By definition 2.2 of VC-type class and [64, Problem 2.5.1, Page 133],
\[ N(\mathcal{F}, \| \cdot \|_{Q^*,2}, 2^{-1} \epsilon \| F\|_{Q^*,2}) \leq \sup_Q N(\mathcal{F}, \| \cdot \|_{Q,2}, 4^{-1} \epsilon \| F\|_{Q,2}) \leq (4A/\epsilon)^\nu, \]
where the \(\sup_Q\) is taken over all finitely supported probability measures on \(S^r\). Thus there exists an integer \(d \leq (4A/\epsilon)^\nu\) and a subset \(\{f_j : 1 \leq j \leq d\} \subset \mathcal{F}\) such that for any \(f \in \mathcal{F}\), there exists \(1 \leq j^* \leq d\) such that
\[ \|f - f_{j^*}\|_{Q^*,2}^2 \leq 2^{-2} \epsilon^2 \|F\|_{Q^*,2}^2 = 4^{-1} \epsilon^2 \int (F^2 + F^4) dP^r \leq 4^{-1} \epsilon^2 \|1 + F^2\|_{P^{r,4}}^2. \]

On the other hand,
\[ \|f - f_{j^*}\|_{Q^*,2}^2 = \int (f - f_{j^*})^2 (1 + F^2) dP^r \geq \|f - f_{j^*}\|_{P^{r,2}}^2, \]
\[ \|f - f_{j^*}\|_{Q^*,2}^2 = \int (f - f_{j^*})^2 (1 + F^2) dP^r \geq 4^{-1} \int (f - f_{j^*})^4 dP^r = 4^{-1} \|f - f_{j^*}\|_{P^{r,4}}^4, \]
which completes the proof of the first claim.

For the second claim, for any \(\tau > 0\) and finite probability measure \(Q\), there exists \(\{f'_j : 1 \leq j \leq d'\} \subset \mathcal{F}\) such that \(d' = N(\mathcal{F}, \| \cdot \|_{Q,2}, \tau \| F\|_{Q,2}) \leq (A/\tau)^\nu\), and for any \(f \in \mathcal{F}\), there exists \(1 \leq j' \leq d'\) such that
\[ \|f - f'_{j'}\|_{Q,2} \leq \tau \|F\|_{Q,2}. \]

By triangle inequality, \(\{f_j - f'_{k} : 1 \leq j, k \leq d'\}\) is a \(\|2F\|_{Q,2}\) cover for \(\mathcal{F} - \mathcal{F} := \{ f - f' : f, f' \in \mathcal{F}\}\).

As a result,
\[ N(\mathcal{F}_\epsilon, \| \cdot \|_{Q,2}, \tau \|2F\|_{Q,2}) \leq N(\mathcal{F} - \mathcal{F}, \| \cdot \|_{Q,2}, \tau \|2F\|_{Q,2}) \leq (A/\tau)^{2\nu}, \]
which completes the proof.

**A.5. Multi-level local maximal inequality for complete U-processes**

In this subsection, let \(\mathcal{F}\) be a collection of symmetric, measurable functions \(f : (S^r, S^r) \to (\mathbb{R}, \mathcal{B}(\mathbb{R}))\) with a measurable envelope function \(F : S^r \to [0, \infty)\) such that \(0 < P^r F^2 < \infty\). For \(f \in \mathcal{F}\), denote by \(U_n^{(r)}(f) := \|I_{n,r}\|^{-1} \sum_{t \in I_{n,r}} f(X_t)\) its associated U-process.
For each \(1 \leq \ell \leq r\), the Hoeffding projection (with respect to \(P\)) is defined by

\[
(\pi_{\ell} f)(x_1, \ldots, x_{\ell}) := (\delta_{x_1} - P) \cdots (\delta_{x_{\ell}} - P)P^{r-\ell} f.
\]

Then the Hoeffding decomposition [42] of \(U_{n}^{(r)}\) is given by

\[
U_{n}^{(r)}(f) - P^{r} f = \sum_{i=1}^{\ell} \binom{r}{\ell} U_{n}^{(i)}(\pi_{\ell} f), \quad \text{for } f \in \mathcal{F}.
\]  

(41)

For \(1 \leq \ell \leq r\), let \(F_{\ell}\) be an envelope function for \(P^{r-\ell}\mathcal{F} := \{P^{r-\ell} f : f \in \mathcal{F}\}\), i.e., \(|P^{r-\ell} f(x)| \leq F_{\ell}(x)\) for any \(f \in \mathcal{F}\) and \(x \in S^{\ell}\). Further for \(1 \leq \ell \leq r\), let \(\sigma_{\ell}\) be such that \(\sup_{f \in \mathcal{F}} \|P^{r-\ell} f\|_{P^{\ell},2} \leq \sigma_{\ell} \leq \|F_{\ell}\|_{P^{\ell},2}\) and define

\[
T_{\ell} := \max_{1 \leq i \leq \lceil n/\ell \rceil} F_{\ell}(X_{(i-1)\ell+1}).
\]

For \(\tau > 0\) and \(1 \leq \ell \leq r\), define the uniform entropy integral

\[
J_{\ell}(\tau) := J_{\ell}(\tau, P^{r-\ell}\mathcal{F}, F_{\ell}) := \int_{0}^{\tau} \left[ 1 + \sup_{Q} \log N(P^{r-\ell}\mathcal{F}, \|\cdot\|_{Q,2}, \epsilon \|F_{\ell}\|_{Q,2}) \right]^{\ell/2} d\epsilon,
\]  

(42)

where the \(\sup_{Q}\) is taken over all finitely supported probability measures on \(S^{\ell}\).

The following Theorem is due to [14, Theorem 5.1 and Corollary 5.6], and included here due to its repeated use in this paper. Together with (41), it provides multi-scale local inequalities for the complete \(U\)-process.

**Theorem A.7.** For \(1 \leq \ell \leq r\), let \(\delta_{\ell} := \sigma_{\ell}/\|F_{\ell}\|_{P^{\ell},2}\). Then

\[
n^{\ell/2} E \left[ \|U_{n}^{(r)}(\pi_{\ell} f)\|_{\mathcal{F}} \right] \lesssim \min \left\{ J_{\ell}(1)\|F_{\ell}\|_{P^{\ell},2}, \ J_{\ell}(\delta_{\ell})\|F_{\ell}\|_{P^{\ell},2} + \frac{J_{\ell}^{2}(\delta_{\ell})\|T_{\ell}\|_{P^{\ell},2}}{\delta_{\ell}^{2}n} \right\},
\]

where \(\|\cdot\|_{\mathcal{F}} = \sup_{f \in \mathcal{F}} \|\cdot\|\), and \(\lesssim\) means up to a multiplicative constant only depending on \(r\). Further, if \(\mathcal{F}\) has a finite cardinality \(d < \infty\), then

\[
n^{\ell/2} E \left[ \|U_{n}^{(r)}(\pi_{\ell} f)\|_{\mathcal{F}} \right] \lesssim \min \left\{ \|F_{\ell}\|_{P^{\ell},2} \log^{\ell/2}(d), \ \sigma_{\ell} \log^{\ell/2}(d) + n^{-1/2}\|T_{\ell}\|_{P^{\ell},2} \log^{\ell/2+1/2}(d) \right\}.
\]

If \((\mathcal{F}, F)\) is VC type class with characteristics \((A, \nu)\) with \(A \geq e \log(2r-1)/16\) and \(\nu \geq 1\), and \(F_{\ell} = P^{r-\ell} F\) for \(1 \leq \ell \leq r\), then there exists a constant \(C\), depending only on \(r\), such that for any \(\tau \in (0, 1]\),

\[
J_{\ell}(\tau) \leq C \tau^{1/2} (\nu \log(A/\tau))^{\ell/2} \quad \text{for } 1 \leq \ell \leq r.
\]

Finally, for any \(q \in [2, \infty]\), \(\|T_{\ell}\|_{P^{\ell},2} \leq n^{1/q}\|F_{\ell}\|_{P^{\ell},q}\), where \(1/q = 0\) if \(q = \infty\).

**Proof.** The first inequality is established in [14, Theorem 5.1 and Corollary 5.6]. The second inequality slightly improves the dependence of the second term inside \(\min\{\cdot, \cdot\}\) on \(\log(d)\) for a finite class. Its proof is essentially the same, except that we use the fact that \(J_{\ell}(\tau) \lesssim \tau^{1/2}(d)\) for any \(\tau > 0\), and thus is omitted. The third claim is established in [14, Corollary 5.3], while the last claim is obvious.
Appendix B: Stratified, incomplete high-dimensional $U$-statistics

In this subsection, we establish Gaussian approximation and bootstrap results for stratified, incomplete high-dimensional $U$-statistics, which is a key step in establishing the distribution approximation for the supremum of the $U$-process. Thus let $\{h_1, \ldots, h_d\}$ be a collection of $d$ elements in $\mathcal{H}$, and define $\bar{h} := (h_1, \ldots, h_d) \in S^r \rightarrow \mathbb{R}^d$. Consider the following complete and stratified, incomplete $d$-dimensional $U$-statistics:

$$U_{n,j} := U_n(h_j) = |I_{n,r}|^{-1} \sum_{i \in I_{n,r}} h_j(X_{i_1}, \ldots, X_{i_r}) := |I_{n,r}|^{-1} \sum_{i \in I_{n,r}} h_j(X_i),$$

$$U'_{n,N,j} := U'_{n,N}(h_j) = (\hat{N}^{(h_j)})^{-1} \sum_{i \in I_{n,r}} Z_i^{(h_j)} h_j(X_i),$$

where we recall that $\hat{N}^{(m)} := \sum_{i \in I_{n,r}} Z_i^{(m)}$ for $m \in [M]$, and $\sigma(h_j) = m$ if and only if $h_j \in \mathcal{H}_m$. Further, define $\Omega := \mathbb{E}[U_n]$, and $d$-by-$d$ matrices $\Gamma_A, \Gamma_B$, and $\Gamma_s$ such that for $1 \leq i, j \leq d$,

$$\Gamma_{A,ij} := \gamma_A(h_i, h_j), \quad \Gamma_{B,ij} := \gamma_B(h_i, h_j), \quad \Gamma_{s,ij} := \gamma_s(h_i, h_j),$$

where the covariance functions $\gamma_A, \gamma_B,$ and $\gamma_s$ are defined in (30). Denote by $\mathcal{R} := \{\prod_{j=1}^d [a_j, b_j] : -\infty \leq a_j \leq b_j \leq \infty\}$ the collection of hyperrectangles in $\mathbb{R}^d$.

We start with the Gaussian approximation results.

**Theorem B.1.** Assume (MT-0)-(MT-2) hold. Then there exists a constant $C$, depending only on $r, q, \sigma$, such that

$$C^{-1} \sup_{R \in \mathcal{R}} |\mathbb{P}(\sqrt{n}(U_n - \bar{\theta}) \in R) - \mathbb{P}(rY_A \in R)| \leq \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/6} + \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/3} + \left( \frac{D_n^{3-2/q} \log^2(d)}{n^{1-1/q}} \right)^{1/2},$$

where $Y_A \sim \mathcal{N}(0, \Gamma_A)$ and $1/q = 0$ if $q = \infty$.

**Proof.** See Section B.2.

**Theorem B.2.** Assume (MT-0)-(MT-4) and (MB) hold. Then there exists a constant $C$, depending only on $r, q, \sigma, c_0, C_0$, such that

$$\sup_{R \in \mathcal{R}} |\mathbb{P}(\sqrt{n}(U'_{n,N} - \bar{\theta}) \in R) - \mathbb{P}(Y \in R)| \leq C \varpi_n^{(1)} + C \varpi_n^{(2)},$$

with

$$\varpi_n^{(1)} := \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/8} + \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/4} + \left( \frac{D_n^{3-2/q} \log^2(d)}{n^{1-1/q}} \right)^{1/2},$$

$$\varpi_n^{(2)} := \left( \frac{B_n^2 \log^7(dn)}{N} \right)^{1/8} + \left( \frac{n^{4r/q} \log^5(dn)B_n^{2-8/q} D_n^{8/q}}{N} \right)^{1/4},$$

where $Y \sim \mathcal{N}(0, r^2 \Gamma_A + \alpha_n \Gamma_B), \alpha_n := n/N$, and $1/q = 0$ if $q = \infty$. 

Proof. See Section B.4. ■

Recall the definitions of $U^*_n, A$, $U^*_n, B$, and $D'_n$ in Section 2.2. Define three $d$-dimensional random vectors as follows: for $1 \leq j \leq d$, 

$$L^*_{n, A, j} := U^*_n(A(h_j)), \quad L^*_{n, B, j} := U^*_n(B(h_j)), \quad L^*_{n, s, j} := U^*_n(s(h_j)).$$

The next theorem establishes the validity of multiplier bootstrap for high-dimensional incomplete $U$-statistics.

**Theorem B.3.** Assume the conditions (MT-0)-(MT-5), and (MB) hold. There exists a constant $C$, depending only on $\sigma, r, q, c_0, C_0$, such that with probability at least $1 - C \log^{1/4}(2M) \mathcal{X}_n$, 

$$\sup_{R \in R} \left| \mathbb{P}_{\mathcal{D}_n} \left( U^*_n, s \in R \right) - \mathbb{P}(rY_A + \alpha Y_B \in R) \right| \leq C \log^{1/4}(2M) \mathcal{X}_n,$$

where $Y_A \sim N(0, \Gamma_A)$, $Y_B \sim N(0, \Gamma_B)$ and $Y_A, Y_B$ are independent, and $\mathcal{X}_n$ is defined as follows:

$$\left( \frac{M^2 q B_n^{2-4/q} D_n^{4/q} \log^3(d)}{N - N_2} \right)^{1/4} + \left( \frac{B_n^{1/4} \log^5(d)}{N - N_2} \right)^{1/8} + \left( \frac{D_n^{3/8} \log^3(d)}{n^{1-2/q}} \right)^{1/4} + \left( \frac{D_n^{5/8} \log^3(d)}{n^{3-4/q}} \right)^{1/14} + \left( \frac{D_n^{3-2/q} \log^3(d)}{n^{1-1/q}} \right)^{2/7}.$$

Proof. See Subsection B.5.3. ■

In the following proofs in this section, we assume without loss of generality that

$$\bar{\theta} = 0,$$

since otherwise we can always center $h$ first.

**B.1. Supporting calculations**

**Lemma B.4.** Let $L \geq N \geq 3$ be positive integers and $p_n := N/L$. Let $M \geq 1$ be an integer and $\log(M) \leq C_0 \log(N)$ for some absolute constant $C_0$. Let $\{Z^{(m)}_\ell : \ell \in [L], m \in [M]\}$ be a collection of Bernoulli random variables with success probability $p_n$ and $\hat{N}^{(m)} := \sum_{\ell \in [L]} Z^{(m)}_\ell$ for $m \in [M]$. Then there exists a constant $C$, depending only on $C_0$, such that

$$\mathbb{P} \left( \bigcup_{m \in [M]} \left\{ \left| N/\hat{N}^{(m)} - 1 \right| > C \sqrt{\frac{\log(N)}{N}} \right\} \right) \leq CN^{-1}.$$

Proof. By Bernstein’s inequality [64, Lemma 2.2.9] with $x = \sqrt{C \log(N)}$ for $C > 0$ and union bound,

$$\mathbb{P} \left( \bigcup_{m \in [M]} \left\{ \left| \hat{N}^{(m)} / N - 1 \right| > \sqrt{\frac{C \log(N)}{N}} \right\} \right) \leq 2M \exp \left( \frac{-C \log(N)/2}{1 + 3^{-1} \sqrt{C \log(N)/N}} \right)$$
we have

\[ \sqrt{x} \]

Then the conclusion holds with

\[ \frac{-C\log(N)/2}{1 + 3^{-1} \sqrt{C\log(N)/N}} + C_0 \log(N) \].

For \( N \geq 3 \), \( \log(N)/N \leq 0.4 \). Thus if we let \( C_1 \) to be large enough such that \( \frac{C_1}{2(1 + 3^{-1} \sqrt{0.4C_1})} - C_0 \geq 1 \), we have

\[ \mathbb{P} \left( \bigcup_{m \in [M]} \left\{ \left| \widehat{N}^{(m)}/N - 1 \right| > \sqrt{\frac{C_1 \log(N)}{N}} \right\} \right) \leq 2N^{-1}. \]

Since \( x \mapsto \log(x)/x \) is a deceasing function on \([e, \infty)\), there exists some \( C_2 > 0 \), such that if \( N \geq C_2 \),

\[ \sqrt{C_1 \log(N)/N} \leq 0.5. \]

Further, since \( |z - 1| \leq 2|z - 1| \) for \( |z - 1| \leq 0.5 \), we have for \( N \geq C_2 \),

\[ \mathbb{P} \left( \bigcup_{m \in [M]} \left\{ \left| N/\widehat{N}^{(m)} - 1 \right| > 2\sqrt{\frac{C_1 \log(N)}{N}} \right\} \right) \leq 2N^{-1}. \]

Then the conclusion holds with \( C = \max\{C_2, 2\sqrt{C_1}\} \).

**Lemma B.5.** Let \( L \geq N \geq 3, M \geq 1 \) be positive integers. Let \( p_n := N/L \), and \( \{Z_{\ell}^{(m)} : \ell \in [L], m \in [M]\} \) be a collection of Bernoulli random variables with success probability \( p_n \). Then there exists an absolute constant \( C \),

\[ \mathbb{E} \left[ \max_{m \in [M]} \left| \sum_{\ell \in [L]} \left( Z_{\ell}^{(m)} - p_n \right) \right|^2 \right] \leq C \left( N \log(2M) + \log^2(2M) \right). \]

**Proof.** By Hoffman-Jørgensen inequality [64, Proposition A.1.6] and [16, Lemma 8],

\[ \mathbb{E} \left[ \max_{m \in [M]} \left| \sum_{\ell \in [L]} \left( Z_{\ell}^{(m)} - p_n \right) \right|^2 \right] \leq \left( \mathbb{E} \left[ \max_{m \in [M]} \left| \sum_{\ell \in [L]} \left( Z_{\ell}^{(m)} - p_n \right) \right| \right] \right)^2 + 1 \]

\[ \leq N \log(2M) + \log^2(2M). \]

**Lemma B.6.** Denote \( S_{n,j} := rn^{-1} \sum_{i=1}^n P^{r-1} h_j(X_i) \) for \( 1 \leq j \leq d \), and recall (45). Assume that (MT-1) and (MT-2) hold, and that

\[ n^{-1} D_n^2 \log(d) \leq 1/6. \]  

(46)

Then there exists a constant \( C \), depending only on \( q, r \), such that

\[ C^{-1} \mathbb{E} \left[ \max_{1 \leq j \leq d} \left| U_{n,j} \right| \right] \leq n^{-1/2} D_n \log^{1/2}(d) + n^{-1+1/q} D_n \log(d) + n^{-3/2+1/q} D_n^{3-2/q} \log^{3/2}(d). \]

\[ C^{-1} \mathbb{E} \left[ \sqrt{n} \max_{1 \leq j \leq d} \left| U_{n,j} - S_{n,j} \right| \right] \leq n^{-1/2} D_n \log(d) + n^{-1+1/q} D_n^{3-2/q} \log^{3/2}(d). \]
Proof. We only prove the second claim, as the proof for the first is almost identical. We apply Theorem A.7 and Hoeffding decomposition (41) to the finite collection \( \{ h_j : 1 \leq j \leq d \} \subset \mathcal{H} \) with envelopes \( \{ P^{r-\ell} H : 2 \leq \ell \leq r \} \):

\[
\mathbb{E} \left[ \max_{1 \leq j \leq d} \left| U_{n,j} - S_{n,j} \right| \right] \lesssim n^{-1} \left( \sup_{1 \leq j \leq d} \left\| P^{r-2} h_j \right\|_{P^2_2} \log(d) + n^{-1/2+1/q} \left\| P^{r-2} H \right\|_{P^2_2} \log^{3/2}(d) \right) + \sum_{\ell=3}^{r} n^{-\ell/2} \left\| P^{r-\ell} H \right\|_{P^2_2} \log^{\ell/2}(d).
\]

Then due to condition (MT-2), we have

\[
\mathbb{E} \left[ \max_{1 \leq j \leq d} \left| U_{n,j} - S_{n,j} \right| \right] \lesssim n^{-1} D_n \log(d) + n^{-3/2+1/q} D_n^{3/2} \log^{3/2}(d) + \sum_{\ell=3}^{r} \left( n^{-1/2} D_n \log^{1/2}(d) \right)^{\ell}.
\]

Due to (46), we have

\[
\mathbb{E} \left[ \sqrt{n} \max_{1 \leq j \leq d} \left| U_{n,j} - S_{n,j} \right| \right] \lesssim n^{-1/2} D_n \log(d) + n^{-1+1/q} D_n^{2} \log(d) + n^{-3/2+1/q} D_n^{4/2} \log^{3/2}(d),
\]

\[
\lesssim n^{-1/2} D_n \log(d) + n^{-1+1/q} D_n^{2} \log(d).
\]

 Lemma B.7. Assume that (46), (MT-2), and (MT-4) holds. Denote

\[
\varphi_n := n^{-1/2} D_n \log(d) + n^{-1+1/q} D_n^{2} \log(d) + n^{-3/2+1/q} D_n^{4/2} \log^{3/2}(d). \tag{47}
\]

Then there exists a constant \( C \), depending only on \( q, r, c_0 \), such that for \( s = 2, 3, 4 \),

\[
\mathbb{E} \left[ \max_{1 \leq j, k \leq d} \left| I_{n,r} \right|^{-1} \sum_{i \in I_{n,r}} \left( \bar{h}_j(X_i) \bar{h}_k(X_i) - P^r \bar{h}_j \bar{h}_k \right) \right] \leq C \varphi_n,
\]

\[
\mathbb{E} \left[ \max_{1 \leq j \leq d} \left| I_{n,r} \right|^{-1} \sum_{i \in I_{n,r}} \left( |\bar{h}_j(X_i)|^s \right) \right] \leq C B_n^{s-2} (1 + \varphi_n),
\]

where \( \bar{h}_j(\cdot) = h_j(\cdot)/\|h_j\|_{P^r,2} \) for \( 1 \leq j \leq d \).

Proof. We only prove the second claim, as the first can be established by the same argument. We apply the Theorem A.7 and Hoeffding decomposition (41) to the finite collection \( \{ |\bar{h}_j|^s : 1 \leq j \leq d \} \subset \mathcal{H} \) with envelopes \( \{ P^{r-\ell} \bar{H}^s : 2 \leq \ell \leq r \} \), where \( \bar{H}(\cdot) := H(\cdot)/\inf_{1 \leq j \leq d} \|h_j\|_{P^r,2} \):

\[
\mathbb{E} \left[ \max_{1 \leq j \leq d} \left| I_{n,r} \right|^{-1} \sum_{i \in I_{n,r}} |\tilde{h}_j(X_i)|^s \right] \lesssim \sup_{1 \leq j \leq d} P^r |\tilde{h}_j|^s +
\]

}\[
Due to (MT-2), (MT-4), and (46), we have
\[ \sum_{\ell=1}^{2} n^{-\ell/2} \left( \sup_{1 \leq j \leq d} \left\| P^{r-\ell} \tilde{h}_j \left( X_t \right) \right\|_{p+2} \log^{\ell/2}(d) + n^{-1/2+1/q} \left\| P^{r-\ell} \tilde{H} \right\|_{p+2} \log^{\ell/2+1/2}(d) \right) + \]
\[ \sum_{\ell=3}^{r} n^{-\ell/2} \left\| P^{r-\ell} \tilde{H} \right\|_{p+2} \log^{\ell/2}(d) \]

Due to (MT-2), (MT-4), and (46), we have
\[
\mathbb{E} \left[ \max_{1 \leq j \leq d} \left\| I_{n,r}^{-1} \sum_{i \in I_{n,r}} \tilde{h}_j (X_i) \left\|^s \right. \right] \lesssim B_n^{s-2} + \sum_{\ell=3}^{r} n^{-\ell/2} B_n^{s-2} D_n^{\ell+1} \log^{\ell/2}(d) + n^{-1/2} B_n^{s-2} D_n \log^{1/2}(d) + n^{-1+1/q} B_n^{s-2} D_n^{2} \log(d) + n^{-3/2+1/q} B_n^{s-2} D_n^{4-2/q} \log^{3/2}(d)
\]
\[ \lesssim B_n^{s-2} + B_n^{s-2} n^{-1/2} D_n \log^{1/2}(d) + B_n^{s-2} n^{-1+1/q} D_n^{2} \log(d) + B_n^{s-2} n^{-3/2+1/q} D_n^{4-2/q} \log^{3/2}(d), \]

which completes the proof.

\[ \Box \]

**B.2. Proof of Theorem B.1**

**Proof of Theorem B.1.** Without loss of generality, we may assume the following hold:
\[
\frac{D_n^2 \log(d)}{n} \leq 1/6, \quad \frac{D_n^2 \log^7(dn)}{n} \leq 1.
\]

(48)
since otherwise we can increase the constant $C$.

**Step 1.** Denote $S_{n,j} := r n^{-1} \sum_{i=1}^{n} P^{r-1} \tilde{h}_j (X_i)$. Due to condition (MT-0), (MT-1) and [17, Proposition 2.1], we have
\[
\sup_{R \in \mathcal{R}} \left\| \mathbb{P} \left( \sqrt{n} (S_n - \theta) \in R \right) - \mathbb{P} (rY_A \in R) \right\| \lesssim \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/6} + \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/3}.
\]

**Step 2.** Fix any rectangle $R = [a, b] \in \mathcal{R}$, where $a, b \in \mathbb{R}^d$ and $a \leq b$. For any $t > 0$,
\[
\mathbb{P} \left( \sqrt{n} \sup_{1 \leq j \leq d} \left| U_{n,j} - S_{n,j} \right| \geq t \right) \leq \mathbb{P} \left( \sqrt{n} \sup_{1 \leq j \leq d} \left| U_{n,j} - S_{n,j} \right| \geq t \cap \sqrt{n} (S_n - \theta) \leq b + t \right) + \mathbb{P} \left( \sqrt{n} (S_n - \theta) \leq -a + t \cap rY_A \leq b + t \right)
\]
\[ \leq (t^{-1} n^{-1/2} D_n \log(d) + n^{-1+1/q} D_n^{3-2/q} \log^{3/2}(d)) + \mathbb{P} (rY_A \leq -a + t \cap rY_A \leq b + t)
\]
\[ + \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/6} + \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/3}, \]
\[
\leq (2) t^{-1} \left( n^{-1/2} D_n \log(d) + n^{-1+1/q} D_n^{3-2/q} \log^{3/2}(d) \right) + C t^2 \log(d) + \mathbb{P}(r_{Y_A} \in R) \\
+ C \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/6} + C \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/3},
\]

where we used Lemma B.6, the Markov inequality and results from Step 1 in (1), and the anti-concentration inequality [17, Lemma A.1] in (2).

Now let \( t = n^{-1/4} D_n^{1/2} \log^{1/4}(d) + n^{-1+1/(2q)} D_n^{3/2-1/q} \log^{1/2}(d) \), and we have

\[
\mathbb{P} \left( \sqrt{n}(U_n - \theta) \in R \right) - \mathbb{P}(r_{Y_A} \in R) \\
\leq \left( \frac{D_n^2 \log^3(d)}{n} \right)^{1/4} + \left( \frac{D_n^{3-2/q} \log^2(d)}{n^{1-1/q}} \right)^{1/2} + \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/6} + \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/3}
\]

\[
\leq \left( \frac{D_n^{3-2/q} \log^2(d)}{n^{1-1/q}} \right)^{1/2} + \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/6} + \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/3} := \epsilon_n,
\]

where we used (48) in the last inequality. By a similar argument, we can show that

\[
\mathbb{P}(r_{Y_A} \in R) - \mathbb{P} \left( \sqrt{n}(U_n - \theta) \in R \right) \leq \epsilon_n,
\]

which completes the proof.

### B.3. Bounding the effect due to sampling

Let \( m \in [M]^d \) such that \( m_j = \sigma(h_j) \) for \( 1 \leq j \leq d \). For \( 1 \leq j \leq d \), let \( \tilde{h}_j(\cdot) = h_j(\cdot)/\|h_j\|_{p^r \cdot 2} \), and define

\[
\zeta_{n,j} := \frac{1}{\sqrt{|I_{n,r}|}} \sum_{i \in I_{n,r}} T_{i,j}, \quad \text{where } T_{i,j} := \frac{Z_{(m_j)}^i - p_n}{\sqrt{p_n(1 - p_n)}} \tilde{h}_j(X_i).
\]

**Lemma B.8.** Assume (MT-2), (MT-3), and (MT-4) hold. Define

\[
\eta_n := \left( \frac{B_n^2 \log^7(dn)}{N} \right)^{1/8}, \quad \omega_n := \left( \frac{n^{4r/q} \log^5(dn) B_n^{2-8/q} D_n^{8/q}}{N} \right)^{1/4},
\]

and recall the definition of \( \varphi_n \) in Lemma B.7. There exists a constant \( C \), depending only on \( r, q, c_0 \), such that with probability at least \( 1 - C \varphi_n^{1/4} \log^{1/2}(d) \),

\[
\mathbb{P}^R_{X_n^{\varphi_n}}(\zeta_n, \Lambda_B^{-1/2} Y_B) := \sup_{R \in R} \left| \mathbb{P}^R_{X_n^{\varphi_n}}(\zeta_n \in R) - \mathbb{P} \left( \Lambda_B^{-1/2} Y \in R \right) \right| \\
\leq C \eta_n + C \omega_n + C \varphi_n^{1/4} \log^{1/2}(d),
\]

where \( Y_B \sim N(0, \Gamma_B) \) and \( \Lambda_B \) is a \( d \times d \) diagonal matrix such that \( \Lambda_{B,jj} := P^r h_j^2 \).
**Proof.** The constants in this proof may depend on \( r, q, c_0 \). Consider conditionally independent (conditioned on \( X^* \)) \( \mathbb{R}^d \)-valued random vectors \( \{ \tilde{X}_i : \iota \in I_{n,r} \} \) such that

\[
\tilde{Y}_i | X^* \sim N(0, \tilde{\Sigma}_i), \quad \text{where } \tilde{\Sigma}_{i,j} = \tilde{h}_i(X_i)\tilde{h}_j(X_j)1 \{ m_i = m_j \}.
\]

Let \( \tilde{Y} := |I_{n,r}|^{-1/2} \sum_{\iota \in I_{n,r}} \tilde{Y}_i \). Further, define

\[
\rho_{|X^*}^R (\zeta_n, \tilde{Y}) := \sup_{R \in \mathbb{R}} \left| \mathbb{P}_{|X^*} (\zeta_n \in R) - \mathbb{P}_{|X^*} (\tilde{Y} \in R) \right|, \quad \rho_{|X^*}^R (\tilde{Y}, \Lambda_B^{-1/2} Y_B) := \sup_{R \in \mathbb{R}} \left| \mathbb{P}_{|X^*} (\tilde{Y} \in R) - \mathbb{P} (\Lambda_B^{-1/2} Y_B \in R) \right|.
\]

By triangle inequality, it then suffices to show that each of the following events happens with probability at least \( 1 - C\varphi_n^{1/4} \log^{1/2}(d) - C\eta_n \),

\[
\rho_{|X^*}^R (\zeta_n, \tilde{Y}) \leq C\eta_n + C\omega_n, \quad \rho_{|X^*}^R (\tilde{Y}, \Lambda_B^{-1/2} Y_B) \leq C\varphi_n^{1/4} \log^{1/2}(d), \quad (50)
\]

on which we now focus. Without loss of generality, we assume

\[
\varphi_n^{1/4} \log^{1/2}(d) \leq 1/6, \quad \eta_n \leq c_1, \quad \omega_n \leq c_1,
\]

for some sufficiently small constant \( c_1 \in (0, 1/2) \) that is to be determined, since otherwise we could always increase \( C \).

**Step 0.** Due to (51), Lemma B.7 and Markov inequality, we have

\[
\mathbb{P} \left( \left\| \text{Cov}_{|X^*} (\tilde{Y}) - \text{Cov} (\Lambda_B^{-1/2} Y_B) \right\|_\infty \geq 1/2 \right) \lesssim \varphi_n \leq \varphi_n^{1/4} \log^{1/2}(d).
\]

(52)

where for \( 1 \leq i, j \leq d \),

\[
\text{Cov}_{|X^*} (\tilde{Y})_{ij} := |I_{n,r}|^{-1} \sum_{\iota \in I_{n,r}} \tilde{h}_i(X_i)\tilde{h}_j(X_j)1 \{ m_i = m_j \}.
\]

By definition, for any \( \iota \in I_{n,r} \) and \( 1 \leq j \leq d \), \( \mathbb{E}_{|X^*} \tilde{Y}_{i,j}^2 = \tilde{h}_j^2(X_j) \), which implies that \( \| \tilde{Y}_{i,j} \|_{\psi_2,|X^*} \lesssim |\tilde{h}_j (X_j) | \). Thus by maximal inequality [64, Lemma 2.2.2], there exists an absolute constant \( C_0 \geq 1 \) such that

\[
\| \max_{1 \leq j \leq d} \tilde{Y}_{i,j} \|_{\psi_1,|X^*} \leq \| \max_{1 \leq j \leq d} \tilde{Y}_{i,j} \|_{\psi_2,|X^*} \leq C_0 \max_{1 \leq j \leq d} |\tilde{h}_j (X_j) | \log^{1/2}(d).
\]

(53)

**Step 1.** The goal is to show that the first event in (50), \( \rho_{|X^*}^R (\zeta_n, \tilde{Y}) \leq C\eta_n + C\omega_n \), holds with probability at least \( 1 - C\varphi_n^{1/4} \log^{1/2}(d) - C\eta_n \).

**Step 1.1.** Define

\[
\tilde{L}_n := \max_{1 \leq j \leq d} |I_{n,r}|^{-1} \sum_{\iota \in I_{n,r}} \mathbb{E}_{|X^*} \left[ |\mathcal{T}_{i,j}|^3 \right].
\]

(54)
Further, $\widehat{M}_n(\phi) := \widehat{M}_{n,X}(\phi) + \widehat{M}_{n,Y}(\phi)$, where

$\widehat{M}_{n,X}(\phi) := |I_{n,r}|^{-1} \sum_{t \in I_{n,r}} \mathbb{E}_{|X|^{t}} \left[ \max_{1 \leq j \leq d} |T_{i,j}| : \max_{1 \leq j \leq d} |T_{i,j}| > \frac{|I_{n,r}|}{4\phi \log d} \right]$, 

$\widehat{M}_{n,Y}(\phi) := |I_{n,r}|^{-1} \sum_{t \in I_{n,r}} \mathbb{E}_{|X|^{t}} \left[ \max_{1 \leq j \leq d} |\hat{Y}_{i,j}| : \max_{1 \leq j \leq d} |\hat{Y}_{i,j}| > \frac{|I_{n,r}|}{4\phi \log d} \right]$. 

(55)

By Theorem 2.1 in [17], there exist absolute constants $K_1$ and $K_2$ such that for any real numbers $\mathcal{L}_n$ and $\mathcal{M}_n$, we have

$\rho_{X_1}^\mathcal{L}_n(\zeta_n, \bar{Y}) \leq K_1 \left( \left( \frac{T_n^2 \log^7(d)}{|I_{n,r}|} \right)^{1/6} + \frac{\mathcal{M}_n}{\mathcal{L}_n} \right)$ with $\phi_n := K_2 \left( \frac{T_n^2 \log^4(d)}{|I_{n,r}|} \right)^{-1/6}$

on the event

$\mathcal{E}_n := \{ \hat{L}_n \leq \mathcal{L}_n \} \cap \{ \mathcal{M}_n(\phi_n) \leq \mathcal{M}_n \} \cap \left\{ \min_{1 \leq j \leq d} \text{Cov}_{|X|^{t}}(\bar{Y})_{jj} \geq 2^{-1} \right\} \cap \{ \phi_n \geq 1 \}$. 

(56)

In Step 0, we have shown $\mathbb{P} \left( \min_{1 \leq j \leq d} \text{Cov}_{|X|^{t}}(\bar{Y})_{jj} \geq 2^{-1} \right) \geq 1 - C\eta_n^1/2 \log^1/2(d)$, since $\text{Cov}(\Lambda_B^{-1/2} \bar{Y}_B)_{jj} = 1$ for $1 \leq j \leq d$. In Step 1.2-1.4, we select proper $\mathcal{L}_n$ and $\mathcal{M}_n$ such that the first two events happen with probability at least $1 - C\eta_n$, and $\phi_n \geq 1$ with small enough $c_1$. In Step 1.5, we plug in these values.

**Step 1.2: Select $\mathcal{L}_n$.** Since $\eta_n \leq 1/2$, $\mathbb{E}|Z^{(\ell)}_i - p_n|^3 \leq C p_n$ for $\ell \in [M]$, and thus

$\hat{L}_n \leq C p_n^{-1/2} T_1$, where $T_1 := \max_{1 \leq j \leq d} \frac{1}{|I_{n,r}|} \sum_{t \in I_{n,r}} |\hat{h}_j(X_i)|^3$.

Due to (51), Lemma B.7 and Markov inequality, we have

$\mathbb{P} \left( T_1 \leq CB_n(\eta_n)^{-1} \right) \geq 1 - \eta_n$.

Thus there exists a constant $C_1$, depending on $q, r, c_0$, such that the following two conditions hold: (i).

$4^{-1} C_0^{-1} K_2^{-1} C_1^{1/3} \geq 3r,

(57)$

where $C_0$ appears in (53), and (ii). if we let

$\mathcal{L}_n := C_1 p_n^{-1/2} B_n(\eta_n)^{-1} \left( 1 + \frac{n^{3r/q} \log^{11/2}(dn) B_n^{2-6/q} D_n^{6/q} \eta_n^{-1-3/q}}{N} \right)$

(58)

then $\mathbb{P} \left( L_n \leq \mathcal{L}_n \right) \geq 1 - \eta_n$. 

With this selection of $L_n$, and due to the definition of $\eta_n$ and (51), we have
\[ \phi_n^{-1} \leq 2K_2^{-1} C_1^{1/3} \left( \frac{B_n^2 \eta_n^{-2} \log^3(dn)}{N} \right)^{1/8} + \left( \frac{n^{2r/q} \log^{5-3/(4q)}(dn) B_n^{2-9/(2q)} D_n^{4/q}}{N^{1-2/(4q)}} \right)^{1/2} \]
\[ \leq 2K_2^{-1} C_1^{1/3} \left( \frac{B_n^3 \log^3(dn)}{N} \right)^{1/8} + \left( \frac{n^{2r/q} \log^{3/2}(dn) B_n^{1-4/q} D_n^{4/q}}{N^{1/2}} \right)^{1/2} \].

Thus, if we select $c_1$ in (51) to be small enough, i.e.,
\[ 4c_1 K_2^{-1} C_1^{1/3} \leq 1, \]
we have $\phi_n^{-1} \leq 1$.

**Step 1.2: bounding $\overline{M}_{n,X}(\phi_n)$.** Since $p_n \leq 1/2$, by its definition in (55), we have $\overline{M}_{n,X}(\phi_n) = 0$ on the event
\[ \left\{ Y_n := \max_{i \in I_{n,x}} \max_{1 \leq j \leq d} \left| \hat{h}_j(X_i) \right| \leq \frac{\sqrt{N}}{4\phi_n \log(d)} \right\}. \]

Observe that by the definition of $\overline{L}_n$ in (58),
\[ \phi_n^{-1} \geq K_2^{-1} C_1^{1/3} \left( p_n^{-1} n^{6r/q} \log^3(dn) B_n^{2-9/(2q)} D_n^{4/q} \right)^{1/2} \]
\[ \geq K_2^{-1} C_1^{1/3} \left( \frac{n^{2r/q} \log^{3/2}(dn) B_n^{1-4/q} D_n^{4/q}}{N} \right)^{1/2}, \]
which implies that
\[ \frac{\sqrt{N}}{4\phi_n \log(d)} \geq 4^{-1} K_2^{-1} C_1^{1/3} n^{r/q} B_n^{1-2/q} D_n^{2/q} \eta_n^{-1/q} \log^{3/2}(dn) \geq n^{r/q} B_n^{1-2/q} D_n^{2/q} \eta_n^{-1/q}, \tag{59} \]
where in the last inequality, we used (57). Due to (MT-3) and (MT-4), and Markov inequality (the case for $q = \infty$ is obvious),
\[ \mathbb{P} \left( Y_n \geq n^{r/q} B_n^{1-2/q} D_n^{2/q} \eta_n^{-1/q} \right) \leq \eta_n. \tag{60} \]
Thus $\mathbb{P} \left( \overline{M}_{n,X}(\phi_n) = 0 \right) \geq 1 - \eta_n$. 
Step 1.4: bounding $\tilde{M}_{n,Y}(\phi_n)$ and selecting $\overline{M}_n$. Due to the calculation in Step 0,\[ \mathbb{P}_{X_1^n} \left( \max_{1 \leq i \leq d} \tilde{Y}_{i,j} \geq t \right) \leq 2 \exp \left( \frac{t}{C_0 \max_{1 \leq i \leq d} |h_j(X_i)| \log^{1/2}(d)} \right), \]where $C_0$ is the absolute constant in (53). In Step 1.3 and 1.2, we have shown that\[ \mathbb{P}(E_n^\prime) \geq 1 - \eta_n, \quad \text{where } E_n^\prime := \left\{ \mathcal{V}_n \leq n^{r/q} B_n^{1-2/q} D_n^{2/q} \eta_n^{-1/4} \leq \frac{\sqrt{N}}{4 \phi_n \log(d)} \right\}, \]\[ \phi_n^{-1} \leq 1, \quad \phi_n^{-1} \geq K_2^{-1} C_1^{1/3} \left( \frac{n^{r/q} \log^3(d) \log^2(d) B_n^{2-4/q} D_n^{4/q} \eta_n^{-2/q}}{N} \right)^{1/2}. \]Thus on the event $E_n^\prime$, we have\[ \mathcal{V}_n \phi_n \leq K_2 C_1^{-1/3} \log^{-3/2}(dn) \log^{-1}(d) N^{1/2}. \]By [17, Lemma C.1], on the event $E_n^\prime$, for each $t \in I_{n,r}$,\[ \mathbb{E}_{X_1^n} \left[ \max_{1 \leq j \leq d} |\tilde{Y}_{i,j}|^3; \max_{1 \leq j \leq d} |\tilde{Y}_{i,j}| > \frac{|I_{n,r}|}{4 \phi_n \log d} \right] \leq 12 C_0^3 \left( \frac{|I_{n,r}|}{4 \phi_n \log d} \right) \mathcal{V}_n \log^{1/2}(d) \exp \left( - \frac{|I_{n,r}|}{4 C_0 \mathcal{V}_n \phi_n \log^{3/2}(d)} \right) \leq 12 C_0^3 n^{3r/2} \exp \left( - \frac{|I_{n,r}|^{1/2}}{4 C_0 K_2 C_1^{-1/3} \log^{-1}(dn) N^{1/2}} \right) \leq 12 C_0^3 n^{3r/2} \exp \left( -4^{-1} C_0^{-1} K_2^{-1} C_1^{1/3} \log(dn) \right). \]Due to (57), we have that on the event $E_n^\prime$, for each $t \in I_{n,r}$,\[ \mathbb{E}_{X_1^n} \left[ \max_{1 \leq j \leq d} |\tilde{Y}_{i,j}|^3; \max_{1 \leq j \leq d} |\tilde{Y}_{i,j}| > \frac{|I_{n,r}|}{4 \phi_n \log d} \right] \leq 12 C_0^3 n^{-3r/2}. \]Thus if we select\[ \overline{M}_n := 12 C_0^3 n^{-3r/2}, \]then $\mathbb{P}(\tilde{M}_{n,Y}(\phi_n) \leq \overline{M}_n) \geq 1 - C \eta_n$.

Step 1.5: plug in $\overline{L}_n$ and $\overline{M}_n$. Recall the definition $\overline{L}_n$ and $\overline{M}_n$ in (58) and (61). With these selections, we have shown that $\mathbb{P}(E_n) \geq 1 - C \phi_n^{1/4} \log^{1/2}(d) - C \eta_n$, where $E_n$ is defined in (56). Further, on the event $E_n$, due to (51), we have\[ \rho_{X_1^n}(\zeta_n, \tilde{Y}) \lesssim \left( \frac{T_n^2 \log^7(dn)}{|I_{n,r}|} \right)^{1/6} \frac{\overline{M}_n}{\overline{L}_n}. \]
The goal is to show that the second event in (50),
holds with probability at least 

\[ n^{-3r/2} p_n^{1/2} B_n^{-1} \eta_n, \]

which completes the proof of Step 1.

**Step 2.** The goal is to show that the second event in (50), \( \rho|_{X_1}^R (\tilde{Y}, \Lambda^{-1/2}_B Y_B) \leq C \varphi_n^{1/4} \log^{1/2}(d), \)
holds with probability at least \( 1 - C \varphi_n^{1/4} \log^{1/2}(d). \)

By the Gaussian comparison inequality [13, Lemma C.5],

\[ \rho|_{X_1}^R (\tilde{Y}, \Lambda^{-1/2}_B Y_B) \lesssim \Delta^{1/3} \log^{2/3}(d), \]
on the event that \( \{ \| \text{Cov}_{X_1}(\tilde{Y}) - \text{Cov}(\Lambda^{-1/2}_B Y_B) \|_\infty \leq \Delta \} \). By Lemma B.7, due to (51), and by Markov inequality,

\[ \mathbb{P} ( \| \text{Cov}_{X_1}(\tilde{Y}) - \text{Cov}(\Lambda^{-1/2}_B Y_B) \|_\infty \leq C \varphi_n^{3/4} \log^{-1/2}(d) ) \geq 1 - C \varphi_n^{1/4} \log^{1/2}(d). \]

Thus if we set \( \Delta := C \varphi_n^{-3/4} \log^{-1/2}(d) \), then with probability at least \( 1 - C \varphi_n^{1/4} \log^{1/2}(d) \),

\[ \rho|_{X_1}^R (\tilde{Y}, \Lambda^{-1/2}_B Y_B) \leq C \varphi_n^{-1/4} \log^{1/2}(d). \]

\[ \boxed{} \]

**B.4. Proof of Theorem B.2**

For \( 1 \leq j \leq d \), let \( \bar{h}_j(\cdot) := h_j(\cdot)/\| h_j \|_{pr,2} \), and let \( m \in [M]^d \) such that \( m_j = \sigma(h_j) \). Recall the definition of \( \zeta_n \) in (49). Let \( Y_A \) and \( Y_B \) be two independent \( d \)-dimensional Gaussian vectors such that

\[ Y_A \sim N(0, \Gamma_A), \quad Y_B \sim N(0, \Gamma_B). \]

Define

\[ Y := rY_A + \sqrt{\alpha_n} Y_B, \quad \tilde{Y} := \Lambda^{-1/2}_s (rY_A + \sqrt{\alpha_n} Y_B), \]

where \( \Lambda_s \) is a \( d \times d \) diagonal matrix such that \( \Lambda_{s,j,j} = \mathbb{E}[Y_j^2] \).

**Proof.** Without loss of generality, we assume (45), and

\[ \varpi_n^{(1)} := \left( \frac{D_n^2 \log^7(dn)}{n} \right)^{1/8} + \left( \frac{D_n^2 \log^3(dn)}{n^{1-2/q}} \right)^{1/4} + \left( \frac{D_n^3 \log^2(dn)}{n^{1-1/q}} \right)^{1/2} \leq 1/2, \]

\[ \varpi_n^{(2)} := \left( \frac{B_n^2 \log^7(dn)}{N} \right)^{1/8} + \left( \frac{n^{4r/q} \log^5(dn)B_n^{2-8/q}D_n^{8/q}}{N} \right)^{1/4} \leq 1/2. \]
We recall the definitions of $\varphi_n$, $\eta_n$, and $\omega_n$ in Lemma B.8. Due to (62),
\[
\varphi_n^{1/4} \log^{1/2}(d) \lesssim \omega_n^{(1)}, \quad \eta_n + \omega_n = \omega_n^{(2)}. \tag{63}
\]
Observe that for $1 \leq j \leq d$,
\[
U'_{n,N,j} = \frac{N}{N(m_j)} \left( \frac{1}{N} \sum_{i \in I_{n,r}} (Z_{i(m_j)} - p_n) \Lambda_B^{1/2} \bar{h}_j(X_i) + \frac{1}{|I_{n,r}|} \sum_{i \in I_{n,r}} h_j(X_i) \right)
= \frac{N}{N(m_j)} \left( \sqrt{\frac{1 - p_n}{n}} \left( \Lambda_B^{1/2} \zeta_n \right)_j + U_{n,j} \right)
= \frac{N}{N(m_j)} \Phi_{n,j}. 
\]
where $\Lambda_B$ is a $d \times d$ diagonal matrix such that $\Lambda_{B,jj} = P^r h_j^2$.

**Step 1:** the goal is to show that
\[
\rho \left( \sqrt{n} \Phi_n, rY_A + \alpha_n^{1/2} Y_B \right) \lesssim \omega_n^{(1)} + \omega_n^{(2)}. 
\]
For any rectangle $R \in \mathcal{R}$, observe that
\[
\mathbb{P}(\sqrt{n} \left( U_n + \sqrt{1 - p_n} N^{-1/2} \Lambda_B^{1/2} \zeta_n \right) \in R)
\leq \mathbb{E} \left[ \mathbb{P}_{X_1^n} \left( \zeta_n \in \left( \frac{1}{\sqrt{\alpha_n(1 - p_n)}} \Lambda_B^{-1/2} R - \sqrt{\frac{N}{1 - p_n} \Lambda_B^{-1/2} U_n} \right) \right) \right] + C \omega_n^{(1)} + C \omega_n^{(2)}
\leq \mathbb{E} \left( \mathbb{P}_{Y_B} \left( \sqrt{n} U_n \in \left[ R - \sqrt{\alpha_n(1 - p_n)} Y_B \right] \right) \right) + C \omega_n^{(1)} + C \omega_n^{(2)},
\]
where we recall that $Y_B$ is independent of all other random variables. Further, by Theorem B.1.
\[
\mathbb{P}(\sqrt{n} \left( U_n + \sqrt{1 - p_n} N^{-1/2} \Lambda_B^{1/2} \zeta_n \right) \in R)
\leq \mathbb{E} \left[ \mathbb{P}_{Y_B} \left( \sqrt{n} U_n \in \left[ R - \sqrt{\alpha_n(1 - p_n)} Y_B \right] \right) \right] + C \omega_n^{(1)} + C \omega_n^{(2)},
\leq \mathbb{E} \left[ \mathbb{P}_{Y_B} \left( rY_A \in \left[ R - \sqrt{\alpha_n(1 - p_n)} Y_B \right] \right) \right] + C \omega_n^{(1)} + C \omega_n^{(2)},
= \mathbb{P} \left( \Lambda_r^{1/2} (rY_A + \sqrt{\alpha_n(1 - p_n)} Y_B) \in \Lambda_r^{-1/2} R \right) + C \omega_n^{(1)} + C \omega_n^{(2)}, 
\]
By definition, $\mathbb{E}[Y_j^2] = 1$ for each $1 \leq j \leq d$. Then by the Gaussian comparison inequality [13, Lemma C.5], and due to (MT-4) and $\alpha_np_n = n/|I_{n,r}| \leq n^{-(r-1)},$

$$
\sup_{R' \in R} \left| \mathbb{P}\left( A_n^{-1/2}(rY_A + \sqrt{\alpha_n(1 - p_n)}Y_B) \in R' \right) - \mathbb{P}\left( \tilde{Y} \in R' \right) \right| 
\lesssim \left( \frac{\alpha_np_n}{r^2\sigma^2} \right)^{1/3} \left( \frac{D_n\log^2(\sigma_n)}{n} \right)^{(r-1)/3} \lesssim \omega_n(1).
$$

As a result,

$$
\mathbb{P}(\sqrt{n}\Phi_n \in R) \leq \mathbb{P}(rY_A + \sqrt{\alpha_n}Y_B \in R) + C\omega_n(1) + C\omega_n(2).
$$

Similarly, we can show $\mathbb{P}(\sqrt{n}\Phi_n \in R) \geq \mathbb{P}(rY_A + \sqrt{\alpha_n}Y_B \in R) - C\omega_n(1) - C\omega_n(2).$ Thus the proof of Step 1 is complete.

**Step 2:** we show that with probability at least $1 - C\omega_n(1) - C\omega_n(2)$,

$$
\max_{1 \leq j \leq d} \left| \frac{N}{N(m_j)} - 1 \right| \sqrt{N}\Phi_{n,j} \leq C\nu_n, \quad \text{where } \nu_n := \left( \frac{D_n^2\log^3(dn)}{n} \right)^{1/2} + \left( \frac{B_n^2\log^3(dn)}{N} \right)^{1/2}.
$$

Due to (MT-1) and (MT-4), $\mathbb{E}[Y_j^2] = r^2\gamma_A(h_j) + \alpha_n\gamma_B(h_j) \lesssim D_n^2 + \alpha_nB_n^2.$ Since $Y$ is a multivariate Gaussian, $\max_{1 \leq j \leq d} \|Y_j\|_{\psi_2} \leq \sqrt{D_n^2 + \alpha_nB_n^2}.$ Then by the maximal inequality [64, Lemma 2.2.2],

$$
\|\max_{1 \leq j \leq d} Y_j\|_{\psi_2} \leq C\sqrt{D_n^2 + \alpha_nB_n^2} \log(d), \quad \text{which further implies that}
$$

$$
\mathbb{P}\left( \max_{1 \leq j \leq d} |Y_j| \geq C\sqrt{D_n^2 + \alpha_nB_n^2} \log(d) \log(n) \right) \leq 2^{-1}.
$$

Since $n^{-1} \lesssim \omega_n(1)$, and from the result in Step 1, we have

$$
\mathbb{P}\left( \|\sqrt{n}\Phi_n\|_{\infty} \geq C\sqrt{D_n^2 + \alpha_nB_n^2} \log(d) \log(n) \right) \leq C\omega_n(1) + C\omega_n(2).
$$

Finally, due to Lemma B.4 and (MB), we have with probability at least $1 - C\omega_n(1) - C\omega_n(2)$,

$$
\max_{1 \leq j \leq d} \left( \frac{N}{N(m_j)} - 1 \right) \sqrt{N}\Phi_{n,j} \leq C\sqrt{D_n^2 + \alpha_nB_n^2} \log(d) \log^2(n)N^{-1}\alpha_n^{1/2} + C\left( \frac{D_n^2\log^3(dn)}{n} \right)^{1/2} + C\left( \frac{B_n^2\log^3(dn)}{N} \right)^{1/2}.
$$

**Step 3:** final step. Recall that $\sqrt{N}U'_{n,j} = \sqrt{N}\Phi_{n,j} + (N/\tilde{N}(m_j) - 1)\sqrt{N}\Phi_{n,j}$ for $1 \leq j \leq d$, and $\nu_n$ is defined in Step 2. For any rectangle $R = [a, b]$ with $a \leq b$, by Step 2,

$$
\mathbb{P}\left( \sqrt{N}U'_{n,N} \in R \right)
$$
Lemma B.9. Assume that (46), (MT-1)- (MT-4), and (MB) holds. Define
\[
\hat{\Delta}_B := \max_{1 \leq j, k \leq d} \left| \tilde{\gamma}_B(h_j, h_k) - \gamma_B(h_j, h_k) \right|,
\]
\[
\chi_{n,B} := \log^{1/4}(2M) \left( \left( \frac{M^{2/q}B_n^{2-4/q}D_n^{4/q} \log^3(d)}{N^{1-2/q}} \right)^{1/4} + \left( \frac{B_n^2 \log^5(dn)}{N} \right)^{1/8} \right.
\]
\[
+ \left( \frac{D_n^2 \log^5(dn)}{n} \right)^{1/8} + \left( \frac{D_n^2 \log^3(d)}{n^{1-1/q}} \right)^{1/4} + \left( \frac{D_n^8 \log^7(d)}{n^{3-2/q}} \right)^{1/8} \right) \left( D_n^{2-2/q} \log^{-2}(d) \chi_{n,B}^3 \right).
\]
Then there exists a constant C, that only depends on q, r, c_0, C_0, such that
\[
\mathbb{P} \left( \hat{\Delta}_B \leq CB_n^2 D_n^{-2} \log^{3/2}(d) \chi_{n,B}^3 \right) \geq 1 - C \chi_{n,B}.
\]

B.5. Proof of Theorem B.3

We will deal with the bootstrap for \( \Gamma_A \) and \( \Gamma_B \) separately.

B.5.1. Bootstrap for \( \Gamma_B \)

Recall the definition of \( \hat{\gamma}_B \) in (32).
**Proof.** Without loss of generality, we assume \( \chi_{n,B} \leq 1/2 \), since we can always let \( C \geq 2 \). For \( 1 \leq j,k \leq d \), and \( \sigma(h_j) = \sigma(h_k) = m \in \{M\}, \)

\[
|\gamma_B(h_j, h_k) - \gamma_B(h_j, h_k)| = \left| \frac{1}{N(m)} \sum_{\ell \in I_{n,r}} Z_{\ell}^{(m)} (h_j(X_\ell) - U_{n,N}(h_j)) \left( h_k(X_\ell) - U_{n,N}(h_k) \right) - P^r(h_j h_k) \right|
\]

\[
\leq \left( \max_{\ell \in \{M\}} N/\tilde{N}(\ell) \right) \left( \Delta_{B,1} + \Delta_{B,2} \right) + \Delta_{B,3} + \left( \max_{\ell \in \{M\}} N/\tilde{N}(\ell) \right)^2 \Delta_{B,4},
\]

\[
\leq \left( \max_{\ell \in \{M\}} N/\tilde{N}(\ell) \right) \left( \Delta_{B,1} + \Delta_{B,2} \right) + \Delta_{B,3} + 2 \left( \max_{\ell \in \{M\}} N/\tilde{N}(\ell) \right)^2 \left( \Delta_{B,5}^2 + \Delta_{B,6}^2 \right).
\]

where we define

\[
\Delta_{B,1} := \max_{1 \leq j,k \leq d} \max_{\ell \in \{M\}} N^{-1} \sum_{\ell \in I_{n,r}} (Z_{\ell}^{(\ell)} - p_n) h_j(X_\ell) h_k(X_\ell),
\]

\[
\Delta_{B,2} := \max_{1 \leq j,k \leq d} |I_{n,r}|^{-1} \sum_{\ell \in I_{n,r}} h_j(X_\ell) h_k(X_\ell) - P^r(h_j h_k),
\]

\[
\Delta_{B,3} := \left( \max_{\ell \in \{M\}} N/\tilde{N}(\ell) - 1 \right) \max_{1 \leq j \leq d} \left| P^r h_j^2 \right|, \quad \Delta_{B,4} := \max_{1 \leq j \leq d} \max_{\ell \in \{M\}} N^{-1} \sum_{\ell \in I_{n,r}} Z_{\ell}^{(\ell)} h_j(X_\ell),
\]

\[
\Delta_{B,5} := \max_{1 \leq j \leq d} \max_{\ell \in \{M\}} N^{-1} \sum_{\ell \in I_{n,r}} (Z_{\ell}^{(\ell)} - p_n) h_j(X_\ell),
\]

\[
\Delta_{B,6} := \max_{1 \leq j \leq d} |I_{n,r}|^{-1} \sum_{\ell \in I_{n,r}} h_j(X_\ell).
\]

(64)

Then by Markov inequality, (MT-4), and due to Lemma B.10 (ahead), Lemma B.7, and Lemma B.4, for \( i = 1, 2, 3 \),

\[
P\left( \Delta_{B,i} \geq C B_n^2 D_n^{-2} \log^{-2}(d) \chi_{B,n}^3 \right) \leq C \chi_{B,n}.
\]

Further, by Lemma B.10 (ahead), and Lemma B.6, since \( B_n \geq D_n \), for \( i = 5, 6 \),

\[
P\left( \Delta_{B,i}^2 \geq C B_n^2 D_n^{-2} \log^{-2}(d) \chi_{B,n}^3 \right) \leq C \chi_{B,n}^{5/2} \leq C \chi_{B,n}.
\]

Then the proof is complete due to (MB) and Lemma B.4.
Lemma B.10. Recall the definition of \( \hat{\Delta}_{B,1} \) and \( \hat{\Delta}_{B,5} \) in (64). Assume that (46), (MT-2), (MT-3), and (MT-4) hold. Then there exists a constant \( C \), depending only on \( q, r, c_0 \), such that

\[
C^{-1} \log^{-1}(2M) \mathbb{E} \left[ \hat{\Delta}_{B,1} \right] \leq B_n^2 D_n^{-2} \left( N^{-1/2+q} M^{2/q} B_n^{2-1/q} D_n^{1/q} \log(d) + N^{-1/2} B_n \log^{1/2}(d) + N^{-1/2} B_n \varphi_n^{1/2} \log^{1/2}(d) \right),
\]

and

\[
C^{-1} \log^{-1}(2M) \mathbb{E} \left[ \hat{\Delta}_{B,5} \right] \leq B_n D_n^{-1} \left( N^{-1+1/q} M^{1/q} B_n^{1-2/q} D_n^{2/q} \log(d) + N^{-1/2} \log^{1/2}(d) + N^{-1/2} \varphi_n^{1/2} \log^{1/2}(d) \right),
\]

where \( \varphi_n \) is defined in (47).

**Proof.** We first focus on \( \hat{\Delta}_{B,1} \), and apply Theorem 7.1 to the finite collection \( \{h_j h_k : 1 \leq j, k \leq d\} \) with envelope \( H^2 \). Since this is a finite collection of functions with cardinality \( d^2 \), we have

\[
\bar{J}(\tau) \leq C \tau \log^{1/2}(d), \text{ for } \tau > 0.
\]

Thus by Theorem 7.1, and Lemma B.7 with \( s = 4 \),

\[
\mathbb{E} \left[ \sqrt{N} \hat{\Delta}_{B,1} \right] \lesssim \sup_{1 \leq j \leq d} ||h_j||_{P^r,2} \log^{1/2}(d) \log^{1/2}(2M) + N^{-1/2+2/q} M^{2/q} ||H^2||_{P^r,q/2} \log(d) \log(2M)
+ B_n^3 D_n^{-2} (1 + \varphi_n^{1/2}) \log^{1/2}(d) \log^{1/2}(2M).
\]

Then due to (MT-2) and (MT-3),

\[
\mathbb{E} \left[ \sqrt{N} \hat{\Delta}_{B,1} \right] \lesssim \log(2M) \left( B_n^3 D_n^{-2} \log^{1/2}(d) + N^{-1/2+2/q} M^{2/q} B_n^{1-4/q} D_n^{1/q-2} \log(d) + B_n^3 D_n^{-2} (1 + \varphi_n^{1/2}) \log^{1/2}(d) \right),
\]

which completes the proof of the first result.

Now for \( \Delta_{B,5} \), we apply Theorem 7.1 to the finite collection \( \{h_j : 1 \leq j \leq d\} \) with envelope \( H \). By Theorem 7.1 and Lemma B.7 with \( s = 2 \),

\[
\mathbb{E} \left[ \sqrt{N} \hat{\Delta}_{B,5} \right] \lesssim \log(2M) \left( \sup_{1 \leq j \leq d} ||h_j||_{P^r,2} \log^{1/2}(d) + N^{-1/2+1/q} M^{1/q} ||H||_{P^r,q} \log(d)
+ B_n D_n^{-1} (1 + \varphi_n^{1/2}) \log^{1/2}(d) \right).
\]

Then due to (MT-3), and (MT-4),

\[
\mathbb{E} \left[ \sqrt{N} \hat{\Delta}_{B,5} \right] \lesssim \log(2M) \left( B_n D_n^{-1} \log^{1/2}(d) + N^{-1/2+1/q} M^{1/q} B_n^{2-2/q} D_n^{2/q-1} \log(d) + B_n D_n^{-1} (1 + \varphi_n^{1/2}) \log^{1/2}(d) \right),
\]

which completes the proof of the second result. \(\blacksquare\)
B.5.2. Bootstrap for $\Gamma_A$.

Recall the definition of $\hat{\gamma}_A$ in (32).

**Lemma B.11.** Assume that (46), (MT-0)- (MT-3), (MT-5), and (MB) holds. Define

$$\tilde{\Delta}_A := \max_{1 \leq i, j \leq d} \left| \gamma_A(h_i, h_j) - \gamma_A(h_i, h_j) \right| / \sqrt{\gamma_A(h_i, h_j)},$$

$$\chi_{n, A} := \left( \log(2M)B_n^2 \log^5(d) \right)^{1/7} + \left( \log(2M)M^{1/q}B_n^2 D_n^{2/3(q-1)\log^{5/2}(d)} \right)^{2/7}$$

$$\left( \frac{D_n^2 \log^5(d)}{n} \right)^{1/8} + \left( \frac{D_n^2 \log^3(d)}{n^{1-2/q}} \right)^{1/4} + \left( \frac{D_n^8 \log^3(d)}{n^{3-4/q}} \right)^{1/14} + \left( \frac{D_n^{3-2/q} \log^3(d)}{n^{1-1/q}} \right)^{2/7}.$$

Then there exists a constant $C$, that only depends on $\sigma^2, q, r, c_0, C_0$, such that

$$\mathbb{P} \left( \tilde{\Delta}_A \leq C \log^{-2}(d) \chi_{n, A}^3 \right) \geq 1 - C \chi_{n, A}.$$

**Proof.** Without loss of generality, we assume $\chi_{n, A} \leq 1/2$, By the same argument as in the proof of [13, Theorem 4.2],

$$\tilde{\Delta}_A \leq \tilde{\Delta}_{A, 1} + \tilde{\Delta}_{A, 2} + \tilde{\Delta}_{A, 3},$$

where we define

$$\tilde{\Delta}_{A, 1} := \max_{1 \leq i, j \leq d} \frac{1}{n} \sum_{k=1}^n \left( G^{(k)}(h_j) - P^{r-1}h_j(X_k) \right)^2,$$

$$\tilde{\Delta}_{A, 2} := \max_{1 \leq i, j \leq d} \left| \frac{1}{\sqrt{\Gamma_{A, i} \Gamma_{A, j}}} \sum_{k=1}^n \left( P^{r-1}h_i(X_k) P^{r-1}h_j(X_k) - \Gamma_{A, ij} \right) \right|,$$

$$\tilde{\Delta}_{A, 3} := \max_{1 \leq i, j \leq d} \left| \frac{1}{\sqrt{\Gamma_{A, j} \Gamma_{A, i}}} \sum_{k=1}^n P^{r-1}h_j(X_k) \right|.$$

By Lemma B.12 (ahead),

$$\mathbb{P} \left( \tilde{\Delta}_{A, 2} \geq C \log^{-2}(d) \chi_{n, A}^3 \right) \leq C \chi_{n, A}, \quad \mathbb{P} \left( \tilde{\Delta}_{A, 3}^2 \geq C \log^{-2}(d) \chi_{n, A}^3 \right) \leq C \chi_{n, A} \leq C \chi_{n, A}.$$

Now we focus on $\tilde{\Delta}_{A, 1}$. By Lemma B.4, and due to (MB) and the union bound, since $N_2 \geq n$,

$$\mathbb{P} (E') \geq 1 - C_1 N_2^{-1},$$

where $E' := \bigcap_{k \in [n], \ell \in [M]} \left\{ \left| N_2 / \tilde{N}^{(k, \ell)}_2 - 1 \right| \leq C_1 \sqrt{\log(N_2)/N_2} \right\}$. Since $N_2 \geq n \geq 4$, on the event $E'$, $\left| N_2 / \tilde{N}^{(k, \ell)}_2 - 1 \right| \leq C_1$ for each $k \in [n], \ell \in [M]$. Then by definition, on the event $E'$, for fixed $k \in [n]$, we have for $1 \leq i \neq j \leq d$,

$$\left( G^{(k)}(h_j) - P^{r-1}h_j(X_k) \right)^2 \leq \left( T^{(k)}_2 \right)^2 + \left( T^{(k)}_3 \right)^2 + \left( T^{(k)}_4 \right)^2.$$
As a result, \( X \) since \( 56 \) hold. Then there exists a constant \( C \) Recall the definition of Lemma B.12. ■ which completes the proof.

where we define

\[
T_2^{(k)} := \max_{\ell \in [M] 1 \leq j \leq [d]} \max_{\ell \in [M]} N_2^{-1} \sum_{i \in I_{n-1,r-1}} (Z_\ell^{(k,\ell)} - q_n) h_j(X_{i,(k)}) \]  

\[
T_3^{(k)} := \max_{1 \leq j \leq d} P^{r-1} h_j(X_k) \max_{\ell \in [M]} N_2^{-1} \sum_{i \in I_{n-1,r-1}} (Z_\ell^{(k,\ell)} - q_n) \]  

As a result, on the event \( \mathcal{E}' \),

\[
\hat{\Delta}_{A,1} \leq T_1 + n^{-1} \sum_{k=1}^{n} \left( (T_2^{(k)})^2 + (T_3^{(k)})^2 \right). 
\]

where we define

\[
T_1 := \max_{1 \leq j \leq d} n^{-1} \sum_{k=1}^{n} \left( |I_{n-1,r-1}|^{-1} \sum_{i \in I_{n-1,r-1}} \left( h_j(X_{i,(k)}) - P^{r-1} h_j(X_k) \right) \right)^2. 
\]

Now by Markov inequality, Lemma B.13 and Lemma B.14 (both ahead),

\[
P \left( T_1 \geq C \log^{-4}(d) \lambda_{n,A}^6 \right) \leq C \chi_{n,A}, 
\]

\[
P \left( n^{-1} \sum_{k=1}^{n} \left( (T_2^{(k)})^2 + (T_3^{(k)})^2 \right) \geq C \log^{-4}(d) \lambda_{n,A}^6 \right) \leq C \chi_{n,A}. 
\]

As a result,

\[
P \left( \hat{\Delta}_{A,1} \geq C \log^{-4}(d) \lambda_{n,A}^6 \right) \leq C \chi_{n,A}. 
\]

Since \( \chi_{n,A} \leq 1/2, \log^{-4}(d) \lambda_{n,A}^6 \leq \log^{-2}(d) \lambda_{n,A}^3 \) thus,

\[
P \left( \hat{\Delta}_{A,1} \geq C \log^{-2}(d) \lambda_{n,A}^3 \right) \leq C \chi_{n,A}, \quad P \left( \hat{\Delta}_{A,1} \geq C \log^{-2}(d) \lambda_{n,A}^3 \right) \leq C \chi_{n,A}, 
\]

which completes the proof. ■

**Lemma B.12.** Recall the definition of \( \hat{\Delta}_{A,2} \) and \( \hat{\Delta}_{A,3} \) in (65). Assume that (46), (MT-0), and (MT-1) hold. Then there exists a constant \( C \), depending only on \( q, \sigma^2 \), such that

\[
C^{-1} \mathbb{E} \left[ \hat{\Delta}_{A,2} \right] \leq n^{-1/2} D_n \log^{1/2}(d) + n^{-1+2/q} D_n^2 \log(d), 
\]
\[ C^{-1} \mathbb{E} \left[ \hat{\Delta}_{A,3} \right] \leq n^{-1/2} \log^{1/2}(d) + n^{-1+1/q} D_n \log(d). \]

**Proof.** For the first result, we apply \([17, \text{Lemma E.1}]\) to the finite collection \(\{P^{r-1}h_i P^{r-1}h_j : 1 \leq i, j \leq d\}\) with envelope \((P^{r-1}H)^2\):

\[
\mathbb{E} \left[ \hat{\Delta}_{A,2} \right] \leq n^{-1/2} \max_{1 \leq j \leq d} \|(P^{r-1}h_j)^2\|_{P_2} \log^{1/2}(d) + n^{-1+2/q}\|(P^{r-1}H)^2\|_{P_2,2} \log(d).
\]

Due to (MT-1),

\[
\mathbb{E} \left[ \hat{\Delta}_{A,2} \right] \leq n^{-1/2} D_n \log^{1/2}(d) + n^{-1+2/q} D_n^2 \log(d).
\]

For the second result, we apply \([17, \text{Lemma E.1}]\) to the finite collection \(\{P^{r-1}h_j : 1 \leq j \leq d\}\) with envelope \(P^{r-1}H\): due to (MT-1),

\[
\mathbb{E} \left[ \hat{\Delta}_{A,3} \right] \leq n^{-1/2} \log^{1/2}(d) + n^{-1+1/q} D_n \log(d),
\]

which completes the proof. \(\blacksquare\)

**Lemma B.13.** Recall the definition of \(T_1\) in (67). Assume that (46), (MT-2), and (MT-5) hold. Then there exists a constant \(C\), depending only on \(q, r\), such that

\[ T_1 \leq C \left( n^{-1} D_n^2 \log(d) + n^{-3/2+2/q} D_n^{4-2/q} \log^{3/2}(d) + n^{-2-2/q} D_n^{6-2/q} \log^2(d) \right). \]

**Proof.** From the proof of \([14, \text{Theorem 3.1, equation (32)}]\), we have

\[
\mathbb{E} [T_1] \lesssim \sum_{\ell=2}^{r-1} n^{-\ell} \|P^{r-\ell-1}H\|^2_{P_{\ell+1,2}} \log^\ell(d) + n^{-1} \max_{1 \leq j \leq d} \|P^{-2}h_j\|^2_{P_2,2} \\
+ n^{-3/2} \max_{1 \leq j \leq d} \|(P^{-2}h_j)^2\|_{P_2,2} \log^{1/2}(d) + n^{-2+2/q} \|(P^{-2}H)^2\|_{P_2,2} \log(d) \\
+ n^{-2} \|(P^{-2}H)^2\|_{P_2,2} \log(d) \\
+ n^{-1} \max_{1 \leq j \leq d} \|(P^{-2}h_j)^2\|_{P_2,2} \log^2(d) + n^{-3/2+2/q} \|(P^{-2}H)^2\|_{P_2,2} \log^{3/2}(d) \\
+ n^{-3/2} \max_{1 \leq j \leq d} \|(P^{-2}h_j)^2\|_{P_2,2} \log^{3/2}(d) + n^{-2+2/q} \|(P^{-2}H)^2\|_{P_2,2} \log^2(d),
\]

and for \(1 \leq j \leq d\), \(\|(P^{-2}h_j)^2\|_{P_2,2} \leq \|P^{-2}h_j\|^2_{P_2,2} \).

Then since \(q \geq 4\), due to (46), (MT-5), (MT-2),

\[
\mathbb{E} [T_1] \lesssim \sum_{\ell=2}^{r-1} n^{-\ell} D_n^{2(\ell+1)} \log^\ell(d) \\
+ n^{-1} \max_{1 \leq j \leq d} \|P^{-2}h_j\|^2_{P_2,2} \log^2(d) + n^{-3/2+2/q} \|(P^{-2}H)^2\|_{P_2,2} \log^{3/2}(d) \\
+ n^{-3/2} \max_{1 \leq j \leq d} \|(P^{-2}h_j)^2\|_{P_2,2} \log^{3/2}(d) + n^{-2+2/q} \|(P^{-2}H)^2\|_{P_2,2} \log^2(d),
\]
\[ \lesssim n^{-2}D_n^0 \log^2(d) + n^{-1}D_n^2 \log(d) + n^{-3/2+2/q}D_n^{4/2} \log^{3/2}(d) + n^{-3/2}D_n^{4/2} \log^{3/2}(d) + n^{-2+2/q}D_n^{6/4q} \log^{2}(d), \]

which completes the proof due to (46).

**Lemma B.14.** Fix \( k \in [n] \), and recall the definitions of \( T_2^{(k)} \) and \( T_3^{(k)} \) in (66). Assume (MT-3) holds. Then there exists an absolute constant \( C \) such that for each \( k \in [n] \),

\[
C^{-1} \mathbb{E}[(T_2^{(k)})^2] \leq \frac{\log(2M)B_n^2 \log(d)}{N_2} + \frac{\log^2(2M)M^{2/q}B_n^{4-4/q}D_n^{4/q-2} \log(d)}{N_2^{2-2/q}},
\]

\[
C^{-1} \mathbb{E}[(T_3^{(k)})^2] \leq \frac{\log(2M)B_n^2}{N_2} + \frac{\log^2(2M)B_n^2}{N_2^2}.
\]

**Proof.** We apply Lemma A.5 to \( \{h_j : 1 \leq j \leq d \} \) conditional on \( X_k \):

\[
\mathbb{E}_{X_k}[(T_2^{(k)})^2] \lesssim N_2^{-1} \log(d) \left( \|H(X_k, \cdot)\|_{\ell_{pr-1},2}^2 \log(2M) + \frac{\log^2(2M)M^{2/q}B_n^{4-4/q}D_n^{4/q-2} \log(d)}{N_2} \right).
\]

Due to (MT-3), \( q \geq 4 \) and Jensen’s inequality, we have

\[
\mathbb{E}[(T_2^{(k)})^2] \leq CN_2^{-1} \log(d) \left( \log(2M)B_n^2 + \frac{\log^2(2M)M^{2/q}B_n^{4-4/q}D_n^{4/q-2}}{N_2^{1-2/q}} \right).
\]

Now we focus on the second inequality. Due to (MT-3), \( \| \max_{1 \leq j \leq d} |P_{pr-1}h_j(X_k)| \|_{\ell_{p,2}}^2 \leq B_n^2 \). By Lemma B.5,

\[
\mathbb{E} \left[ \max_{\ell \in [M]} \left| \sum_{i \in I_{n-1,r-1}^{(k)}} (Z_i^{(k,\ell)} - q_n) \right|^2 \right] \lesssim N_2 \log(2M) + \log^2(2M).
\]

As a result, due to independence,

\[
\mathbb{E}[(T_3^{(k)})^2] \lesssim B_n^2 N_2^{-1} \log(2M) + B_n^2 N_2^{-2} \log^2(2M).
\]

---

**B.5.3. Proof of Theorem B.3**

The constants in the following proof may depend on \( r, \sigma, q, c_0, C_0 \), and may vary from line to line.

**Proof of Theorem B.3.** Without loss of generality, we can assume \( Y_A \) and \( Y_B \) are independent of all other random variables. Recall the definition of \( \mathcal{X}_{n,A} \) and \( \mathcal{X}_{n,B} \) in Lemma B.11 and B.9. Define two \( d \times d \) diagonal matrices \( \Lambda_A \) and \( \Lambda_B \) such that

\[
\Lambda_{A,jj} = \gamma_A(h_j), \quad \Lambda_{B,jj} = \gamma_B(h_j), \quad \text{for } 1 \leq j \leq d.
\]
Testing for regression curvature

Step 1. Due to Lemma B.9 and (MT-4),

$$\mathbb{P}(\mathcal{E}_1) \geq 1 - C\chi_{n,B}, \text{ where } \mathcal{E}_1 := \left\{ \max_{1 \leq j, k \leq d} \frac{\hat{\gamma}_B(h_j, h_k) - \gamma_B(h_j, h_k)}{\sqrt{\gamma_B(h_j)\gamma_B(h_k)}} \leq C\log^{-2}(d)\lambda_{n,B}^3 \right\}. $$

Then by the Gaussian comparison inequality [13, Lemma C.5], on the event $\mathcal{E}_1$,

$$\sup_{R \in \mathcal{R}} \left| \mathbb{P}|_{\mathcal{D}_n'}(U_{n,B}^\# R) - \mathbb{P}(Y_B \in R) \right| = \sup_{R \in \mathcal{R}} \left| \mathbb{P}|_{\mathcal{D}_n'}(\Lambda^{-1/2}_{B} U_{n,B}^\# R) - \mathbb{P}(\Lambda^{-1/2}_{B} Y_B \in R) \right| \leq \left( \log^{-2}(d)\lambda_{n,B}^3 \right)^{1/3} \log^{2/3}(d) = \chi_{n,B}. $$

Step 2. Due to Lemma B.11,

$$\mathbb{P}(\mathcal{E}_2) \geq 1 - C\chi_{n,A}, \text{ where } \mathcal{E}_2 := \left\{ \hat{\Delta}_A \leq C\log^{-2}(d)\lambda_{n,A}^3 \right\}, $$

where $\hat{\Delta}_A$ is defined in Lemma B.11. Then by the Gaussian comparison inequality [13, Lemma C.5], on the event $\mathcal{E}_2$,

$$\sup_{R \in \mathcal{R}} \left| \mathbb{P}|_{\mathcal{D}_n'}(U_{n,A}^\# R) - \mathbb{P}(Y_A \in R) \right| = \sup_{R \in \mathcal{R}} \left| \mathbb{P}|_{\mathcal{D}_n'}(\Lambda^{-1/2}_{A} U_{n,A}^\# R) - \mathbb{P}(\Lambda^{-1/2}_{A} Y_A \in R) \right| \leq \left( \log^{-2}(d)\lambda_{n,A}^3 \right)^{1/3} \log^{2/3}(d) = \chi_{n,A}. $$

Step 3. Now we focus on the event $\mathcal{E}_1 \cup \mathcal{E}_2$, which occurs with probability at least $1 - C\chi_{n,A} - C\chi_{n,B}$.

Fix $R \in \mathcal{R}$.

On the event $\mathcal{E}_1 \cup \mathcal{E}_2$, by the results in Step 1 and 2,

$$\mathbb{P}|_{\mathcal{D}_n}(U_{n,*}^\# R) = \mathbb{P}|_{\mathcal{D}_n}(\alpha_{n/2}^1 U_{n,B}^\# + r U_{n,A}^\# R) = \mathbb{P}|_{\mathcal{D}_n}(U_{n,B}^\# \in \alpha_{n/2}^{-1}(R - r U_{n,A}^\#)) \leq \mathbb{P}|_{\mathcal{D}_n}(Y_B \in \alpha_{n/2}^{-1}(R - r U_{n,A}^\#)) + C\chi_{n,B} = \mathbb{P}|_{\mathcal{D}_n}(U_{n,A}^\# \in r^{-1}(R - \alpha_{n/2}^{-1} Y_B)) + C\chi_{n,B} \leq \mathbb{P}(Y_A \in r^{-1}(R - \alpha_{n/2}^{-1} Y_B)) + C\chi_{n,B} + C\chi_{n,A} = \mathbb{P}(r Y_A + \alpha_{n/2}^{-1} Y_B \in R) + C\chi_{n,B} + C\chi_{n,A}. $$

The reverse inequality is similar. Then the proof is complete by noticing that $\chi_{n,A} + \chi_{n,B} \leq \log^{1/4}(M)\lambda_n$. 

\hfill \blacksquare
Appendix C: Proofs regarding stratified, incomplete $U$-processes

First, define
\[ \partial \mathcal{H}_t := \{ h - h' : h, h' \in \mathcal{H}, \max\{ \| h - h' \|_{P^r,2}, \| h - h' \|_{P^{r,4}} \} \leq \epsilon \}. \] (68)

By Lemma A.6, \{ \partial \mathcal{H}_t, 2H \} is a VC-type class with characteristics \((A, 2\nu)\). Then due to [18, Corollary A.1], \{ (\partial \mathcal{H}_t), (2H)^2 \} is also VC-type with characteristics \((\sqrt{2}A, 4\nu)\).

Due to (MT-2), (MT-4), if (72) holds, we have
\[ \log(\| H \|_{P^r,2}) \leq C \log(n), \quad \log(\| H^2 \|_{P^r,2}) \leq C \log(n), \quad n^{-1} D_n^2 K_n \leq 1. \] (69)

where the constant $C$ depends on $r$.

C.1. Supporting calculations

**Lemma C.1.** Assume (69), (VC), (MT-1), (MT-2) and (MT-4) hold. Let $\epsilon^{-1} := N\| 1 + H^2 \|_{P^r,2}$. Then there exists a constant $C$, depending only on $q, r$, such that
\[ C^{-1} \mathbb{E} \left[ \| \sqrt{n} (U_n(h) - P^n h) \|_{\partial \mathcal{H}_n} \right] \leq n^{-1/2 + 1/q} D_n K_n + n^{-1 + 1/q} D_n^{3 - 2/q} K_n. \]

**Proof.** By definition, for $1 \leq \ell \leq r$, $\sup_{h \in \partial \mathcal{H}_n} \| P^{r-E} h \|_{P^{r,2}} \leq \sup_{h \in \partial \mathcal{H}_n} \| h \|_{P^{r,2}} \leq N^{-1}$. Thus let
\[ \sigma_\ell := N^{-1}, \quad \delta_\ell := \sigma_\ell / (2 P^{r-E} H \| P^{r,2} \| \geq (2 N \| H \|_{P^{r,2}})^{-1}. \]

Now we apply Theorem A.7 to the class \{ \partial \mathcal{H}_t, 2H \} with envelopes \{ 2 P^{r-E} H : 1 \leq \ell \leq r \}. Note that by Theorem A.7, due to (VC) and (69),
\[ J_\ell(\delta_\ell) \leq \delta_\ell (4 \log(A/\delta_\ell))^\ell/2 \leq \delta_\ell K_\ell^{\ell/2}. \]

Thus by Theorem A.7, due to (MT-1), (MT-2), (69), and $N \geq n/r$,
\[ \mathbb{E} \left[ \| U_n(h) - P^n h \|_{\partial \mathcal{H}_n} \right] \leq n^{-1/2} N^{-1} K_n^{1/2} + n^{-1 + 1/q} \| P^{r-E} H \|_{P^{r,2}} K_n \]
\[ + n^{-1} N^{-1} K_n + n^{-3/2 + 1/q} \| P^{r-E} H \|_{P^{r,2}} K_n^2 + \sum_{\ell=3}^r n^{-\ell/2} \| P^{r-E} H \|_{P^{r,2}} K_n^{\ell/2} \]
\[ \leq n^{-1 + 1/q} D_n K_n + n^{-3/2 + 1/q} D_n^{3 - 2/q} K_n^2 + n^{-3/2} D_n^{3/2} K_n^3 \]
\[ \leq n^{-1 + 1/q} D_n K_n + n^{-3/2 + 1/q} D_n^{3 - 2/q} K_n^2, \]

which completes the proof.

**Lemma C.2.** Assume (69), (VC), (MT-2), and (MT-4) hold. Let $\epsilon^{-1} := N\| 1 + H^2 \|_{P^r,2}$. Then there exists a constant $C$, depending only on $q, r, C_0$, such that
\[ C^{-1} \mathbb{E} \left[ \left\| \frac{1}{| I_{n,r} |} \sum_{i \in I_{n,r}} h^2(X_i) \right\|_{\partial \mathcal{H}_n} \right] \leq \left( \inf_{h \in \mathcal{H}} \gamma_B(h) \right) \left( n^{-1 + 1/q} D_n^2 K_n + n^{-3/2 + 1/q} D_n^{4 - 2/q} K_n^2 \right). \]
Lemma C.3. Assume the conditions (PM), (VC), (MB), and (MT-0). Then for $m \in [M]$, define

$$H_m := \left\{ h / \sqrt{\gamma_s(h)} : h \in H_m \right\}, \quad d_m^2(h_1, h_2) := \mathbb{E} \left[ (W_P(h_1) - W_P(h_2))^2 \right],$$

for $h_1, h_2 \in H_m$. Then for $m \in [M]$ and $h_1, h_2 \in H_m$, by definition (recall $W_P$ is prelinear [23, Theorem 3.1.1]) and Jensen’s inequality,

$$d_m^2(h_1, h_2) = \mathbb{E} \left[ W_P^2(h_1 - h_2) \right] \leq r^2 \mathbb{E} \left[ (P^{r-1}(h_1 - h_2)(X_1))^2 \right] + \alpha_n \mathbb{E} \left[ (h_1 - h_2)(X_1))^2 \right] \leq (r^2 + r) \|h_1 - h_2\|_{P^{r-2}}^2.$$
Due to (VC) and (MT-0), \( \{ \tilde{H}_m, \sigma^{-1} H \} \) is a VC-type class with characteristics \((A, \nu + 1)\) for \( m \in [M] \). As a result, for any \( \tau > 0 \) and \( m \in [M] \),

\[
N(\tilde{H}_m, d_m, \tau \sqrt{r^2 + r^2} \| \sigma^{-1} H \|_{p^{r,2}}) \\
\leq N(\tilde{H}_m, \sqrt{r^2 + r^2} \| \sigma^{-1} H \|_{p^{r,2}}, \tau \sqrt{r^2 + r^2}) \leq (A/\tau)^{\nu + 1}.
\]

Since \( \mathbb{E} [W_{n}^2 (h)] = 1 \) for any \( h \in \tilde{H}_m \), by the entropy integral bound [64, Corollary 2.2.5] and due to (MT-3), for \( m \in [M] \),

\[
\mathbb{E} \left[ \| W_P \|_{\tilde{H}_m} \right] \leq \int_{0}^{2} \sqrt{1 + (\nu + 1) \log (2Ar \| \sigma^{-1} H \|_{p^{r,2}} / \tau)} \, d\tau \lesssim K_n^{1/2}.
\]

By the Borell-Sudakov-Tsirelson concentration inequality [31, Theorem 2.2.7], for \( m \in [M] \),

\[
\mathbb{P} \left( \| W_P \|_{\tilde{H}_m} \geq \mathbb{E} \left[ \| W_P \|_{\tilde{H}_m} \right] + \sqrt{2 \log (Mn)} \right) \leq M^{-1} n^{-1}.
\]

Then the proof is complete due to (MB) and the union bound. \( \blacksquare \)

**C.2. Proof of the Gaussian approximation for the suprema**

Now we prove Theorem 6.1. For \( \epsilon \in (0, 1) \) and \( m \in [M] \), denote

\[
\partial \mathcal{H}_{m,\epsilon} := \{ h - h' : h, h' \in \mathcal{H}_m, \max\{\| h - h' \|_{p^{r,2}}, \| h - h' \|_{p^{r,4}} \} \leq \epsilon \| 1 + H^2 \|_{p^{r,2}} \}. \quad (70)
\]

By Lemma A.6, due to condition (VC), \( \{ \partial \mathcal{H}_{m,\epsilon}, 2H \} \) is a VC-type class with characteristics \((A, 2\nu)\). For each \( m \in [M] \) and \( h_1, h_2 \in \mathcal{H}_m \) such that \( \max\{\| h_1 - h_2 \|_{p^{r,2}}, \| h_1 - h_2 \|_{p^{r,4}} \} \leq \epsilon \| 1 + H^2 \|_{p^{r,2}} \), we define for \( h := h_1 - h_2 \),

\[
\bar{U}^\prime_{n,N}(h) := U^\prime_{n,N}(h_1) - U^\prime_{n,N}(h_2), \quad \bar{W}_P(h) := W_P(h_1) - W_P(h_2).
\]

\( \bar{U}^\prime_{n,N}(\cdot) \) is well defined (i.e. independent of the choice of \( h_1, h_2 \)) since \( U^\prime_{n,N}(\cdot) \) is linear in its argument. Further, by [23, Theorem 3.1.1], \( W_P \) can be extended to the linear hull of \( \mathcal{H}_m \). With above discussions, we will simply write \( \bar{U}^\prime_{n,N} \) and \( \bar{W}_P \) for their extensions \( U^\prime_{n,N} \) and \( W_P \) to \( \partial \mathcal{H}_{m,\epsilon} \). Similar convention applies to \( U_{\hat{n},N} \).

Further, recall and define

\[
\gamma_{s}(h, h') := r^2 \gamma_A(h, h') + \alpha_n \gamma_B(h, h') \quad \text{for} \quad h, h' \in \mathcal{H}, \quad \gamma_{s} := \inf_{h \in \mathcal{H}} \gamma_{s}(h, h), \quad (71)
\]

where we recall that \( \gamma_A(\cdot, \cdot), \gamma_B(\cdot, \cdot) \), and \( \gamma_s(\cdot, \cdot) \) are defined in (30), and \( \alpha_n = n/N \).

In this section, \( C \) denotes a constant that depends only on \( r, q, \sigma, c_0, C_0 \), and that may vary from line to line. The notation \( \lesssim \) means that the left hand side is bounded by the right hand side up to a constant that depends only on \( r, q, \sigma, c_0, C_0 \). Clearly, in proving Theorem 6.1, without loss of generality, we may assume

\[
\eta_n^{(1)} \leq 1/2, \quad \eta_n^{(2)} \leq 1/2. \quad (72)
\]
Proof of Theorem 6.1. Fix some $t \in \mathbb{R}$. Let $\epsilon^{-1} := N\|1 + H^2\|_{pr,2}$. By Lemma A.6 and (MB), there exists a finite collection $\{h_j : 1 \leq j \leq d\} \subset \mathcal{H}$ such that the following two conditions hold: (i) $\log(d) \leq \log(M(4A/\epsilon)) \leq K_n$; (ii) for any $h \in \mathcal{H}$, there exists $1 \leq j^* \leq d$ such that $\sigma(h) = \sigma(h_{j^*})$, and

$$\max \left\{ \|h - h_{j^*}\|_{pr,2}, \|h - h_{j^*}\|_{pr,4} \right\} \leq \epsilon + 1 + H^2 \|_{pr,2}.$$ 

Define $M_n^\epsilon := \max_{1 \leq j \leq d} U'_n,h_j, \quad \tilde{M}_n^\epsilon := \max_{1 \leq j \leq d} W_P(h_j).$ Then by definition,

$$M_n^\epsilon \leq M_n \leq M_n^\epsilon + \max_{m \in [M]} \left[ U'_{n,N}(h) \right] \leq \tilde{M}_n \leq \tilde{M}_n^\epsilon + \max_{m \in [M]} \|W_P(h)\|_{\partial \mathcal{H}_{m,c}}.$$ 

Observe that $E[\gamma_n^{-1/2}(h_j)W_P(h_j)] = 1$ for $1 \leq j \leq d$. Then for any $\Delta > 0$, by Gaussian anti-concentration inequality [17, Lemma A.1],

$$P \left( \tilde{M}_n \leq t - \Delta \gamma_n^{-1/2} \right) = P \left( \bigcap_{j=1}^{d} \left\{ W_P(h_{j}) \leq t - \Delta \gamma_n^{-1/2} \right\} \right)$$

$$= P \left( \bigcap_{j=1}^{d} \left\{ \gamma_n^{-1/2}(h_j)W_P(h_j) \leq \gamma_n^{-1/2}(h_j)t - \Delta \gamma_n^{-1/2}(h_j) \gamma_n^{-1/2} \right\} \right)$$

$$\geq P \left( \bigcap_{j=1}^{d} \left\{ \gamma_n^{-1/2}(h_j)W_P(h_j) \leq \gamma_n^{-1/2}(h_j)t - \Delta \right\} \right)$$

$$\geq P \left( \bigcap_{j=1}^{d} \left\{ \gamma_n^{-1/2}(h_j)W_P(h_j) \leq \gamma_n^{-1/2}(h_j)t \right\} \right) - C \Delta \log^1/(d) \geq P \left( \tilde{M}_n \leq t \right) - C \Delta K_n^{1/2}.$$ 

Thus for any $\Delta > 0$, we have

$$P(\tilde{M}_n \leq t) \leq P(\tilde{M}_n^\epsilon \leq t) \leq P(\tilde{M}_n^\epsilon \leq t - \Delta \gamma_n^{-1/2}) + C \Delta K_n^{1/2}$$

$$\leq (1) P(\tilde{M}_n^\epsilon \leq t - \Delta \gamma_n^{-1/2}) + C \Delta K_n^{1/2} + C \eta_n^{(1)} + C \eta_n^{(2)}$$

$$\leq P(\tilde{M}_n \leq t) + P \left( \max_{m \in [M]} \left[ U'_{n,N}(h) \right] \geq \Delta \gamma_n^{-1/2} \right) + C \Delta K_n^{1/2} + C \eta_n^{(1)} + C \eta_n^{(2)}$$

$$\leq (2) P(\tilde{M}_n \leq t) + C \Delta K_n^{1/2} + C \eta_n^{(1)} + C \eta_n^{(2)}$$

$$\quad + \frac{1}{\Delta} \left( \frac{M_{1/q}^N_{B_n 1-2/q}}{n^{1/2-1/q}} + \frac{D_n K_{n}^{3/2}}{n^{1/2-1/q}} + \frac{D_n^{2-1/q} K_n^2}{n^{3/4-1/(2q)}} + \frac{D_n^3 K_{n}^2}{n^{1-1/q}} \right) + \frac{1}{N},$$

where (1) is due to Theorem B.2, and (2) is due to Lemma C.4 (ahead). Now let $\Delta$ be the following

$$\left( \frac{M_{1/q}^N_{B_n 1-2/q}}{n^{1/2-1/q}} \right)^{1/2} + \left( \frac{D_n K_{n}^{3/2}}{n^{1/2-1/q}} \right)^{1/2} + \left( \frac{D_n^{2-1/q} K_n^2}{n^{3/4-1/(2q)}} \right)^{1/2} + \left( \frac{D_n^3 K_{n}^2}{n^{1-1/q}} \right)^{1/2}.$$
Then due to (72), we have
\[ P(\tilde{M}_n \leq t) \leq P(M_n \leq t) + Cn(1) + Cn(2). \]

By a similar argument (using the bound on \( P(\max_{m \in [M]} \| W_P(h) \|_{\partial H_{m, \epsilon}} \geq \Delta) \) instead of the one on \( P(\max_{m \in [M]} \| U'_{n,N}(h) \|_{\partial H_{m, \epsilon}} \geq \Delta^2 \) in Lemma C.4), we have
\[ P(M_n \leq t) \leq P(\tilde{M}_n \leq t) + Cn(1) + Cn(2), \]
which completes the proof.

### C.3. A lemma for establishing validity of Gaussian approximation

Recall the definition of \( \partial H_{m, \epsilon} \) in (70). The next Lemma controls the size of \( U'_{n,N} \) and \( W_P \) over \( \partial H_{m, \epsilon} \).

In this section, the notation \( \lesssim \) means that the left hand side is bounded by the right hand side up to a multiplicative constant that only depends on \( r, C_0, \sigma, \sigma \). It is clear that for \( m \in [M] \), \( \partial H_{m, \epsilon} \subset \partial H_{\epsilon} \), where \( H_{\epsilon} \) is defined in (68).

**Lemma C.4.** Assume (72), (PM), (VC), (MB), (MT-0)-(MT-4) hold. Let \( \epsilon^{-1} := N \| 1 + H^2 \|_{p^r, 2} \). Recall the definition of \( \gamma_* \) in (71). For any \( \Delta > 0 \),
\[ P \left( \max_{m \in [M]} \| U'_{n,N}(h) \|_{\partial H_{m, \epsilon}} \geq \Delta \gamma_*^{1/2} \right) \lesssim \frac{1}{\Delta} \left( \frac{M^{1/q} B_n^{1-2/q} D_n^{2/q} K_n^2}{N^{1/2-1/q}} + \frac{D_n K_n^{3/2}}{n^{1/2-1/q}} + \frac{D_n^{2-1/q} K_n^2}{n^{3/4-1/(2q)}} + \frac{D_n^{3-2/q} K_n^2}{n^{1-1/q}} \right) + \frac{1}{N}, \]
\[ P \left( \max_{m \in [M]} \| W_P(h) \|_{\partial H_{m, \epsilon}} \geq \Delta \right) \leq \Delta^{-1} N^{-1} K_n. \]

**Proof.** We start with the first claim. Observe that for \( m \in [M] \) and \( h \in \partial H_{m, \epsilon} \),
\[ \left( \hat{N}(m)/N \right) \sqrt{n} U'_{n,N}(h) - P h = \alpha_n^{1/2} \frac{1}{\sqrt{N}} \sum_{i \in I_{n,r}} (Z_i^{(m)} - p_n) h(X_i) \]
\[ - \alpha_n^{1/2} P h \frac{1}{\sqrt{N}} \sum_{i \in I_{n,r}} (Z_i^{(m)} - p_n) + \sqrt{n} \frac{1}{|I_{n,r}|} \sum_{i \in I_{n,r}} (h(X_i) - P h). \]

As a result, \( \max_{m \in [M]} \left( \hat{N}(m)/N \| U'_{n,N}(h) \|_{\partial H_{m, \epsilon}} \right) \leq \alpha_n^{1/2} I + \alpha_n^{1/2} II + III \), where
\[ I := \max_{m \in [M]} \sup_{h \in \partial H_{\epsilon}} \left| \frac{1}{\sqrt{N}} \sum_{i \in I_{n,r}} (Z_i^{(m)} - p_n) h(X_i) \right|, \]
\[ II := \sup_{h \in \partial H_{\epsilon}} |P h| \max_{m \in [M]} \left| \frac{1}{\sqrt{N}} \sum_{i \in I_{n,r}} (Z_i^{(m)} - p_n) \right|. \]
Due to \((MT-3)\) and \((MT-4)\), and since \(\int \) Testing for regression curvature.

Then by Lemma B.4 and by the Markov inequality,

\[
\sup_{h \in \partial H_c} \|h\|_{p_r,2} \leq N^{-1} := \sigma_r, \quad \delta_r := \sigma_r/(M^{1/2}\|H\|_{p_r,2}) \geq (2NM^{1/2}\|H\|_{p_r,2})^{-1}.
\]

By Theorem 7.1 and due to \((MB)\) and \((69)\), \(\tilde{J}(\delta_r) \lesssim \delta_r K_n^{1/2} \) and \(\log(2M) \lesssim K_n\). Then due to Theorem 7.1 and Lemma C.2,

\[
\mathbb{E}[I] \lesssim N^{-1} K_n + M^{1/q} N^{-1/2+1/q}\|H\|_{p_r,2}^2 K_n^2
\]

\[
+ \left( \inf_{h \in H} \gamma_B(h) \right)^{1/2} \left( n^{-1/2+1/(2q)} D_n K_n^{3/2} + n^{-3/4+1/(2q)} D_n^{2-1/q} K_n^2 \right).
\]

Due to \((MT-3)\) and \((MT-4)\), and since \(N \geq n/r\),

\[
\alpha_n^{1/2} \mathbb{E}[I] \lesssim \left( \alpha_n \inf_{h \in H} \gamma_B(h) \right)^{1/2} \left( M^{1/q} B_n^{1-2/q} D_n^{2/q} K_n^2 \right) \left( n^{1/2-1/q} + n^{-3/4-1/(2q)} D_n^{2-1/q} K_n^2 \right).
\]

For the second term, by Lemma B.5,

\[
\mathbb{E}[II] \lesssim N^{-1} \left( K_n^{1/2} + N^{-1/2} K_n \right) = N^{-1} K_n^{1/2} + N^{-3/2} K_n.
\]

Finally, due to Lemma C.1, we have

\[
\mathbb{E} \left[ \max_{m \in [M]} \left( \hat{N}^{(m)}/N \|U_{n,N}^{\prime}(h)\|_{\partial H_{m,v}} \right) \right] \lesssim \frac{D_n K_n}{n^{1/2-1/q}} + \frac{D_n^{3-2/q} K_n^2}{n^{1-1/q}}
\]

\[
\left( \alpha_n \inf_{h \in H} \gamma_B(h) \right)^{1/2} \left( M^{1/q} B_n^{1-2/q} D_n^{2/q} K_n^2 \right) \left( n^{1/2-1/q} + n^{-3/4-1/(2q)} D_n^{2-1/q} K_n^2 \right).
\]

Recall \(\gamma_* := \inf_{h \in H} \gamma_*(h)\) (in \((71)\)). Clearly, by definition and due to \((MT-0)\),

\[
\gamma_* \geq \max \left\{ r^2 \mathbb{E}_2^2, \alpha_n \inf_{h \in H} \gamma_B(h) \right\}.
\]

Then by Lemma B.4 and by the Markov inequality,

\[
P \left( \max_{m \in [M]} \|U_{n,N}^{\prime}(h)\|_{\partial H_{m,v}} \geq \Delta_{\gamma_*}^{1/2} \right)
\]

\[
\leq P \left( \max_{m \in [M]} \|U_{n,N}^{\prime}(h)\|_{\partial H_{m,v}} \geq \Delta_{\gamma_*}^{1/2}, \max_{m \in [M]} N/\hat{N}^{(m)} \leq C \right) + CN^{-1}
\]

\[
\leq P \left( \max_{m \in [M]} \left( (\hat{N}^{(m)}/N) \|U_{n,N}^{\prime}(h)\|_{\partial H_{m,v}} \right) \geq \Delta_{\gamma_*}^{1/2}/C \right) + CN^{-1},
\]
Observe that for which completes the proof of the first claim.

By Lemma A.7 and (69), for

\[ \text{Assume the conditions (PM), (VC), (MB), and Lemma C.5.} \]

domain from \( H \)

\[ \text{Then the proof is complete by maximal inequality [64, Lemma 2.2.2], and Markov inequality.} \]

Since \( \{ \partial H_{m,\epsilon}, 2H \} \) is VC type with characteristics \( (A,2\nu) \), by entropy integral bound [64, Theorem 2.3.7], if we denote \( D := \sup_{h \in \partial H_{m,\epsilon}}, \| h \|_{P^r,2} \leq N^{-1} \), we have for \( m \in [M] \),

\[ \| W_P(h) \|_{\partial H_{m,\epsilon}} \leq 1 + \log N(\partial H_{m,\epsilon}, \| \cdot \|_{P^r,2}, \tau) d\tau \]

\[ \leq 2^2 \| P^r \|_{P^r,2} \int_0^D \sqrt{1 + \log N(\partial H_{m,\epsilon}, \| \cdot \|_{P^r,2}, \tau) 2H \|_{P^r,2}) d\tau,} \]

By Lemma A.7 and (69), for \( m \in [M] \),

\[ \| W_P(h) \|_{\partial H_{m,\epsilon}} \|_{\psi_2} \leq N^{-1} K_n^{1/2}. \]

Then the proof is complete by maximal inequality [64, Lemma 2.2.2], and Markov inequality.

C.4. Proof of the validity of bootstrap for stratified, incomplete \( U \)-processes

In this section, \( C \) denotes a constant that depends only on \( r, q, \sigma, c_0, C_0 \), and that may vary from line to line. Recall the definition of \( \partial H_{m,\epsilon} \) for \( m \in [M] \) in (70). The next Lemma establishes a high probability bound on the size of \( W_P \) and \( \cup_{n,s} \) over \( \partial H_{m,\epsilon} \) (recall the discussions in Section C.2 on extending the domain from \( H_m \) to \( \partial H_{m,\epsilon} \); similar convention applies to \( \cup_{n,s} \)).

Lemma C.5. Assume the conditions (PM), (VC), (MB), and (MT-0)-(MT-5), and for some \( C_1 > 0 \),

\[ \log(B_n) + \log(D_n) \leq C_1 \log(n), \quad n^{-1} D_n^2 K_n \leq C_1, \quad N_2^{-1/2} B_n \leq C_1. \]

Let \( \epsilon^{-1} := N \| 1 + H^2 \|_{P^r,2} \). Then there exists a constant \( C \), depending only on \( r, C_0 \), such that

\[ \mathbb{P} \left( \max_{m \in [M]} \| W_P(h) \|_{\partial H_{m,\epsilon}} \geq C N^{-1} K_n^{1/2} \right) \leq n^{-1}. \]
Further, there exists a constant $C'$, depending only on $r, q, c_0, \sigma, C_0, C_1$, such that for any $\Delta > 0$, with probability at least $1 - C'(N \wedge N_2)^{-1} - C'\Delta - C'\Delta^2$,

$$\Pr_{|D_n} \left( \max_{m \in [M]} \|\mathbb{U}^\#_{n,*} \|_{\partial H_{m,*}} \geq C' \Delta^1/2 N^{-1/2} B_n K_n^{1/2} + C' \Delta^{1/2} \chi^\#_{n,*} \right) \leq n^{-1}, \text{ where}$$

$$\chi^\#_{n,*} := (N \wedge N_2)^{-1/2 + 1/q} M^1/q B_n^{1-2/q} D_n^{2/q} K_n^{2} + n^{-1/2 + 1/q} D_n K_n^{3/2} + n^{-3/4 + 1/q} D_n^{2-2/q} K_n^{2} + n^{-1 + 1/q} D_n^{3-2/q} K_n^{2}.$$  

**Proof.** See Section C.5. \[\blacksquare\]

**Proof of Theorem 6.2.** Without loss of generality, we may assume $\theta_n \leq 1$.

Let $\epsilon^{-1} := N \|1 + H^2\|_{\Pr,2}^2$. By Lemma A.6 and (MB), there exists a finite collection $\{h_j : 1 \leq j \leq d\} \subset \mathcal{H}$ such that the following two conditions hold: (i) $\log(d) \leq \log(M(4A/\epsilon)^p) \leq K_n$; (ii). for any $h \in \mathcal{H}$, there exists $1 \leq j^* \leq d$ such that $\sigma(h) = \sigma(h_{j^*})$, and

$$\max \left\{ \|h - h_{j^*}\|_{\Pr,2}, \|h - h_{j^*}\|^2_{\Pr,4} \right\} \leq \epsilon \|1 + H^2\|_{\Pr,2}.$$  

Define $M^\#_{n,*} := \max_{1 \leq j \leq d} \mathbb{U}^\#_{n,*}(h_j)$, $M^\#_{n} := \max_{1 \leq j \leq d} WP(h_j)$. Then

$$M^\#_{n,*} \leq M^\#_{n} \leq \max_{m \in [M]} \|\mathbb{U}^\#_{n,*} \|_{\partial H_{m,*}} \text{ and } \mathbb{M}^\#_{n,*} \leq \mathbb{M}^\#_{n} \leq \mathbb{M}^\#_{n,*} + \max_{m \in [M]} \|WP\|_{\partial H_{m,*}}.$$  

Fix $t \in \mathbb{R}$. For some $\Delta > 0$ to be determined, denote

$$\Delta' := C' N^{-1/2} B_n K_n^{1/2} + C' \Delta^{-1} \chi^\#_{n,*},$$  

where $C', \chi^\#_{n,*}$ are defined in Lemma C.5. We have shown in the proof of Theorem 6.1 that

$$\Pr(\mathbb{M}^\#_{n} \leq t) \leq \Pr(\mathbb{M}^\#_{n,*} \leq t - \Delta^1/2) + C \Delta' K_n^{1/2}.$$  

Then, by Theorem B.3, with probability at least $1 - C\theta_n$,

$$\Pr(\mathbb{M}^\#_{n} \leq t) \leq \Pr_{|D_n} \left( \mathbb{M}^\#_{n,*} \leq t - \Delta^1/2 \right) + C\theta_n + C \Delta' K_n^{1/2}.$$  

Finally, due to Lemma C.5 and union bound, with probability at least $1 - C\theta_n - C\Delta - C\Delta^2$,

$$\Pr(\mathbb{M}^\#_{n} \leq t) \leq \Pr_{|D_n} \left( \mathbb{M}^\#_{n,*} \leq t \right) + \Pr_{|D_n} \left( \max_{m \in [M]} \|\mathbb{U}^\#_{n,*} \|_{\partial H_{m,*}} \geq \Delta^1/2 \right) + C\theta_n + C \Delta' K_n^{1/2}$$

$$\leq \Pr_{|D_n} \left( \mathbb{M}^\#_{n,*} \leq t \right) + n^{-1} + C\theta_n + C \Delta' K_n^{1/2}$$

$$\leq \Pr_{|D_n} \left( \mathbb{M}^\#_{n} \leq t \right) + C\theta_n + C \Delta^{-1} \chi^\#_{n,*} K_n^{1/2}.$$  

Now let $\Delta = (\chi^\#_{n,*})^{1/4} K_n^{1/4}$. Since $\theta_n \leq 1$, we have that with probability at least $1 - C\theta_n$

$$\Pr(\mathbb{M}^\#_{n} \leq t) \leq \Pr_{|D_n} \left( \mathbb{M}^\#_{n} \leq t \right) + C\theta_n.$$
By a similar argument (using the bound in Lemma C.5 for $\max_{m \in [M]} \|W_P\|_{\partial H_m, \epsilon}$),
\[
P(\mathcal{D}_n \left( M_n^\# \leq t \right)) \leq P(\tilde{M}_n \leq t) + C \vartheta_n,
\]
with probability at least $1 - C \vartheta_n$. Thus the proof is complete. 

C.5. Proof of Lemma C.5

In this section, the constants may depend on $r, q, c_0, C_0, \bar{\sigma}$, and vary from line to line. Recall the definitions of $U_n^A, U_n^B, U_n^\#$ in (15) and (16).

**Proof.** First claim. In the proof of Lemma C.4, we have shown that for $m \in [M],$
\[
E \left[ \|W_P(h)\|_{\partial H_m, \epsilon} \right] \lesssim N^{-1} K_n^{1/2}.
\]
Further, by definition of $\partial H_m, \epsilon$ (70), we have
\[
\sup_{h \in \partial H_m, \epsilon} E \left[ (W_P(h))^2 \right] = \sup_{h \in \partial H_m, \epsilon} \left( r^2 \text{Var}(P_r^{-1} h(X_1)) + \alpha_n \text{Var}(h(X_1^r)) \right) \lesssim \sup_{h \in \partial H_m, \epsilon} \|h\|_{\tilde{P}_r, 2}^2 \lesssim N^{-2}.
\]
By the Borell-Sudakov-Tsirelson concentration inequality [31, Theorem 2.2.7], for $m \in [M],$
\[
P \left( \|W_P\|_{\partial H_m, \epsilon} \geq E \left[ \|W_P\|_{\partial H_m, \epsilon} \right] + \sqrt{2 \sup_{h \in \partial H_m, \epsilon} E \left[ (W_P(h))^2 \right] \log(Mn}) \right) \leq M^{-1} n^{-1}.
\]
Thus by union bound and due to (MB),
\[
P \left( \max_{m \in [M]} \|W_P\|_{\partial H_m, \epsilon} \geq CN^{-1} K_n^{1/2} \right) \leq n^{-1},
\]
which completes the proof of the first claim.

Second claim. By the Borell-Sudakov-Tsirelson concentration inequality [31, Theorem 2.2.7], for $m \in [M],$
\[
P \left( \mathcal{D}_n \left( \|U_n^\#(h)\|_{\partial H_m, \epsilon} \right) \right) \geq E \left[ \|U_n^\#(h)\|_{\partial H_m, \epsilon} \right] + \sqrt{2 \Sigma_n \log(Mn}) \leq M^{-1} n^{-1},
\]
where $\Sigma_n := \sup_{h \in \partial H_m, \epsilon} E \left[ (U_n^\#(h))^2 \right]$. Conditioned on $\mathcal{D}_n$, for $m \in [M],$
\[
E \left[ \|U_n^\#(h)\|_{\partial H_m, \epsilon} \right] \leq r E \left[ \|U_n^\#(h)\|_{\partial H_m, \epsilon} \right] + \alpha_n \Sigma_n^{(m)} \lesssim r \Sigma_n + \alpha_n \Sigma_n^{(m)}.
\]
where $\Sigma^{(m)}_{n,A}$ and $\Sigma^{(m)}_{n,B}$ are defined in Lemma C.6 and C.7 (both ahead) respectively.

Recall that $\gamma_* := \inf_{h \in H} \gamma_s(h)$ in (71). In particular, due to (MT-0) and (MT-4),

$$\gamma_* \leq \max \left\{ r^2 \sigma^2, \alpha_n c_0 B_n^2 D_n^{-2} \right\}$$

Then by Lemma C.6 (ahead), for any $\Delta > 0$, with probability at least $1 - C N^{-1} - C \Delta - C \Delta^2$, for each $m \in [M]$,

$$C^{-1} \Delta \gamma_*^{-1/2} \alpha_n \left( \mathbb{E}_{D_n^r} \left[ \left\| \mathbb{U}_{n,B}^{\#} \right\|_{\partial H_{m,s}} \right] + (\Sigma^{(m)}_{n,B} \log(M n))^{1/2} \right) \leq M^{1/q} N^{1/2+1/q} B_n^{1-2/q} D_n^{2/q} K_n^2 + n^{-1/2+1/(2q)} D_n K_n^{3/2} + n^{-3/4+1/(2q)} D_n^{2-1/q} K_n^2.$$

Further, by Lemma C.7 and C.8 (both ahead), for any $\Delta > 0$, with probability at least $1 - C \Delta^2 - C N_2^{-1}$, for each $m \in [M]$,

$$C^{-1} \Delta \gamma_*^{-1/2} \left( \mathbb{E}_{D_n^r} \left[ \left\| \mathbb{U}_{n,A}^{\#} \right\|_{\partial H_{m,s}} \right] + (\Sigma^{(m)}_{n,A} \log(M n))^{1/2} \right) \leq (\Delta N^{1/2} B_n K_n^{1/2}) + N_2^{-1/2} B_n K_n^{3/2} + N_2^{-1+1/q} M^{1/q} B_n^{2-2/q} D_n^{2-1/q} K_n^2 + n^{-1/2+1/q} D_n K_n + n^{-3/4+1/q} D_n^{2-2/q} K_n^{3/2} + n^{-1+1/q} D_n^{3-2/q} K_n^2.$$

Combining above results and by union bound, for any $\Delta > 0$, with probability at least $1 - C' (N \land N_2)^{-1} - C' \Delta - C' \Delta^2$,

$$\mathbb{P}_{D_n^r} \left( \max_{m \in [M]} \left\| \mathbb{U}_{n,B}^{\#}(h) \right\|_{\partial H_{m,s}} \geq \frac{C' \gamma_*^{1/2} N^{-1/2} B_n K_n^{1/2} + C' \Delta^{1/2} \gamma_s \gamma_*}{\gamma_* \gamma_s} \right) \leq n^{-1},$$

which completes the proof. \[\blacksquare\]

Recall the definition of $\mathbb{U}_{n,B}^{\#}$ in (15).

**Lemma C.6.** Let $\epsilon := \epsilon = N^1 + H^2 \|_{Pr,2}$, and denote $\Sigma^{(m)}_{n,B} := \sup_{h \in \partial H_{m,s}} \mathbb{E}_{D_n^r} \left[ \left( \mathbb{U}_{n,B}^{\#}(h) \right)^2 \right]$ for $m \in [M]$. Assume (69), (PM), (VC), (MB), (MT-2), (MT-3), and (MT-4) hold. Then there exists a constant $C$, depending only on $q, r, c_0$, such that for any $\Delta > 0$, with probability at least $1 - C \Delta - C \Delta^2 - CN_2^{-1}$, the following two events hold:

$$C^{-1} \Delta \max_{m \in [M]} \mathbb{E}_{D_n^r} \left[ \left\| \mathbb{U}_{n,B}^{\#} \right\|_{\partial H_{m,s}} \right] \leq M^{1/q} N^{-1/2+1/q} B_n^{2-2/q} D_n^{2-1/q} K_n^2 + n^{-1/2+1/(2q)} B_n K_n^{3/2} + n^{-3/4+1/(2q)} B_n D_n^{1-1/q} K_n^2.$$

$$C^{-1} \Delta^2 \max_{m \in [M]} \Sigma^{(m)}_{n,B} \leq N^{-1+2/q} M^{-2/q} B_n^{4-4/q} D_n^{4-2/q} K_n^2 + n^{-1+1/q} B_n^2 K_n + n^{-3/2+1/q} B_n^2 D_n^{2-2/q} K_n^2.$$
Proof. First event. Note that for \( m \in [M] \), and \( h_1, h_2 \in \partial \mathcal{H}_{m, \varepsilon} \),

\[
\| \mathbb{U}^\#_{m,B}(h_1) - \mathbb{U}^\#_{m,B}(h_2) \|_{\psi_2[D^\prime_n]}^2 \lesssim \frac{1}{N(m)} \sum_{i \in I_{n,r}} Z_i^{(m)}(h_1(X_i) - h_2(X_i)) - U_{n,N}(h_1) + U_{n,N}(h_2))^2
\]

\[
= \frac{1}{N(m)} \sum_{i \in I_{n,r}} Z_i^{(m)}(h_1(X_i) - h_2(X_i))^2 - (U_{n,N}(h_1) - U_{n,N}(h_2))^2
\]

\[
\leq \left( N/N^{(m)} \right) \| h_1 - h_2 \|_{Q(m,2)}^2,
\]

where recall that \( Q(m) \) is defined in (35). Recall that \( \hat{V}_n := \max_{m \in [M]} \sup_{h \in \partial \mathcal{H}_\varepsilon} \| h \|_{Q(m,2)} \) (see (36) with \( \mathcal{F} \) replaced by \( \partial \mathcal{H}_\varepsilon \)), that \( \hat{Q} \), which dominates \( Q(m) \) for \( m \in [M] \), is defined in (35), and that \( \partial \mathcal{H}_\varepsilon \) is defined in (68). Then by the entropy integral bound [64, Corollary 2.2.5],

\[
\left\| \sqrt{N^{(m)}} / N \| \mathbb{U}^\#_{m,B}(h) \|_{\partial \mathcal{H}_{m,\varepsilon}} \right\|_{\psi_2[D^\prime_n]} \lesssim \int_0^{\hat{V}_n} \sqrt{1 + \log N(\partial \mathcal{H}_\varepsilon, \| \cdot \|_{Q(m,2)}, \tau)} d\tau \lesssim \| H \|_{\hat{Q},2} J(\hat{V}_n/\| H \|_{\hat{Q},2}).
\]

By maximal inequality [64, Lemma 2.2.2] and Corollary A.3,

\[
E \left[ \max_{m \in [M]} \sqrt{N^{(m)}} / N \| \mathbb{U}^\#_{m,B}(h) \|_{\partial \mathcal{H}_{m,\varepsilon}} \right] \lesssim \sqrt{\log(2M)} E \left[ \| H \|_{\hat{Q},2} J(\hat{V}_n/\| H \|_{\hat{Q},2}) \right] \lesssim V_{\hat{Q},2} \| H \|_{\hat{Q},2} + \frac{\log(2M) M^{1/q} \| H \|_{\delta r} J^2(\delta_r)}{N^{1/2-1/q}} + \sqrt{\Delta' \log(2M)} J(\delta_r)/\delta_r,
\]

where due to definition of \( \partial \mathcal{H}_\varepsilon \), we may take

\[
\sigma_r := N^{-1}, \quad \delta_r := \sigma_r/\left( \sqrt{M} 2H \right) \geq (2N M^{1/2} \| H \|_{\delta r})^{-1},
\]

\[
\Delta' := E \left[ \sup_{h \in \partial \mathcal{H}_\varepsilon} | I_{n,r} |^{-1} \sum_{i \in I_{n,r}} h^2(X_i) \right].
\]

Due to Theorem 7.1, (MB), and (69), \( J(\delta_r)/\delta_r \lesssim K_n^{1/2} \). Thus due to Lemma C.2, (MB), (MT-3) and (MT-4),

\[
E \left[ \max_{m \in [M]} \sqrt{N^{(m)}} / N \| \mathbb{U}^\#_{m,B}(h) \|_{\partial \mathcal{H}_{m,\varepsilon}} \right] \lesssim N^{-1} K_n + M^{1/q} N^{-1/2+1/q} B_n^{2-2/q} D_n^{2/q-1} K_n^{2} + B_n D_n^{-1} \left( n^{-1/2+1/(2q)} D_n K_n^{1/2} + n^{-3/4+1/(2q)} D_n^{2/q} K_n \right) K_n.
\]

Then the proof for the first inequality is complete due to Markov inequality and Lemma B.4.

Second event. Observe that

\[
\max_{m \in [M]} \sum_{n,B} Z_i^{(m)}(h(X_i) - U_{n,N}(h)) \leq \max_{m \in [M]} \sup_{h \in \partial \mathcal{H}_{m,\varepsilon}} \left( \hat{N}^{(m)} \right)^{-1} \sum_{i \in I_{n,r}} Z_i^{(m)}(h(X_i) - U_{n,N}(h))^2
\]
Proof. Observe first that by definition of Lemma C.7. Then the proof is complete by Markov inequality and Lemma B.4.

Due to Corollary A.3, Lemma C.2, (MT-3), (MT-4), (MB), and above calculations,

\[
\mathbb{E} \left[ \hat{V}_n^2 \right] \leq B_n^2 D_n^{-2} \left( n^{-1+1/q} D_n^2 K_n + n^{-3/2+1/q} D_n^{4-2/q} K_n^2 \right) \\
+ N^{-2} + N^{-1+2/q} M^2 / B_n^{4-4/q} D_n^{4-2/q} K_n^2.
\]

Then the proof is complete by Markov inequality and Lemma B.4.

Recall the definition of \( U_{n,A}^{\#} \) in (15).

**Lemma C.7.** Let \( \epsilon^{-1} := N \|1 + H^2\|_{TV,2} \), and denote \( \Sigma_{n,A}^{(m)} := \sup_{h \in \partial H_{m,\epsilon}} \mathbb{E}_{\mathcal{D}_n^\epsilon} \left[ \left( \hat{\eta}_{n,A}^{\#}(h) \right)^2 \right] \) for \( m \in [m] \). Assume (69), (PM), (VC) (MB), (MT-1), (MT-2), (MT-3), and (MT-5) hold. Then there exists a constant \( C \), depending only on \( q,r \), such that for any \( \Delta > 0 \), with probability at least \( 1 - C \Delta^2 - C N_2^{-1} \),

\[
C^{-1} \Delta^2 \max_{m \in [M]} \Sigma_{n,A}^{(m)} \leq N_2^{-1} B_n^2 D_n^2 K_n^2 + N_2^{-2+2/q} M^2 / B_n^{4-4/q} D_n^{4-2/q} K_n^2 \\
+ n^{-1+2/q} D_n^2 K_n + n^{-3/2+2/q} D_n^{4-4/q} K_n^2 + n^{-2+2/q} D_n^{6-4/q} K_n^2.
\]

**Proof.** Observe first that by definition of \( \partial H_{\epsilon} \) in (68), \( \sup_{h \in \partial H_{\epsilon}} \left\{ \|h\|_{TV,2} \lor \|h\|_{TV,4}^2 \right\} \leq N^{-1} \). By definition of \( U_{n,A}^{\#} \), for \( m \in [M] \) and \( h \in \partial H_{m,\epsilon} \),

\[
\Sigma_{n,A}^{(m)} = \sup_{h \in \partial H_{m,\epsilon}} \left( \sum_{k=1}^{n} \left( \xi^{(k)}(h) - \hat{\xi}(h) \right)^2 \right) \leq \sup_{h \in \partial H_{m,\epsilon}} \left( \sum_{k=1}^{n} \left( \xi^{(k)}(h) \right)^2 \right)
\]

\[
\leq 4 \left( \max_{1 \leq k \leq n} N_2 / N_2^{(k,m)} \right)^2 \left( I + II + III \right),
\]

where

\[
I := \max_{m \in [M]} \sup_{h \in \partial H_{m,\epsilon}} \left( \sum_{k=1}^{n} \left( Z_{(k,m)}^{(k,m)} - q_h(X_{(k)}) \right)^2 \right),
\]

\[
II := \sum_{k=1}^{n} \left( \sum_{i \in I_{n-1,r-1}^{(k)}} \left( h(X_{(i)}) - P^{r-1} h(X_k) \right)^2 \right),
\]

\[
III := \sum_{k=1}^{n} \left( P^{r-1} h(X_k) \right)^2.
\]
As a result, \( \max_{m \in [M]} \sum_{n,A}^m \leq \left( \max_{k \in [n], m \in [M]} N_2 / \hat{N}_2^{(k,m)} \right)^2 (I + II + III) \).

Due to Lemma B.4 and (MB),

\[
\mathbb{P} \left( \max_{k \in [n], m \in [M]} N_2 / \hat{N}_2^{(k,m)} \leq C \right) \geq 1 - C N_2^{-1}.
\] (73)

By Lemma A.5 and due to (VC) and (MB), for each \( k \in [n] \),

\[
\mathbb{E} \left| I_k \right| \leq N_2^{-1} B_n^2 K_n^2 + N_2^{-2+2/q} M_2^2 q B_n^{4-4/q} D_n^4 K_n^3.
\] (74)

From the proof of [14, Theorem 3.1] and similar to the proof for Lemma B.13,

\[
\mathbb{E} \left| II \right| \leq \sum_{\ell=2}^{r-1} n^{-\ell} \left\| P^{r-\ell-1} H \right\|_{P^{r+1},2}^2 K_n^\ell + n^{-1} \sup_{h \in \partial \mathcal{H}_c} \left\| P^{r-2} h \right\|_{P^{r+2},2}^2
\]

\[
+ n^{-3/2} \sup_{h \in \partial \mathcal{H}_c} \left\| (P^{r-2} h)^2 \right\|_{P^{r+2},2} K_n^{1/2} + n^{-2+2/q} \left\| (P^{r-2} H)^2 \right\|_{P^{r+2},q/2} K_n
\]

\[
+ n^{-2} \left\| (P^{r-2} H)^2 \right\|_{P^{r+2},2} K_n
\]

\[
+ n^{-1} \sup_{h \in \partial \mathcal{H}_c} \left\| (P^{r-2} h)^2 \right\|_{P^{r+2},2} K_n^{3/2} + n^{-3+2/q} \left\| (P^{r-2} H)^2 \right\|_{P^{r+2},q/2}^2 K_n
\]

\[
+ n^{-3/2} \sup_{h \in \partial \mathcal{H}_c} \left\| (P^{r-2} h)^2 \right\|_{P^{r+2},2} K_n^{3/2} + n^{-2+2/q} \left\| (P^{r-2} H)^2 \right\|_{P^{r+2},q/2}^2 K_n
\]

Thus due to the definition of \( \partial \mathcal{H}_c \), (69), (MT-5), and (MT-2),

\[
\mathbb{E} \left| II \right| \leq n^{-3+2/q} D_n^4 K_n^2 + n^{-2+2/q} D_n^6 K_n^3.
\] (75)

By [18, Theorem 5.2], and due to (VC), (69), and (MT-1),

\[
\mathbb{E} \left| III \right| = \mathbb{E} \left[ \sup_{h \in \partial \mathcal{H}_c} n^{-1} \sum_{k=1}^n \left( P^{r-1} h(X_k) \right)^2 \right]
\]

\[
\leq n^{-1/2} N^{-1} K_n^{1/2} + n^{-1+2/q} \left\| (P^{r-1} H)^2 \right\|_{P^{r+2},q/2} K_n \leq n^{-1+2/q} D_n^2 K_n.
\] (76)

Then the proof is complete by Markov inequality, (73), (74), (75), and (76).
Lemma C.8. Let $\epsilon > 1: N + H^2 \|_{P^{2}}^{2}$, and recall the definition of $\Sigma^{(m)}_{n,A}$ in Lemma C.7. Assume the conditions in Lemma C.7 hold. Then there exists a constant $C$, depending only on $r$, such that with probability at least $1 - CN^{-1}$,

$$C^{-1} \max_{m \in [M]} \mathbb{E}[\mathcal{D}_n] \left[ \| U_{n,A}^{\#} \|_{\partial \mathcal{H}_{m,\epsilon}} \right] \leq N^{-1/2} B_n K_n^{1/2} + \left( \max_{m \in [M]} \Sigma^{(m)}_{n,A} \right)^{1/2} K_n^{1/2}.$$

Proof. Define $d_n(h_1, h_2) := \| U_{n,A}^{\#}(h_1) - U_{n,A}^{\#}(h_2) \|_{\psi_2[\mathcal{D}_n]}$ for $m \in [M]$ and $h_1, h_2 \in \partial \mathcal{H}_{m,\epsilon}$. By Cauchy-Schwarz inequality, for $m \in [M]$ and $h_1, h_2 \in \partial \mathcal{H}_{m,\epsilon}$,

$$d_n^2(h_1, h_2) \leq n^{-1} \sum_{i=1}^{n} \left( \mathcal{G}^{(k)}(h_1) - \mathcal{G}^{(k)}(h_2) \right)^2$$

$$\leq n^{-1} \sum_{i=1}^{n} \left( \mathcal{G}^{(k)}(h_1) - \mathcal{G}^{(k)}(h_2) \right)^2$$

$$\leq n^{-1} \sum_{i=1}^{n} \left( \mathcal{G}^{(k)}(h_1) - \mathcal{G}^{(k)}(h_2) \right)^2$$

$$\leq n^{-1} \sum_{i=1}^{n} \left( \mathcal{G}^{(k)}(h_1) - \mathcal{G}^{(k)}(h_2) \right)^2$$

where $\mathcal{G} := n^{-1} \sum_{k=1}^{n} \sum_{i \in I_{k, r-1}}^{k} \delta_{X_{i}(k)}$ is a random measure on $\mathcal{S}$. Since $(\partial \mathcal{H}_{m,\epsilon}, 2H)$ is a VC type class with characteristics $(A, 2\nu)$, we have for $\tau > 0$,

$$N(\partial \mathcal{H}_{m,\epsilon}, d_n(\cdot, \cdot), \| 2H \|_{\mathcal{Q}, 2}) \leq N(\partial \mathcal{H}_{m,\epsilon}, \| \cdot \|_{\mathcal{Q}, 2}, \| 2H \|_{\mathcal{Q}, 2}) \leq (A/\tau)^{2\nu}.$$

By Markov inequality and since $N_2 \leq |I_{n-1, r-1}|$,

$$P(\mathcal{E}') \geq 1 - N_2^{-1},$$

where $\mathcal{E}' := \left\{ \| H \|_{\mathcal{Q}, 2} \leq n^{r-1} \| H \|_{P^{2}} \right\}$.

By entropy integral bound [64, Theorem 2.3.7], if we use $2 \left( N^{-1/2} \| H \|_{P^{2}} \vee (\Sigma^{(m)}_{n,A})^{1/2} \right)$ as a $d_m$- diameter for $\partial \mathcal{H}_{m,\epsilon}$, we have on the event $\mathcal{E}'$, for $m \in [M]$,

$$\mathbb{E}[\mathcal{D}_n] \left[ \| U_{n,A}^{\#} \|_{\partial \mathcal{H}_{m,\epsilon}} \right] \lesssim \int_{0}^{N^{-1/2} || H ||_{P^{2}} \vee (\Sigma^{(m)}_{n,A})^{1/2}} \sqrt{\nu \log (A \| H \|_{\mathcal{Q}, 2}/\tau)} d\tau$$

$$\lesssim \left( N^{-1/2} \| H \|_{P^{2}} \vee (\Sigma^{(m)}_{n,A})^{1/2} \right) \sqrt{\nu \log (A n^{r-1} N^{1/2})}$$

$$\lesssim \left( N^{-1/2} \| H \|_{P^{2}} \vee (\Sigma^{(m)}_{n,A})^{1/2} \right) K_n^{1/2}.$$

Then the proof is complete due to (MT-3).
Appendix D: More simulation results

We present more simulation results in the same setup as in Section 5, except that in Subsection D.2, the distribution of \( \varepsilon \) in (1) has a different distribution than the centered Gaussian.

D.1. A figure about locally convex regression function in (29)

In Figure 2, we plot the regression function \( f \) in (29) with \( c_2 = 0.2, \omega_2 = 0.15 \), together with one realization of dataset with the sample size \( n = 1000 \) and the variance \( \sigma^2 = 0.2^2 \).

![Figure 2: The regression function \( f \) in (29) with a realization of the data points.](image)

D.2. Asymmetric and heavy tailed noise.

The use of \( \mathcal{H}^g \) requires the conditional distribution of \( \varepsilon \) to be symmetric about zero, but otherwise allows \( \varepsilon \) to have a heavy tail. On the other hand, to use \( \mathcal{H}^{id} \), our theory requires \( \varepsilon \) to a light tail, but otherwise imposes no additional restriction. In this subsection, we consider the following two types of error distributions.

Asymmetric distribution. In the first, the distribution of \( \varepsilon \) is a mixture of two Gaussian distributions: \( G_{\varepsilon} := 0.5 \times N(-0.1, 0.06) + 0.5 \times N(0.1, 0.24) \), under which \( \mathbb{P}(\varepsilon < 0) > 0.5 \). Further, if \((\Lambda_1, \ldots, \Lambda_{d+1})\) has a uniform distribution on the simplex \( \{ (v_1, \ldots, v_{d+1}) : \sum_{i=1}^{d+1} v_i = 1, v_i > 0 \} \), and \( \varepsilon_1, \ldots, \varepsilon_{d+2} \) are i.i.d. with common distribution \( G_{\varepsilon} \), then \( \mathbb{P}(S < 0) < 0.5 \), where \( S := \sum_{i=1}^{d+1} \Lambda_i \varepsilon_i - \varepsilon_{d+2} \). The density of \( G_{\varepsilon} \) and the histogram of \( S \) are plotted in Figure 3. In this case, \( \mathcal{H}^g \) fails to achieve the prescribed level as \( \mathbb{P}(\mathcal{H}^g > 0) > \mathbb{P}(\mathcal{H}^{id} > 0) \) for \( v \in \mathcal{H}^{id} \), while \( \mathcal{H}^{id} \) is valid, which agrees with results in Table 8.

Heavy tail distribution. In the second, the distribution of \( \varepsilon \) is \( 0.2/\sqrt{3} \times t_3 \), where \( t_3 \) means standard \( t \) distribution with 3 degree of freedom. From Table 8, \( \mathcal{H}^{id} \) still achieves valid size, but its power is significantly smaller than that of \( \mathcal{H}^g \).

In Figure 4, we plot the probability of rejection for \( \mathcal{H}^g \) under the asymmetric noise \( \varepsilon \sim G_{\varepsilon} \), and \( \mathcal{H}^{id} \) under the heavy tail, when the regression function is linear. As we can see, both tests are slightly undersized, but the approximation by bootstrap is reasonable over all levels, as predicted by our theory.
Testing for regression curvature

Figure 3: The left is the density of $G_\epsilon$, while the right the histogram for $S$.

<table>
<thead>
<tr>
<th>$\kappa_0 = 1$ (size)</th>
<th>HT</th>
<th>Asymm</th>
<th>$\kappa_0 = 1.5$ (alternative)</th>
<th>HT</th>
<th>Asymm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ID</td>
<td>7.4</td>
<td>7.5</td>
<td>ID</td>
<td>60.4</td>
<td>60.3</td>
</tr>
<tr>
<td>SG</td>
<td>9.3</td>
<td>89.3**</td>
<td>SG</td>
<td>80.9</td>
<td>—</td>
</tr>
</tbody>
</table>

Table 8. The rejection probability (in percentage) at level 10% for $d = 2$, $n = 1000$, polynomial $f$ (27), and two types of noise distributions. “HT” is for heavy tail, while “Asymm” for asymmetric. ‘***’ indicates the serious size inflation, and thus the corresponding power is irrelevant (‘—’).

Figure 4: The x axis is prescribed level. The dashed line is $y = x$, and the solid line with crosses is the actual probability of rejection under a linear regression function.

D.3. Size validity - Gaussian noise

In Table 9, 10 and 11, we list the size for different bandwidth $b_0$ and error variance $\sigma^2$ at levels 5% and 10% for $d = 3$ and $d = 4$ (the column with $\kappa_0 = 1$), as well as $d = 2$, $n = 1500$. In Figure 5, we
also show the probability of rejection over all levels ranging from \((0, 1)\). Similar to \(d = 2\), the proposed procedure is consistently on the conservative side.

\[
\begin{array}{cccccc}
  d = 3 & n = 500 & n = 1000 \\
  \sigma = 0.1 & b_n = 0.7 & b_n = 0.65 & b_n = 0.6 & b_n = 0.65 & b_n = 0.6 & b_n = 0.55 \\
  \text{Level 5\%} & 2.5 & 2.3 & 1.8 & 3.2 & 2.8 & 2.5 \\
  \text{Level 10\%} & 6.3 & 4.8 & 3.3 & 7.1 & 7.1 & 5.2 \\
  \sigma = 0.2 & b_n = 0.7 & b_n = 0.65 & b_n = 0.6 & b_n = 0.65 & b_n = 0.6 & b_n = 0.55 \\
  \text{Level 5\%} & 2.9 & 1.4 & 1.2 & 3.5 & 3.8 & 1.8 \\
  \text{Level 10\%} & 6.8 & 4.3 & 4.1 & 7.4 & 8.1 & 5.5 \\
  \end{array}
\]

Table 9. Size validity using \(H_{sg}\) for \(d = 3\) under the Gaussian noise. The sizes are in the unit of percentage.

\[
\begin{array}{cccc}
  \kappa_0 & 1 \ (\text{size}) & 1.2 & 1.5 \\
  \text{Level 5\%} & 3.4 & 23.6 & 83.3 \\
  \text{Level 10\%} & 6.8 & 37.7 & 95.1 \\
  \end{array}
\]

Table 10. The rejection probability using \(H_{sg}\) (in percentage) at level 5\% and 10\% for \(d = 4\), \(n = 2000\), \(b_n = 0.7\), Gaussian noise \(N(0, 0.2^2)\), and polynomial regression function (27). Note that \(\kappa_0 = 1\) corresponds to a linear function.

\[
\begin{array}{cccc}
  d = 2, n = 1500 & \sigma = 0.2 & b_n = 0.45 & b_n = 0.35 \\
  \text{Level 5\%} & b_n = 0.45 & b_n = 0.4 & b_n = 0.35 \\
  \text{ID} & 3.9 & 3.6 & 3.1 & 8.4 & 7.4 & 6.9 \\
  \text{SG} & 4.0 & 3.9 & 2.6 & 7.4 & 8.6 & 7.3 \\
  \end{array}
\]

Table 11. Size validity using \(H_{sg}\) for \(d = 2, n = 1500\) under the Gaussian noise. The sizes are in the unit of percentage.

### D.4. Power - Gaussian Noise

For the polynomial regression functions (27), in Table 12 and 10, we list the power using \(H_{sg}\) for \(d = 3\) and \(d = 4\). In Table 12, the power for locally convex regression functions (29) and \(d = 3\) is also listed.
Testing for regression curvature

Figure 5: The x axis is prescribed level. The dashed line is \( y = x \), and the solid line with crosses is the actual rejection probability using \( H^g \) under a linear regression function and \( \varepsilon \sim N(0, \sigma^2) \).

<table>
<thead>
<tr>
<th>( d = 3 )</th>
<th>Level 5%</th>
<th>Level 10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,2,0.1)</td>
<td>29.7</td>
<td>51.5</td>
</tr>
<tr>
<td>(1,2,0.2)</td>
<td>9.5</td>
<td>22.6</td>
</tr>
<tr>
<td>(1,5,0.1)</td>
<td>91.4</td>
<td>98.5</td>
</tr>
<tr>
<td>(1,5,0.2)</td>
<td>38.7</td>
<td>61.2</td>
</tr>
</tbody>
</table>

(a) Polynomial \( f \) (27) for \( H^g \), varying \( \kappa_0, \sigma \) and \( \varepsilon \sim N(0, \sigma^2) \)

<table>
<thead>
<tr>
<th>( d = 3, n = 1500, b_n = 0.55 )</th>
<th>Level 5%</th>
<th>Level 10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \omega_2 = 0.15 )</td>
<td>12.0</td>
<td>21.0</td>
</tr>
<tr>
<td>( \omega_2 = 0.2 )</td>
<td>35.3</td>
<td>46.5</td>
</tr>
<tr>
<td>( \omega_2 = 0.4 )</td>
<td>64.4</td>
<td>73.9</td>
</tr>
<tr>
<td>( \omega_2 = 0.5 )</td>
<td>79.7</td>
<td>86.6</td>
</tr>
<tr>
<td>( \omega_2 = 0.6 )</td>
<td>89.9</td>
<td>95.0</td>
</tr>
</tbody>
</table>

(b) Locally convex \( f \) (29) for \( H^g \), varying \( (c_2, \omega_2) \), and \( \varepsilon \sim N(0, \sigma^2) \).

Table 12. The rejection probability using \( H^g \) (in percentage) at level 5% and 10% for \( d = 3 \).

D.5. Multiple testing - Gaussian Noise

Another way to combine multiple bandwidths, \( B_n \), is to use Bonferroni correction. Specifically, for each \( b_n \in B_n \), we run separately the proposed test in (21) with a single bandwidth \( b_n \) at level \( \alpha / |B_n| \). Then we reject the null if and only if at least one of the multiple tests does so.

In Table 13, we list its size, as well as power against two alternatives, for \( d = 2, n = 1000, \sigma = 0.5 \) and \( B_n = \{0.6, 0.8, 1\} \). Compared to Table 7, it seems that if \( |B_n| \) is small and one of \( b_n \in B_n \) has power close to one, then this multiple testing approach enjoys reasonable power.

Table 13.
Rejection Probability

<table>
<thead>
<tr>
<th>Description</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polynomial $f (27)$ with $\kappa_0 = 1$ at 10% (size)</td>
<td>7.5</td>
</tr>
<tr>
<td>Polynomial $f (27)$ with $\kappa_0 = 1.5$ at 5% (power)</td>
<td>90.1</td>
</tr>
<tr>
<td>Locally convex $f (29)$ with $\omega_2 = 0.15, c_2 = 0.3$ at 10% (power)</td>
<td>26.4</td>
</tr>
</tbody>
</table>

Table 13. The rejection probabilities of using Bonferroni correction to combine multiple proposed tests corresponding to $b = 0.6, 0.8, 1$ for $d = 2, n = 1000$, and $\sigma = 0.5$.

Appendix E: Proofs and discussions for concavity test

E.1. Proof of Theorem 3.2 - Identity kernel

We will prove Theorem 3.2 for $\mathcal{H}_{\text{id}}$ under the following condition (C6-id), instead of (C6-id'), and apply Theorem 6.1 and 6.2, instead of Theorem 2.3.

(C6-id). Assume that $\sup_{v \in \mathcal{V}_b} |f(v)| \leq C_0$, and that for some $\beta > 0$,

$$\inf_{v \in \mathcal{V}_b} \text{Var}(\varepsilon|V = v) \geq 1/C_0, \quad \sup_{v \in \mathcal{V}_b} \|\varepsilon|\psi_\beta|V = v \leq C_0. \quad (77)$$

**Remark E.1.** Clearly, (C6-id') implies (C6-id), since (C6-id) only requires $\varepsilon$ to have a light tail, instead of being bounded. Further, under the condition (C6-id), in Theorem 3.2, Corollary 3.4 and Corollary 3.5, the constant $C$ may thus depend on $\beta$.

**Proof of Theorem 3.2 under (C6-id) - Identity kernel.** First, let

$$q := \max \left\{ \frac{4r}{\kappa}, \frac{2C_0 + 2 + C_0}{\kappa \wedge \kappa'}, \frac{2 + C_0}{3}, 6 \right\} + 1. \quad (78)$$

By (C2) and (C3), $M \leq nC_0$ and $b_n^{-d/2} \leq C_0n(1-1/C_0)/3 \leq C_0n^{1/3}$. Then due to Theorem 6.1, Theorem 6.2, and the definition of $q$ in (78), it suffices to verify that (MT-1)-(MT-5) holds with above $q$, and

$$D_n := Cb_n^{-d/2}, \quad B_n := Cb_n^{-dr/2}, \quad K_n \leq C\log(n), \quad (79)$$

in addition to (PM), (VC), (MB), and (MT-0).

Due to (C1) and (C6-id), we consider the envelope function(s) $H_n : \mathbb{R}^{(d+1)\times r} \rightarrow \mathbb{R}$ for $\mathcal{H}_{\text{id}}$.

$$H_n(x_1, \ldots, x_r) := \left( 2C_0 + \sum_{i=1}^r |y_i - f(v_i)| \right) C_0^r \times b_n^{-d(r-1/2)} \prod_{1 \leq i < j \leq r} \mathbb{I} \left\{ \frac{|v_i - v_j|}{b_n} \in (-1, 1)^d \right\} \prod_{i=1}^r \mathbb{I} \left\{ v_i \in \mathcal{V}_b \right\}, \quad (80)$$

where for $i \in [r]$, $x_i := (v_i, y_i)$ with $v_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$.
Verify (PM), (VC), (MB), and (MT-0). By [31, Proposition 3.6.12], if \( L(\cdot) \) is of bounded variation (see (C1)), \((H^{\nu}, H_n)\) is a VC type class for some absolute constants \((A, \nu)\), which also implies that \( K_n \leq C_0 \log(n) \). The conditions (PM), (MB), and (MT-0) are satisfied due to (C1), (C2), and (C5) respectively.

Verify the bounds involving \( H_n \) in (MT-1)-(MT-5). Due to (C6-id), for \( q \) in (78) and \( 1 \leq s \leq 4 \), there exists a constant \( C \) depending on \( \beta, C_0, r, \kappa, \kappa' \) such that

\[
E [ |e|^q | V = v ] \leq C, \quad \text{for any } v \in \mathcal{V}^{b_0}, \text{ and } t \leq 4q. \tag{81}
\]

Then for \( 1 \leq s \leq 4 \) and \( 1 \leq \ell \leq r \), due to (C4),

\[
P^{r-\ell} H_n^s \lesssim (1 + \sum_{i=1}^{\ell} |e_i|^s) b_n^{s(d(r-1)/2)} \times \\
\int \prod_{1 \leq i < j \leq r} 1 \left\{ \frac{|v_i - v_j|}{b_n} \in (-1, 1)^d \right\} \prod_{i=1}^{\ell} 1 \{ v_i \in \mathcal{V}^{b_0} \} p(v_i) dv_{\ell+1} \cdots dv_r \\
\lesssim (1 + \sum_{i=1}^{\ell} |e_i|^s) b_n^{-sd(r-1)/2} b_n^{d(r-\ell)} \prod_{1 \leq i < j \leq \ell} 1 \left\{ \frac{|v_i - v_j|}{b_n} \in (-1, 1)^d \right\} \prod_{i=1}^{\ell} 1 \{ v_i \in \mathcal{V}^{b_0} \}.
\]

Now again due to (81) and (C4), for \( 1 \leq s \leq 4 \) and \( 1 \leq \ell \leq r \),

\[
\| P^{r-\ell} H_n^s \|_{P^{\ell,q}} \lesssim b_n^{-sd(r-1)/2} b_n^{d(r-\ell)} b_n^{d(\ell-1)/2} = b_n^{-d(\ell(s-1)+1)} b_n^{d(\ell(s-1)-1)} \\
\| P^{r-\ell} H_n^s \|_{P^{\ell,2}} \lesssim b_n^{-sd(r-1)/2} b_n^{d(r-\ell)} b_n^{d(\ell-1)/2} = b_n^{-d(s-1)+\ell/2} b_n^{d(s-1)-1/2}.
\]

Recall in (79) that \( D_n = Cb_n^{-d/2} \) and \( B_n = Cb_n^{-dr/2} \). Then the bounds involving \( H_n \) in (MT-1)-(MT-5) are verified, except for \( \| (P^{r-2} H) \mathcal{O}^2(x_1, x_2) \|_{P^{2,q}/2} \) in (MT-5), on which we now focus. With \( \ell = 2, s = 1 \), we have

\[
(P^{r-2} H) \mathcal{O}^2(X_1, X_2) \lesssim \\
(1 + |e_1| + |e_2|) b_n^{-2d(r-1)/2} b_n^{2d(r-2)} \left\{ 1 \{ V_1 \in \mathcal{V}^{b_0} \} 1 \{ V_2 \in \mathcal{V}^{b_0} \} \times \\
\int \prod_{1 \leq i < j \leq 2} 1 \left\{ \frac{|v_i - v_j|}{b_n} \in (-1, 1)^d \right\} \left\{ \frac{|v_3 - v_2|}{b_n} \in (-1, 1)^d \right\} \prod_{i=1}^{2} 1 \{ v_i \in \mathcal{V}^{b_0} \} p(v_i) dv_3 \\
\lesssim (1 + |e_1| + |e_2|) b_n^{-2d} \left\{ \frac{|V_1 - V_2|}{b_n} \in (-2, 2)^d \right\} \prod_{i=1}^{2} 1 \{ V_i \in \mathcal{V}^{b_0} \} 1 \{ V_2 \in \mathcal{V}^{b_0} \},
\]

which implies that \( \| (P^{r-2} H) \mathcal{O}^2(x_1, x_2) \|_{P^{2,q}/2} \leq D_n^{4-4q} \).

Verify the upper bounds involving \( \{ h_v^{id} : v \in \mathcal{V} \} \) in (MT-1)-(MT-5). We will write \( h_v^{id} \) for \( h_v^{id} \) to simplify notations. Due to (81), (C4), and (C6-id), for \( 1 \leq s \leq 4 \), \( 0 \leq \ell \leq r \), and \( v \in \mathcal{V} \),

\[
P^{r-\ell} |h_v|^s \lesssim (1 + \sum_{i=1}^{\ell} |e_i|^s) b_n^{-sd(r-1)/2} b_n^{d(r-\ell)} \prod_{i=1}^{\ell} \left( \frac{v - V_i}{b_n} \right)^s,
\]
which implies that for \( q' \in \{2, 3, 4, q \}, \)
\[
\|P^{r-\ell} \{h_v|v| \} P^r \|_{p,q} \lesssim b_n^{d(r-1/2)} b_n^{d(r-\ell)/q'} \lesssim b_n^{-d(r-1)+\ell(1-1/q')-s/2}.
\]

Recall in (79) that \( D_n = C b_n^{-d/2} \) and \( B_n = C b_n^{-dr/2} \). Then the upper bounds involving \( \{h_n^v : v \in V\} \) in (MT-1)-(MT-5) are verified.

**Verify the lower bound in (MT-4).** By definition of \( w(\cdot) \) in (19) and due to (C6-id),
\[
\text{Var}(h_v(X_1^r) \mid V_1^r) = b_n^{-2d(r-1/2)} \prod_{i=1}^r L^2 \left( \frac{v - V_i}{b_n} \right) \times
\sum_{j=1}^r \mathbb{1} \{ V_1^r \in S_j \} \mathbb{E} \left[ \left( \sum_{i \in [r] \setminus \{j\}} \tau_i^{(j)} (v_r^i) \varepsilon_i - \varepsilon_j \right)^2 \mid V_1^r \right]
\geq \frac{1}{C_0} b_n^{-2d(r-1/2)} \prod_{i=1}^r L^2 \left( \frac{v - V_i}{b_n} \right) \mathbb{1} \{ V_1^r \in S \}.
\]

Then for \( v \in V \), due to (C4) and \( \{(v_1, \ldots, v_r) \in S \} = \{(\frac{v,v_1}{b_n}, \ldots, \frac{v,v_r}{b_n}) \in S \} \), we have
\[
\text{Var}(h_v(X_1^r)) \geq \mathbb{E} \left[ \text{Var}(h_v(X_1^r) | V_1^r) \right]
\geq \frac{1}{C_0} b_n^{-2d(r-1/2)} b_n^{dr} \int \prod_{i=1}^r L^2 (u_i) \mathbb{1} \{ u_1^r \in S \} \prod_{i=1}^r p(v - b_n u_i) du_1 \ldots du_r
\geq \frac{1}{C_0^{-1} + d} \int \prod_{i=1}^r L^2 (u_i) \mathbb{1} \{ u_1^r \in S \} du_1 \ldots du_r,
\]
which verifies the lower bound in (MT-4) due to (C1) and the definitions of \( B_n, D_n \) in (79).

---

**E.2. Proof of Theorem 3.2 - Sign kernel**

We will prove Theorem 3.2 for \( \mathcal{H}_{\mathbb{R}} \) under the following condition (C6-sg), instead of (C6-sg').

(C6-sg). Assume that \( |f(v) - f(v')| \leq 1/C_0 \) for \( v, v' \in \mathbb{V}^{b_n} \) such that \( \|v - v'\|_\infty \leq 1/C_0; |b_n| \leq 1/C_0 \) for \( n \geq C_0 \); for each \( v \in \mathbb{V}^{b_n} \), conditional on \( V = v, \varepsilon \) has a symmetric distribution, i.e., \( \mathbb{P}(\varepsilon > t | V = v) = \mathbb{P}(\varepsilon < -t | V = v) \) for any \( t > 0 \), and that
\[
\inf_{v \in \mathbb{V}^{b_n}} \mathbb{P}(|\varepsilon| \geq C_0^{-1} | V = v) \geq C_0^{-1}.
\]

**Remark E.2.** Although (C6-sg') does not implies (C6-sg), the only difference is in the proof of Lemma E.3, which follows from similar but simpler arguments if we work with the condition (C6-sg').
Proof of Theorem 3.2 under (C6-sg) - Sign kernel. Now we focus on the class $\mathcal{H}^g$ and apply Theorem 2.3. Due to (C1), we consider the envelope function(s) $H_n : \mathbb{R}^{(d+1) \times r} \to \mathbb{R}$ for $\mathcal{H}^g$:

$$H_n(x_1, \ldots, x_r) := C_0 b_n^{-d(r-1)/2} \prod_{1 \leq i < j \leq r} \mathbb{1}\left\{ \frac{|v_i - v_j|}{b_n} \in (-1, 1)^d \right\} \prod_{i=1}^r \mathbb{1}\{ v_i \in V_{b_n} \},$$

where for $i \in [r]$, $x_i := (v_i, y_i)$ with $v_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$. The other conditions in Theorem 2.3, except for the lower bound in (MT-4) (about $\text{Var}(h(X_1^r))$), can be verified in the same way as for $\mathcal{H}^d$ (see Subsection E.1) with $D_n = Cb_n^{-d/2}$; since $H_n$ and $\{h_v^g : v \in \mathcal{V}\}$ are bounded, the arguments are simpler, and thus omitted. Now we focus on verifying the lower bound in (MT-4), and we will write $h_v$ for $h_v^g$ to simplify notations.

By Lemma E.3 (ahead), there exists a constant $C$ only depending on $C_0$ such that for any $(u_1, \ldots, u_r) \in (-1/2, 1/2)^r \cap S$ and $v \in \mathcal{V}$,

$$\text{Var}(w(X_1, \ldots, X_r) \mid V_1 = v - b_n u_1, \ldots, V_r = v - b_n u_r) \geq C^{-1}.$$ 

By definition of $w(\cdot)$ in (19),

$$\text{Var}(h_v(X_1^r)) = b_n^{-2d(r-1)/2} \prod_{i=1}^r L^2 \left( \frac{v - V_i}{b_n} \right) \text{Var}(w(X_1, \ldots, X_r) \mid V_1^r)$$

Thus due to (C6-sg), we have

$$\text{Var}(h_v(X_1^r)) \geq \mathbb{E}[\text{Var}(h_v(X_1^r)|V_1^r)] = b_n^{-2d(r-1)/2} b_n^{dr} \times \int \left( \prod_{i=1}^r L^2(u_i) p(v - b_n u_i) \right) \text{Var}(w(X_1, \ldots, X_r) \mid V_i = v - b_n u_i \text{ for } i \in [r] ) \, du_1 \ldots du_r$$

$$\geq C_0^{-r} b_n^{-dr+d} C^{-1} \int \left( \prod_{i=1}^r L^2(u_i) \right) \mathbb{1}\{ u_1^r \in S \} \, du_1 \ldots du_r,$$

which verifies the lower bound in (MT-4) due to (C1).

Lemma E.3. Assume (C6-sg) holds. There exists a constant $C$ only depending on $C_0$ such that for any $(u_1, \ldots, u_r) \in (-1/2, 1/2)^r \cap S$ and $v \in \mathcal{V}$,

$$\text{Var} \left( \text{sign} \left( \sum_{i=1}^{r-1} \tau_i^{(r)} (u_i^r) Y_i - Y_r \right) \right) \mid V_1 = v - b_n u_1, \ldots, V_r = v - b_n u_r \geq C^{-1}.$$

Proof. Fix any $v \in \mathcal{V}$ and $(u_1, \ldots, u_r) \in (-1/2, 1/2)^r \cap S$. Note that

$$\text{Var} \left( \text{sign} \left( \sum_{i=1}^{r-1} \tau_i^{(r)} (u_i^r) Y_i - Y_r \right) \bigg| V_k = v - b_n u_k, \text{ for } k \in [r] \right)$$

$$= 1 - \left( 2^p \left( \sum_{i=1}^{r-1} \tau_i^{(r)} (u_i^r) Y_i - Y_r > 0 \right) \bigg| V_k = v - b_n u_k, \text{ for } k \in [r] \right) - 1 \right)^2.$$
Since $Y_i = f(v - b_n u_i) + \varepsilon_i$ for $i \in [r]$, due to (C6-sg), for $n \geq C_0$,
\[
    P\left( \sum_{i=1}^{r-1} \tau_i^{(r)}(u_i^r) Y_i - Y_r > 0 \ \mid \ V_k = v - b_n u_k, \ for \ k \in [r] \right) 
\]
\[
    \leq P\left( \sum_{i=1}^{r-1} \tau_i^{(r)}(u_i^r) \varepsilon_i - \varepsilon_r > -1/C_0 \ \mid \ V_k = v - b_n u_k, \ for \ k \in [r] \right) 
\]
\[
    = 1 - P\left( \sum_{i=1}^{r-1} \tau_i^{(r)}(u_i^r) \varepsilon_i - \varepsilon_r \leq -1/C_0 \ \mid \ V_k = v - b_n u_k, \ for \ k \in [r] \right) 
\]
\[
    \leq 1 - \left( \prod_{i=1}^{r-1} P(\varepsilon_i \leq 0 | V_i = v - b_n u_i) \right) P(\varepsilon_r \geq 1/C_0 | V_r = v - b_n u_r) \leq 1 - \frac{1}{2^{r/C_0}}. 
\]

By a similar argument, $P\left( \sum_{i=1}^{r-1} \tau_i^{(r)}(u_i^r) Y_i - Y_r > 0 \ \mid \ V_k = v - b_n u_k, \ for \ k \in [r] \right) \geq \frac{1}{2^{r/C_0}}$. Then the proof is complete.

**E.3. Proofs related to the power of the proposed concavity test**

**Proof of Corollary 3.5.** By Theorem 6.2 (the conditions have been verified in the proof of Theorem 3.2), with probability at least $1 - Cn^{-1/C}$,
\[
P_{D_n} \left( \widetilde{M}_n \geq q^\#_\alpha \right) > \alpha - Cn^{-1/C}.
\]

In the proof of Theorem 3.2, we have shown that
\[
    \sup_{v \in \mathcal{V}} \left\{ r^2 \gamma_A(h^*_v) + \alpha_n \gamma_B(h^*_v) \right\} \leq C \alpha_n b_n^{-d \gamma + d} = C + Cn^{1-\kappa} b_n^d.
\]

(83)

Then due to Lemma C.3,
\[
P \left( q^\#_\alpha \geq C K_n^{1/2} (1 + n^{1-\kappa}/b_n^d) \right) \leq Cn^{-1/C}.
\]

(84)

Observe that
\[
P \left( \sup_{v \in \mathcal{V}} \sqrt{n} U_{n,N}(h^*_v) \geq q^\#_\alpha \right) \geq P \left( \sqrt{n} \left( U_{n,N}^*(h_{v_n}^*) - P^* h_{v_n}^* \right) \geq q^\#_\alpha - \sqrt{n} P^* h_{v_n}^* \right).
\]

By Theorem B.1 with $d = 1$ (the conditions have been verified in the proof of Theorem 3.2), we have
\[
P \left( \sup_{v \in \mathcal{V}} \sqrt{n} U_{n,N}(h^*_v) \geq q^\#_\alpha \right) \geq P \left( Y \geq q^\#_\alpha - \sqrt{n} P^* h_{v_n}^* \right) - Cn^{-1/C},
\]

where $Y \sim N(0, r^2 \gamma_A(h_{v_n}^*) + \alpha_n \gamma_B(h_{v_n}^*))$ and is independent of $D_n'$. Then due to (83) and (84), and $\kappa'' > (1-\kappa)/2$, we have with probability at least $1 - Cn^{-1/C}$,
\[
    \frac{\sqrt{n} P^* h_{v_n}^* - q^\#_\alpha}{\sqrt{\text{Var}(Y)}} \geq C^{-1} n^{1/2},
\]
By Taylor’s Theorem, if

\[ P^r_{h_{v_0}} = b_n^{d/2} \int \left( \sum_{j=1}^{r} \left( \sum_{i \in [r] \setminus \{j\}} \tau_i^{(j)} (u_i^r) f(v_0 - b_n u_i) - f(v_0 - b_n u_j) \right) 1 \{ u_i^r \in S_j \} \right) \prod_{i=1}^{r} L(u_i) p(v - b_n u_i) du_1 \ldots du_r, \]

(85)

By Taylor’s Theorem, if \( \|u\|_\infty < 1/2 \),

\[ f(v_0 - b_n u) = f(v_0) - b_n \nabla f(v_0) u + \frac{b_n^2}{2} u^T \nabla^2 f(v_0) u + R(u, b_n), \]

where \( \nabla f(v_0) \) and \( \nabla^2 f(v_0) \) are the gradient and the Hessian matrix of \( f \) at \( v_0 \) respectively, and

\[ |R(u, b_n)| \leq C b_n^2 R(b_n), \]

where \( R(b_n) := \max_{\|\xi\|_\infty \leq b_n/2} \|\nabla^2 f(v_0) - \nabla^2 f(v_0 - \xi)\|_{\text{op}}, \]

with \( \|\cdot\|_{\text{op}} \) being the operator norm of a matrix. As a result, due to (C1) and (C4),

\[ P^r_{h_{v_0}} \geq \left( C^{-1} b_n^{2+d/2} \int \left( \sum_{j=1}^{r} \left( \sum_{i \in [r] \setminus \{j\}} \tau_i^{(j)} (u_i^r) u_i^T \nabla^2 f(v_0) u_i - u_j^T \nabla^2 f(v_0) u_j \right) 1 \{ u_i^r \in S_j \} \right) \prod_{i=1}^{r} L(u_i) du_1 \ldots du_r \right)^{-1} - C b_n^{2+d/2} R(b_n). \]

Since \( f \) is twice continuously differentiable at \( v_0 \) and \( \nabla^2 f(v_0) \) is positive definite, we have \( R(b_n) \to 0 \) as \( b_n \to 0 \), and \( \lim \inf_{n \to \infty} P^r_{h_{v_0}} / \left( b_n^{2+d/2} \right) > 0. \)

**Proof of Corollary 3.9.** Since \( f_n \) is a convex function, due to the condition (C4) and in view of (85), we have \( P^r_{h_{v_n}} \) is lower bounded by

\[ C_0^{-1} b_n^{d/2} \int \left( \sum_{j=1}^{r} \left( \sum_{i \in [r] \setminus \{j\}} \tau_i^{(j)} (u_i^r) f_n(v_n - b_n u_i) - f_n(v_n - b_n u_j) \right) 1 \{ u_i^r \in S_j \} \right) \prod_{i=1}^{r} L(u_i) du_i. \]

Now for \( i \in [r] \), since \( f_{n,1}(v_n) = f_{n,2}(v_n) \), we have

\[ f_n(v_n - b_n u_i) = f_n(v_n) - b_n g_n(u_i) + b_n \| \theta_{n,1} - \theta_{n,2} \|_2 h_n(u_i), \]

where \( g_n(u) := \theta_{n,1}^T u \) and \( h_n(u) := \max \{ 0, (\theta_{n,1} - \theta_{n,2})^T u / \| \theta_{n,1} - \theta_{n,2} \|_2 \}. \)
Since \( g_n \) is linear, we have

\[
P^r h_{v_n}^\text{id} \geq C_0^{-1} \theta_n^{1+d/2} \| \theta_{n,1} - \theta_{n,2} \|_2 \sum_{j=1}^r \left( \sum_{i \in [r] \setminus \{j\}} \tau_j^{(j)}(u_i^r) h_n(u_i) - h_n(u_j) \right) 1 \{ u_1^r \in \mathcal{S}_j \} \prod_{i=1}^r L(u_i) du_i.
\]

Now pick an arbitrary \( \theta_* \in \mathbb{R}^d \) such that \( \| \theta_* \|_2 = 1 \), and define \( h_*(u) = \max \{ 0, \theta^T u \} \). Then due to rotation invariance,

\[
P^r h_{v_n}^\text{id} \geq C_0^{-1} \theta_n^{1+d/2} \| \theta_{n,1} - \theta_{n,2} \|_2 \sum_{j=1}^r \left( \sum_{i \in [r] \setminus \{j\}} \tau_j^{(j)}(u_i^r) h_*(u_i) - h_*(u_j) \right) 1 \{ u_1^r \in \mathcal{S}_j \} \prod_{i=1}^r L(u_i) du_i,
\]

which completes the proof as the integral does not depend on \( n \).

\[\square\]

### E.4. \( L_2 \) minimax separation rate and the FS test

We follow the definition of \( L_2 \) minimax separation rate in [44]. We will ignore logarithmic factors in describing rates.

First, consider the univariate case, i.e., \( d = 1 \). Denote \( C \) the collection of concave functions on \( S = [0, 1] \), and \( S_s \) the collection of Hölder continuous functions with smoothness parameter \( s \) (see [44] for precise definitions). For any \( f \in S_s \), define

\[
\Phi_2(f) = \inf \{ \| f - g \|_2 : g \in C \cap S_s \}, \quad \text{where} \quad \| h \|_2^2 := \int_0^1 |h(x)|^2 dx.
\]

Fix some \( p \in (0, 1/8) \). Define the \( L_2 \) minimax separation rate \( \mathcal{R}_n^* \) to be the smallest \( \epsilon > 0 \) such that there exists a test \( T \) for which

\[
\sup_{f \in C \cap S_s} P_f(T \text{ rejects } H_0) + \sup_{f \in S_s, \Phi_2(f) \geq \epsilon} P_f(T \text{ accepts } H_0) \leq p.
\]

In [44], which considers the Gaussian white noise model, it is shown that if \( s \geq 2 \), then \( \mathcal{R}_n^* = C n^{-s/(2s+1)} \), which is of the same order as the minimax rate of estimating \( f \in S_s \) itself. If \( s < 2 \), based on the remark following [44][Theorem 1], \( \mathcal{R}_n^* = C n^{-(2/5) \wedge (2s/(4s+1))} \). Specifically, for \( f \in S_s \), denote \( f^* \) the projection of \( f \) onto \( C \), i.e. \( f^* \in C \cap S_s \) such that \( \Phi_2(f) = \| f - f^* \|_2 = \| f \|_2 - \| f^* \|_2 \); here, \( \| f \|_2 \) can be estimated at the rate of \( n^{-2s/(4s+1)} \) [51], and \( \| f^* \|_2 \) at the rate of \( n^{-2/5} \) [52][Corollary 4.2] (see also [34][Theorem 6.1]).

For \( d \geq 2 \), to the best of our knowledge, the minimax separation rate is not known in the literature. In view of the results for \( d = 1 \), for smooth functions (say Hölder continuous with smoothness parameter \( s \geq 2 \) [4][Section 3.1]), it is reasonable to conjecture that \( \mathcal{R}_n^* = C n^{-s/(2s+d)} \), the minimax rate of estimating \( f \) itself. For \( s < 2 \), although an upper bound on the rate of recovering \( \| f^* \|_2 \) is established
recently in [52][Corollary 4.2] for $d \geq 2$, the rate of estimating $\|f\|_2$ seems unknown for $d \geq 2$.

FS test [27]. [27] proposes a projection framework for testing shape restrictions including concavity. Specifically, [27] proposes to first estimate the regression function $f$ by *unconstrained, nonparametric* methods, say, by sieved B-splines, and then evaluate and calibrate the $L^2$ distance between the estimator and the space of concave functions.

Denote $k_n$ the number of B-spline terms of order $s_0$ used to estimate $f$ without constraint [27]. There are two important components in the FS test [27]: under-smoothing and strong approximation. For Hölder continuous functions with smoothness parameter $s$, under-smoothing requires that $k_n \gg n^{d/(2(s\wedge s_0)+d)}$, while the strong approximation requires $k_n \ll n^{-1/5}$ [4][Theorem 4.4] (see also [19][Example 5]).

Thus if $s \wedge s_0 \leq 2d$, then there is no choice of $k_n$ that can simultaneously meet these two requirements. In particular, if $d = 2$, it requires the smoothness parameter $s > 4$ and the order of B-splines $s_0 > 4$. This explains why the FS test fails to control the size properly for concave, piecewise affine functions in Section 5.

On the other hand, if $s \wedge s_0 > 2d$ and the under-smoothing is moderate (say by a logarithmic amount), then the FS test achieves the separation rate $n^{-s/(2s+d)}$ [27][Theorem 3.2] (ignoring logarithmic factors), which is minimax for smooth functions for $d = 1$ and may be minimax for $d \geq 2$ as discussed above.

E.5. An algorithm without stratification

In this section, we present an algorithm to compute the test statistics $U'_{n,N}(h^{(s)}_v)$ over $\mathcal{Y}_n$ without stratification. It has a similar computational complexity as Algorithm 1 in theory with $d$ fixed, but it is not computationally feasible since the multiplicative constant is of order $2^{dr}$. We adopt the notations in Section 3.

Without partitioning, there is a single sampling plan $\{Z_i : i \in I_{n,r}\}$. The key insight is that for $i \in I_{n,r}$ and $v \in \mathcal{Y}_n$,

$$h_v(X_i) = 0, \text{ if } V_j \not\in \mathcal{N}(V_{j'}, 2b_n) \text{ for some } j, j' \in i.$$ 

As a result, it suffices to focus on those $r$-tuples such that their feature vectors are within $2b_n$-neighbourhood of each other (in $\|\cdot\|_\infty$).

The pseudocode is listed in Algorithm 2, whose computational complexity is

$$n \approx \left( \frac{n(2b_n)^d}{r-1} \right) n^s b_n^{-(dr)} \log(n) \cdot |\mathcal{Y}_n| k_n^d \lesssim 2^{dr} |\mathcal{Y}_n| n^s \log(n) b_n.$$

The factor $2^{dr}$ is due to the fact that we need to focus on a $2b_n$-neighbourhood, instead of a $b_n$-neighbourhood as in Algorithm 1.
Input: Observations \( \{ X_i = (V_i, Y_i) \in \mathbb{R}^{d+1} : i \in \{ n \} \} \), budget \( N \), kernel \( L(\cdot) \), bandwidth \( b_n \), query points \( \mathcal{V}_n \).

Output: \( U'_{n,N} \) a list of length \( |\mathcal{V}_n| \)

**Initialization:** \( p_n = N / \binom{n}{r} \), \( \tilde{N} = 0 \), \( U'_{n,N} \) set zero;

1. Compute \( A \), a length \( n \) list, where \( A[i] = \{ j > i : V_j \in \mathcal{N}(V_i, 2b_n) \} \) for \( i \in \{ n \} \);
2. Compute \( B \), a length \( n \) list, where \( B[i] = \{ v \in \mathcal{V}_n : v \in \mathcal{N}(V_i, b_n) \} \) for \( i \in \{ n \} \);
3. for \( i \leftarrow 1 \) to \( n \) do
   4. Generate \( T_1 \sim \text{Binomial}(\frac{|A[i]|}{r-1}, p_n) \), \( T_2 \sim \text{Binomial}(\frac{n-i}{r-1} - \frac{|A[i]|}{r-1}, p_n) \);
   5. Compute \( \tilde{N} \leftarrow \tilde{N} + T_1 + T_2 \);
6. Sample \( T_1 \) terms \( \{ i'_{\ell} : 1 \leq \ell \leq T_1 \} \) without replacement from \( \{ (s_1, \ldots, s_{r-1}) : s_j \in A[i] \text{ for each } j \in [r-1] \} \):
   7. for \( \ell \leftarrow 1 \) to \( T_1 \) do
   8. for \( v \in B[i] \) do
   9. \( U'_{n,N}[v] \leftarrow U'_{n,N}[v] + h^*_v(X_{i'}) \);
   10. end
11. end
12. end
13. \( U'_{n,N} \leftarrow U'_{n,N} / \tilde{N} \) /* Operations are element-wise */

Algorithm 2: Algorithm to compute \( U'_{n,N} \) for the concavity test without partitioning.