ISOTONIC REGRESSION IN MULTI-DIMENSIONAL SPACES AND GRAPHS

BY HANG DENG, AND CUN-HUI ZHANG

Department of Statistics, Rutger University

In this paper we study minimax and adaptation rates in general isotonic regression. For uniform deterministic and random designs in $[0,1]^d$ with $d \geq 2$ and $N(0,1)$ noise, the minimax rate for the $\ell_2$ risk is known to be bounded from below by $n^{-1/d}$ when the unknown mean function $f$ is non-decreasing and its range is bounded by a constant, while the least squares estimator (LSE) is known to nearly achieve the minimax rate up to a factor $(\log n)^\gamma$ where $n$ is the sample size, $\gamma = 4$ in the lattice design and $\gamma = \max\{9/2, (d^2 + d + 1)/2\}$ in the random design. Moreover, the LSE is known to achieve the adaptation rate $(K/n)^{1 - \log(n/K)/d}$ when $f$ is piecewise constant on $K$ hyper-rectangles in a partition of $[0,1]^d$.

Due to the minimax theorem, the LSE is identical on every design point to both the max-min and min-max estimators over all upper and lower sets containing the design point. This motivates our consideration of estimators which lie in-between the max-min and min-max estimators over possibly smaller classes of upper and lower sets, including a subclass of block estimators. Under a $q$-th moment condition on the noise, we develop $\ell_q$ risk bounds for such general estimators for isotonic regression on graphs. For uniform deterministic and random designs in $[0,1]^d$ with $d \geq 3$, our $\ell_2$ risk bound for the block estimator matches the minimax rate $n^{-1/d}$ when the range of $f$ is bounded and achieves the near parametric adaptation rate $(K/n)^{1 - \log(n/K)/d}$ when $f$ is $K$-piecewise constant. Furthermore, the block estimator possesses the following oracle property in variable selection: When $f$ depends on only a subset $S$ of variables, the $\ell_2$ risk of the block estimator automatically achieves up to a poly-logarithmic factor the minimax rate based on the oracular knowledge of $S$.

Keywords: Isotonic regression, multiple isotonic regression, isotonic regression on graphs, max-min estimator, min-max estimator, block estimator, lattice design, random design, minimax rate, adaptive estimation, variable selection, oracle property.

1. Introduction. Let $G = (V, E)$ be a directed graph with vertex set $V$ and edge set $E$. For $a$ and $b$ in $V$, we say that $a$ is a descendant of $b$ if $E$ contains a chain of edges from $v_j$ to $v_{j+1}$ such that $b = v_0$ and $a = v_m$ for some finite $m \geq 0$. We write $a \preceq b$ if $a = b$ or $a$ is a descendant of $b$. A function $f : V \to \mathbb{R}$ is non-decreasing on the graph $G$ if $f(a) \leq f(b)$ whenever $a \preceq b$. Let $\mathcal{F}$ be the class of all non-decreasing functions on $G$. In isotonic regression, we observe $x_i \in V$ and $y_i \in \mathbb{R}$ satisfying

$$ y_i = f(x_i) + \varepsilon_i, \quad i = 1, \ldots, n, \text{ for some } f \in \mathcal{F}, $$

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where \( \varepsilon_1, \ldots, \varepsilon_n \) are independent noise variables with \( \mathbb{E} \varepsilon_i = 0 \) and \( \text{Var}(\varepsilon_i) \leq \sigma^2 \) given the (deterministic or random) design points \( \{x_i\} \). Note that we allow \( |V| > n \).

An interesting special case of (1) is the multiple isotonic regression where \( V \subset \mathbb{R}^d \) is a subset of a certain Euclidean space of dimension \( d \), and for \( a = (a_1, \ldots, a_d)^T \in \mathbb{R}^d \) and \( b = (b_1, \ldots, b_d)^T \in \mathbb{R}^d \), \( a \preceq b \) iff \( a_j \leq b_j \) for all \( 1 \leq j \leq d \). In this case, \( \mathcal{F} \) is the class of all non-decreasing functions on \( V \).

Let \( f_n = (f(x_1), \ldots, f(x_n))^T \) and \( \hat{f}_n = (\hat{f}_n(x_1), \ldots, \hat{f}_n(x_n))^T \) for any estimator \( \hat{f}_n \) of \( f \).

We are interested in the estimation of \( f \) under the (normalized) \( \ell_q \) risk

\[
R_q(f_n, f) = \frac{1}{n} \mathbb{E} \left\| \hat{f}_n - f \right\|_q^q = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left| \hat{f}_n(x_i) - f(x_i) \right|^q.
\]

In this case, a specification of \( \hat{f}_n \) is sufficient for the definition of \( \hat{f}_n \). For multiple isotonic regression with random design in \( V \subset \mathbb{R}^d \), we are also interested in the \( L_q \) risk

\[
R_q^*(\hat{f}_n, f) = \mathbb{E} \left\| \hat{f}_n - f \right\|_{L_q(V)}^q = \mathbb{E} \int_V \left| \hat{f}_n(x) - f(x) \right|^q dx.
\]

The literature of univariate isotonic regression \((d = 1)\) encompasses at least the past six decades; See for example Brunk (1955), Ayer et al. (1955), Grenander (1956), Rao (1969), Groeneboom (1984), van de Geer (1990, 1993), Donoho (1990), Birgé and Massart (1993), Woodroofe and Sun (1993), Wang and Chen (1996), Durot (2007), Durot (2008), and Yang and Barber (2017) among many others for some key developments. The least squares estimator (LSE), say \( \hat{f}_n^{lse} \), has been the focus of this literature. We describe in some detail here existing results on minimax and adaptation rates as they are directly related to our study. For any \( a < b \), the \( \ell_q \) risk of the LSE in the interval \([a, b]\) is bounded by

\[
\mathbb{E} \sum_{a \leq x_i \leq b} \left| \hat{f}_n^{lse}(x_i) - f(x_i) \right|^q \leq C_q \sigma^q \left\{ n_{a,b} \left( \frac{\Delta_{a,b}(f_n/\sigma)}{n_{a,b}} \wedge 1 \right) + \sum_{j=1}^{n_{a,b}} j^{-q/2} \right\},
\]

where \( \Delta_{a,b}(f_n/\sigma) = \max_{a \leq x_i, x_j \leq b} \{ f(x_j) - f(x_i) \} / \sigma \) is the range-to-noise ratio for the mean vector \( f_n \) in \([a, b]\), \( n_{a,b} = \#\{ j : a \leq x_j \leq b \} \) is the number of design points in the interval, and \( C_q \) is a constant depending on \( q \) only. This result can be found in Meyer and Woodroofe (2000) for \( n_{a,b} = n, q = 2 \) and \( \varepsilon_i \sim N(0, \sigma^2) \), and in Zhang (2002) for general \( a < b \) and \( 1 \leq q < 3 \) under a \((q \vee 2)\)-th moment condition on \( \varepsilon_i \). For \( \Delta_{-\infty,\infty}(f_n/\sigma) \leq \Delta^*_a \times 1, (4) \) yields the cube-root rate \( \sigma^q(\Delta^*_a/n)^{q/3} \) for the LSE in terms of the \( \ell_q \) risk in (2). By summing over the risk bound (4) over \( K \) intervals \([a_k, b_k]\) with \( \Delta_{a_k,b_k}(f_n/\sigma) = 0 \), the LSE can be seen to achieve the near parametric adaptation rate \((K/n)^{1 \vee \log(n/K)} \) in the mean squared risk when the unknown \( f \) is piecewise constant on the \( K \) intervals and \( x_i \in \bigcup_{k=1}^{K} [a_k, b_k] \) for all \( i \leq n \). This adaptation rate was explicitly given in Chatterjee et al. (2015). However, Gao et al. (2017) proved that the sharp adaptation rate in the mean squared risk, achieved by a penalized LSE, is \((K/n) \log \log(16n/K) \) in the piecewise
constant case. Moreover, by summing over the risk bound (4) over a growing number of disjoint intervals, the LSE has been shown to converge faster than the cube root rate when the measure \( f(dx) \) is singular to the Lebesgue measure (Zhang, 2002).

Compared with the rich literature on univariate isotonic regression, our understanding of the multiple isotonic regression, i.e. \( V \subset \mathbb{R}^d \) with \( d > 1 \), is quite limited. A major difficulty is that the design points are typically only partially ordered. Univariate risk bounds can be directly applied to linearly ordered paths in \( V \), but this typically does not yield a nearly minimax rate. However, significant advances have been made recently on the minimax and adaptation rates for the LSE. For \( n_1 \times \cdots \times n_d \) lattice designs with \( n = \prod_{j=1}^d n_j \), the LSE provides

\[
R_2(\hat{f}^{(lse)}_n, f_n) \leq C_d \sigma^2 \left\{ \Delta(f_n/\sigma)n^{-1/d}(\log n)^\gamma + n^{-2/d}(\log n)^{2\gamma} \right\}
\]

in certain settings, where \( \Delta(f_n/\sigma) = \max_{1 \leq i < j \leq n} |f(x_i) - f(x_j)|/\sigma \) is the range-to-noise ratio of the mean over the design points. For Gaussian \( \varepsilon_i \) and \( n_1 = \cdots = n_d \), the minimax rate is bounded from below by

\[
\inf_{\hat{f}_n} \sup_{\Delta(f_n/\sigma) \leq \Delta_n^*} R_2(\hat{f}_n, f_n) \geq \sigma^2 \min \left\{ 1, C_0 n^{-1/d} \Delta_n^* \right\}.
\]

Moreover, when \( f \) is piecewise constant on \( K \) hyper-rectangles in a partition of the lattice,

\[
R_2(\hat{f}^{(lse)}_n, f_n) \leq C_d \sigma^2 (K/n)^{2/d} \{ 1 \vee \log(n/K) \}^{2\gamma}.
\]

For \( d = 2 \) and Gaussian noise, Chatterjee et al. (2018) proved the above mean squared risk bounds with \( \gamma = 4 \). Thus, up to a logarithmic factor, the LSE is nearly rate minimax for a wide range of \( \Delta_n^* \) and also nearly adaptive to the parametric rate \( \sigma^2 K/n \) when \( f \) is piecewise constant on \( K \) rectangles. Han et al. (2017) extended the results of Chatterjee et al. (2018) from \( d = 2 \) to \( d > 2 \) under the conditions \( n_1 = \cdots = n_d \) and \( \Delta(f_n/\sigma) \leq \Delta_n^* = 1 \) in (5) and (6), and also proved parallel results for random designs with a larger \( \gamma = \max \{ 9/2, (d^2 + d + 1)/2 \} \). However, there is still a gap of a poly-logarithmic factor between such upper and lower minimax bounds for \( d \geq 2 \), and it is still unclear from (7) the feasibility of near adaptation to the parametric rate \( \sigma^2 K/n \) for \( d \geq 3 \) when \( f \) is piecewise constant on \( K \) hyper-rectangles.

We have also seen some progresses in adaptive estimation to variable selection in isotonic regression on lattices with \( \max_{j \leq d} n_j \leq C_d n^{1/d} \). When the unknown mean function depends on only a known subset of \( s \) variables, say \( f(x) = f_S(x_S) \) where \( x_S = (x_j, j \in S)^T \) with \( |S| = s \), one may use the LSE, say \( \hat{f}^{(lse)}_{n,S} \), based on the average of \( y_i \) given \( x_S \) to attain

\[
R_2(\hat{f}^{(lse)}_{n,S}, f_n) \leq \begin{cases} 
C_d \sigma_S^2 \left\{ \Delta(f_n/\sigma_S)n^{-1/d}(\log n)^\gamma + n^{-2/d}(\log n)^{2\gamma} \right\}, & s \geq 2, \\
C_d \sigma_S^2 \{ (\Delta(f_n/\sigma_S)n^{-1/d}) \wedge 1 \}^{2/3} + n^{-1/d}(\log n), & s = 1,
\end{cases}
\]

with \( \sigma_S^2 = \sigma^2 / \prod_{j \notin S} n_j \leq C_d \sigma^2 / n^{1-s/d} \), which would match the minimax rate for Gaussian \( \varepsilon_i \) for a proper range of \( \Delta(f_n/\sigma_S) \) as we discussed in the previous paragraph. For unknown \( S \) with
\(d \geq 2\) and \(\Delta(f_n/\sigma) \leq 1 = \sigma\). Han et al. (2017) proved that the LSE \(\hat{f}^{\text{lse}}_n\) for the general \(f\) automatically achieves the rate \(n^{-4/(3d)}(\log n)^{16/3}\) for \(d = 2\) and \(n^{-2/d}(\log n)^{8}\) for \(d = 2\). As \(\Delta(f_n/\sigma) \leq n^{(d-s)/(2d)}\) in their setting, \((8)\) would yield the rates \(n^{-(d-s)/(2d) - 1/d}\) for \(s \geq 2\) and \(n^{-(d-1)/d - (3-d) + (3d)}\) for \(s = 1\) up to a logarithmic factor. These oracle minimax rates nearly match the adaptation rates in Han et al. (2017) for \(d = 2\) or \((d, s) = (2, 1)\), but not for other configurations of \((d, s)\).

We consider isotonic regression on directed graphs, i.e. with general domain \(V\) in \((1)\), including \(V \subset \mathbb{R}^d\) as a special case. In this general setting, Robertson et al. (1988) proved the following minimax formula for the LSE on the design points:

\[
\hat{f}^{\text{lse}}_n(x) = \max_{U \ni x} \min_{L \ni x} \bar{y}_U \wedge \bar{y}_L = \min_{L \ni x} \max_{U \ni x} \bar{y}_U \wedge \bar{y}_L
\]

for \(x = x_i, i = 1, \ldots, n\), where the maximum is taken over all upper sets \(U\) containing \(x\), the minimum over all lower sets \(L\) containing \(x\), and \(\bar{y}_A\) is the average of the observed \(y_i\) over \(x_i\) for any \(A \subseteq V\). As the high complexity of the upper and lower sets for \(d \geq 2\) could be the culprit behind the possible suboptimal performance of the LSE in convergence and adaptation rates, we consider a class of block estimators involving rectangular upper and lower sets. As the minimax theorem no longer holds in this setting in general, the block estimator, say \(\hat{f}^{(\text{block})}_n(x)\), is defined as any estimator in-between the following max-min and min-max estimators,

\[
\hat{f}^{\text{max-min}}_n(x) = \max_{u \ni x, n_{u,v} > 0} \min_{x \ni v, n_{u,v} > 0} \bar{y}_{[u,v]}, \quad \forall x \in V,
\]

\[
\hat{f}^{\text{min-max}}_n(x) = \min_{x \ni v, n_{u,v} > 0} \max_{u \ni x, n_{u,v} > 0} \bar{y}_{[u,v]}, \quad \forall x \in V,
\]

where \([u,v] = \{x: u \leq x \leq v\}, n_{u,v} = \#\{i \leq n:\ x_{i} \in [u,v]\}\), \(n_{u,v} = \#\{i \leq n: u \leq x_{i}\}\), and \(n_{u,v} = \#\{i \leq n: x_{i} \leq v\}\). The idea of replacing the general level sets \(U \cap L\) by rectangular blocks \([u,v]\) is not new as a preliminary version of the block estimator in the case of \(V = [0, 1]^d\) was considered in Fokianos et al. (2017). Some more delicate details of different versions of the block estimator are discussed in Section 2.

We derive in Section 3 a general \(\ell_q\) risk bound for the above block estimator on graphs. For \(n_1 \times \cdots \times n_d\) lattice designs with \(d \geq 2\), our general risk bound yields

\[
R_2\left(\hat{f}^{(\text{block})}_n, f_n\right) \leq C_d \sigma^2 \min\left\{1, \Delta(f_n/\sigma) n^{-1/d}(\log n)^{1/(d+2)} + n^{-1}(\log n)^d\right\}
\]

when \(\max_{j \leq d} n_j \leq C_d n^{1/d}\), compared with \((5)\) and \((6)\), and the adaptation rate

\[
R_2\left(\hat{f}^{(\text{block})}_n, f_n\right) \leq C_d \sigma^2 (K/n)^{\{1 \lor \log(n/K)\}^d}
\]

when the true \(f\) is non-decreasing and piecewise constant on \(K\) hyper-rectangles, compared with \((7)\).

We also explore the phase transition of the risk bounds, both the minimax lower bound and the upper risk bound for the block estimator, by presenting them using its effective dimension \(s\) in
the sense that the risk bound only depends on the largest \( s \) \( n_j \)'s. For example, when \( n_1 \geq n_2 \geq \cdots \geq n_d \) and \( n_2^{3/2} / n_1^{1/2} \leq \Delta(f_n / \sigma) \), we show that the risk bound for the block estimator in \( d \)-dimensional isotonic regression with \( n \) design points is almost no different from that in univariate isotonic regression with \( n_1 \) design points. This phase transition, captured by effective dimension, proved for \( d = 2 \) in Chatterjee et al. (2018), is new for \( d > 2 \).

Moreover, perhaps more interestingly, we prove that when the unknown \( f \) depends on an unknown set of \( s \) variables, the block estimator achieves near adaptation to the oracle selection in the sense that for \( \Delta(f_n / \sigma) \leq \Delta^*_s \).

\[
R_2(\hat{f}_n^{(block)}, f_n) \leq \begin{cases} 
C_d \sigma^2 \min \left( (\log n)^{-d-s}, \Delta^*_n n^{(d-s-2)/(2d)}(\log n)^{I(s=2)} + n^{-s/d}(\log n)^d \right), & s \geq 2, \\
C_d \sigma^2 \min \left( (\log n)^{-d-1}, \left( \Delta^*_n n^{(d-s-2)/(2d)} \right)^{2/3} + n^{-1/d}(\log n)^d \right), & s = 1,
\end{cases}
\]

with \( \sigma^2_S = \sigma^2 / \prod_{j \notin S} n_j \leq C_d \sigma^2 / n^{1-s/d} \), while the oracle minimax rate with the knowledge of \( S \) is bounded from below by

\[
\inf \sup \left\{ R_2(\hat{f}_n, f_n) : f_n \in \mathcal{F}_n, f(x) = f_S(x_S), \Delta(f_n / \sigma) \leq \Delta^*_n \right\} \geq \begin{cases} 
C_d \sigma^2 n^{-1+s/d} \min \left( 1, \Delta^*_n n^{(d-s-2)/(2d)} \right), & s \geq 2, \\
C_d \sigma^2 n^{-1+1/d} \min \left( 1, \left( \Delta^*_n n^{(d-3)/(2d)} \right)^{2/3} \right), & s = 1,
\end{cases}
\]

where \( \mathcal{F}_n = \{ f_n : f \in \mathcal{F} \} \).

Let \( \bar{f}_n^* \) be the noiseless version of the block estimator. When the isotonic regression model is misspecified in the sense of having a non-monotone regression function, we prove that the error bounds discussed above still hold if \( \mathcal{F}_n \) is treated as the estimation target; (11), (12) and (13) are valid with \( f_n \) replaced by \( \bar{f}_n^* \), when \( f \notin \mathcal{F} \) in (1) . However, such results are of a less ideal form compared with the existing oracle inequalities for the LSE under misspecified monotonicity assumption (Chatterjee et al., 2015; Bellec, 2018; Chatterjee et al., 2018; Han et al., 2017).

We summarize our main results as follows. In terms of the mean squared risk, the block estimator is rate minimax for \( \Delta(f_n / \sigma) \leq \Delta^*_n \) with a wide range of \( \Delta^*_n \) (with no extra logarithmic factor for \( d \neq 2 \)), achieves near parametric adaptation in the piecewise constant case, and also achieves near adaptation to the oracle minimax rate in variable selection. Furthermore, we prove parallel results for the integrated risk for i.i.d. random designs in \([0, 1]^d\) when the joint density of the design point is uniformly bounded away from zero and infinity. In addition to Sections 2 and 3, we present in Section 4 some simulation results to demonstrate the advantage of the block estimator over the LSE in multiple isotonic regression. The full proofs of all theorems, propositions and lemmas in this paper are relegated to the supplement (Deng and Zhang, 2019).

Here and in the sequel, the following notation is used. For \( \{a, b\} \subset V \), we say \( b \) is larger than \( a \) when \( a \preceq b \), and we set \( [a, b] = \{x \in V : a \preceq x \preceq b\} \) as a block in \( G = (V, E) \). We denote
It is clear from (where estimators risk of the LSE and the optimal minimax and adaptation rates, we consider in this paper block in the minimax formula seems to be the cause of the analytical or possibly real gap between the is better known in the univariate case. As the high complexity of the general upper and lower sets formula (Stout efficient algorithms for the LSE have been developed in than where

\[ \hat{f}^{(\text{lse})}_n = \arg\min_{f \in \mathcal{F}} \sum_{i=1}^{n} \{ y_i - f(x_i) \}^2, \]

where \( \mathcal{F} = \{ f : f(u) \leq f(v) \ \forall \ u \leq v \} \) is the set of all non-decreasing functions on the directed graph \( G = (V, E) \). As the squared loss only involves the value of \( f \) at the design points, this LSE is any non-decreasing extension of the LSE of the mean vector \( f_n = (f(x_1), \ldots, f(x_n))^T \) in (1),

\[ \hat{f}^{(\text{lse})}_n = \arg\min_{f_n \in \mathcal{F}_n} \| y - f_n \|_2^2, \]

where \( y = (y_1, \ldots, y_n)^T \) and \( \mathcal{F}_n = \{ f_n : f \in \mathcal{F} \} \subset \mathbb{R}^n \). As \( \mathcal{F}_n \) is defined with no more than \( \binom{n}{2} \) linear constraints, \( \hat{f}^{(\text{lse})}_n \) can be computed with quadratic programming. Potentially more efficient algorithms for the LSE have been developed in Dijkstra (1983), Kyng et al. (2015) and Stout (2015), among others.

As mentioned in the introduction, the LSE \( \hat{f}^{(\text{lse})}_n \) has an explicit representation in the minimax formula (9) for isotonic regression on graphs in general (Robertson et al., 1988), although this fact is better known in the univariate case. As the high complexity of the general upper and lower sets in the minimax formula seems to be the cause of the analytical or possibly real gap between the risk of the LSE and the optimal minimax and adaptation rates, we consider in this paper block estimators \( \hat{f}^{(\text{block})}_n \) of the form

\[ \min \left\{ \hat{f}^{(\text{max-min})}_n(x), \hat{f}^{(\text{min-max})}_n(x) \right\} \leq \hat{f}^{(\text{block})}_n(x) \leq \max \left\{ \hat{f}^{(\text{max-min})}_n(x), \hat{f}^{(\text{min-max})}_n(x) \right\}, \quad \forall x \in V, \]

where \( \hat{f}^{(\text{max-min})}_n \) and \( \hat{f}^{(\text{min-max})}_n \) are the block max-min and min-max estimators given in (10). It is clear from (10) that both the max-min and min-max estimators are non-decreasing on the graph \( G = (V, E) \) as the maximum is taken over increasing classes indexed by \( x \in V \) and the minimum
over decreasing classes. However, the monotonicity of the block estimator, \( \hat{f}_n^{(\text{block})} \in \mathcal{F} \) or even \( \hat{f}_n^{(\text{block})} \in \mathcal{F}_n \), is optional in our analysis. A practical monotone solution is

\[
\hat{f}_n^{(\text{block})}(x) = \frac{1}{2} \left( \hat{f}_n^{(\text{max-min})}(x) + \hat{f}_n^{(\text{min-max})}(x) \right), \quad \forall x \in V.
\]

(17) We note that the estimator (16) is defined on the entire \( V \). This is needed as we shall consider the \( \ell_q \) risk (3) as well as the \( \ell_q \) risk (2). It would be tempting to define the block estimator by

\[
\max_{u \leq x \leq v} \min_{u \leq x \leq v} \overline{y}_{[u,v]} \leq \hat{f}_n^{(\text{block})}(x) \leq \min_{u \leq x \leq v} \max_{u \leq x \leq v} \overline{y}_{[u,v]}
\]

(Fokianos et al., 2017). However, unfortunately, when \( x \) is not a design point, \( \overline{y}_{[u,v]} \) is undefined when \([u, v]\) contains no data point, and \( \hat{f}_n^{(\text{max-min})}(x) \leq \hat{f}_n^{(\text{min-max})}(x) \) is not guaranteed to hold even for properly defined max-min and min-max estimators in (10), even in the univariate case. For example, for \( V = [0, 1] \) with two data points \((x_1, y_1) = (0, 1)\) and \((x_2, y_2) = (1, 2)\), (10) gives \( \hat{f}_n^{(\text{max-min})}(0.5) = 2 > 1 = \hat{f}_n^{(\text{min-max})}(0.5) \). We do have

\[
\hat{f}_n^{(\text{max-min})}(x_i) \leq \hat{f}_n^{(\text{min-max})}(x_i), \quad i = 1, \ldots, n,
\]

(18) but the minimax formula \( \hat{f}_n^{(\text{max-min})} = \hat{f}_n^{(\text{min-max})} \) may fail even on the design points as the example in Figure 1 demonstrates.

![Figure 1](image_url)

**Figure 1.** Responses \( y_i \) on a \( 4 \times 2 \) lattice design: At design point \( x = (4, 1) \), \( \hat{f}_n^{(\text{max-min})}(x) = 0.4 \) is attained by the mean inside the magenta box and \( \hat{f}_n^{(\text{min-max})}(x) = 0.725 \) attained by the mean inside the green box.

In the rest of this section, we prove that the max-min and min-max estimators defined with upper and lower sets in a graph \( G \), including the LSE, can always be expressed as the block estimators defined as in (16) but over a larger graph than \( G \), so that our analysis of general block estimators is also relevant to the LSE. We present our argument in a more general setting as follows.

Formally, a subset of vertices \( U \subseteq V \) is called an upper set if \( U = \{x : f(x) > t\} \) for some \( f \in \mathcal{F} \) and real \( t \), or equivalently the indicator function \( 1_U \) is non-decreasing on \( G \), i.e. \( 1_U \in \mathcal{F} \); a subset \( L \subseteq V \) is called a lower set if \( L = \{x : f(x) \leq t\} \) for some \( f \in \mathcal{F} \) and \( t \in \mathbb{R} \), i.e. the
complement of an upper set. Let \( \mathcal{U} \) be the collection of all upper sets, \( \mathcal{L} \) the collection of all lower sets, and

\[
\mathcal{U}_x \subseteq \{ U \in \mathcal{U} : x \in U \} \quad \text{and} \quad \mathcal{L}_x \subseteq \{ L \in \mathcal{L} : x \in L \}
\]

be certain subsets of the collections of upper and lower sets containing \( x \). The max-min and min-max estimator can be defined in general as

\[
\hat{f}_n^{(\text{max-min})}(x) = \max_{U \in \mathcal{U}_x} \min_{L \in \mathcal{L}_x, n_L > 0} \overline{f}_{U \cap L}, \quad x \in V;
\]

\[
\hat{f}_n^{(\text{min-max})}(x) = \min_{L \in \mathcal{L}_x} \max_{U \in \mathcal{U}_x, n_U > 0} \overline{f}_{U \cap L}, \quad x \in V,
\]

where \( n_A = \{ i \leq n : x_i \in A \} \). These max-min and min-max estimators are non-decreasing in \( x \) on the entire graph if \( \mathcal{U}_x \) is non-decreasing in \( x \) and \( \mathcal{L}_x \) non-increasing in \( x \); \( \mathcal{U}_x \subseteq \mathcal{U}_x' \) and \( \mathcal{L}_x \supseteq \mathcal{L}_x' \) for all ordered pairs \( x \preceq x' \).

By (9), the LSE is a special case of (19) when \( \mathcal{U}_x \) and \( \mathcal{L}_x \) are taken to be the largest possible. The block max-min and min-max estimators (10) are special cases of (19) with \( \mathcal{U}_x = \{ [u, *) : u \preceq x \} \) and \( \mathcal{L}_x = \{ (*, v) : x \preceq v \} \). Conversely, the LSE, and more generally (19), can be written as

\[
\hat{f}_n^{(\text{max-min})}(x) = \max_{u \in A_x, n_u > 0} \min_{v \in B_x, n_v > 0} \overline{f}_{[u, v]}, \quad x \in V;
\]

\[
\hat{f}_n^{(\text{min-max})}(x) = \min_{v \in B_x, n_v > 0} \max_{u \in A_x, n_u > 0} \overline{f}_{[u, v]}, \quad x \in V,
\]

based on the average response in blocks \([u, v]\) for suitable \( A_x \) and \( B_x \) in a larger graph \( G^* \) in which \( G \) is a subgraph. We define \( G^* \) by amending \( G \) with new nodes and edges as follows. For each upper
set \( U \), we amend \( G \) with node \( u^{(\text{new})} = u^{(\text{new},U)} \) and edges \( \{ u \to u^{(\text{new})} : u \in U \} \), whereas for each lower set \( L \), we amend \( G \) with node \( v^{(\text{new})} = v^{(\text{new},L)} \) and edges \( \{ v^{(\text{new})} \to v : v \in L \} \).

Define in the new graph \( G^* \) the estimators (20) with \( A_x = \{ u^{(\text{new},U)} : U \in \mathcal{U}_x \} \) and \( B_x = \{ v^{(\text{new},L)} : L \in \mathcal{L}_x \} \). Then, the restriction of (20) on \( G \) is identical to (19) as \( [u^{(\text{new},U)}, v^{(\text{new},L)}] \) contains the same set of design points as \( U \cap L \). This can be seen as follows. For any pair of upper and lower sets \( U \) and \( L \), \([u^{(\text{new},U)}, v^{(\text{new},L)}] \supseteq U \cap L \) by the definition of \( u^{(\text{new},U)} \) and \( v^{(\text{new},L)} \) and the associated collections of new edges. On the other hand, for any design point \( x_i \in [u^{(\text{new},U)}, v^{(\text{new},L)}] \), \( u^{(\text{new},U)} \preceq x_i \) could happen only if \( u \preceq x_i \) for some \( u \in U \) as there is no other way to connect to \( u^{(\text{new},U)} \) in \( G^* \), while \( x_i \preceq v^{(\text{new},L)} \) could happen only if \( x_i \preceq v \) for some \( v \in L \). Thus, \( \overline{G}_{U \cap L} = \overline{G}_{[u^{(\text{new},U)}, v^{(\text{new},L)}]} \). Figure 2 demonstrate a \([u^{(\text{new})}, v^{(\text{new})}] \) when \( G \) is a 2-dimensional lattice.

Our theoretical results on general graph in Subsection 3.1 below are applicable to the LSE by writing the LSE as a block estimator on a much larger amended graph. However, the more specific results in multiple isotonic regression in Subsections 3.2-3.7 are not applicable to the LSE as they are based on the calculation of the variability bounds in (21) and (22) below for the lattice and random designs, not on the enlarged graph.

### 3. Theoretical results

In this section, we first analyze the block estimator \( \hat{f}_n^{(\text{block})} (x) \) in (16) for graphs under the most general setting. Specific risk bounds are then given for multiple isotonic regression with fixed lattice designs and random designs.

#### 3.1. General isotonic regression on graph

We shall extend the risk bounds of Zhang (2002) from the real line to general graphs. To this end, we first derive an upper bound for the total risk in subsets \( V_0 \subseteq V \),

\[
T_q(V_0) = \sum_{x_i \in V_0} \mathbb{E} \left| \hat{f}_n^{(\text{block})}(x_i) - f(x_i) \right|^q,
\]

based on the value of the true \( f \) on \( V_0 \). Such bounds automatically produce adaptive risk bounds when the true \( f \) is “piecewise constant” in a partition of \( V \). Given \( V_0 \), let \( r_{q,+}(m) \) be a non-increasing function of \( m \in \mathbb{N}^+ \) satisfying

\[
(21) \quad r_{q,+}(m) \geq \max \left\{ \mathbb{E} \left( \max_{u \preceq x} \sum_{x_i \in [u,v]} \frac{\varepsilon_i}{n_{u,v}} \right)^q : n_{x,v} = m, x \preceq v \text{ and } v \in V_0 \right\}.
\]

This function bounds the error of the block estimator from the positive side when the positive part of its bias is no greater than the positive part of the maximum average of at least \( m \) noise variables. Similarly, to control the estimation error from the negative side, let \( r_{q,-}(m) \) be a non-increasing function satisfying

\[
(22) \quad r_{q,-}(m) \geq \max \left\{ \mathbb{E} \left( \min_{u \preceq x} \sum_{x_i \in [u,v]} \frac{\varepsilon_i}{n_{u,v}} \right)^q : n_{u,x} = m, u \preceq x \text{ and } u \in V_0 \right\}.
\]
With the above functions $r_{q,\pm}(m)$, we define for $x \in V_0$

$$m_{x,-} = \max \left\{ n_{x,u} : f(u) \geq f(x) - r_{q,-}^{1/q}(n_{x,u}), u \leq x \text{ and } u \in V_0 \right\},$$

(23)

$$u_x = \arg \max_{u \in V_0 : u \leq x} \left\{ n_{x,u} : f(u) \geq f(x) - r_{q,-}^{1/q}(n_{x,u}) \right\},$$

$$m_x = m_{x,+} = \max \left\{ n_{x,v} : f(v) \leq f(x) + r_{q,+}^{1/q}(n_{x,v}), x \leq v \text{ and } v \in V_0 \right\},$$

$$v_x = \arg \max_{v \in V_0 : x \leq v} \left\{ n_{x,v} : f(v) \leq f(x) + r_{q,+}^{1/q}(n_{x,v}) \right\}.$$  

Roughly speaking, the above quantities provide configurations in which the bias of $\widehat{f}_n(x_i)$ is of no greater order than its variability from the negative and positive sides, so that the error of the block estimator is of no greater order than an average of $m_{x,-}$ noise variables on the negative side and the average of $m_x = m_{x,+}$ noise variables on the positive side. Thus, it makes sense to count the frequencies of $m_{x,-}$ and $m_x$ as follows,

$$\ell_{-}(m) = \# \left\{ i : x_i \in V_0, m_{x,-} \leq m \right\}, \quad \ell_{+}(m) = \# \left\{ i : x_i \in V_0, m_x \leq m \right\}.$$  

(24)

We note that the functions $r_{q,\pm}$ in (21) and (22) do not depend on $f$, and all the quantities in (23) and (24) depend on the true $f$ only through $\{f(x) : x \in V_0\}$.

**Theorem 1.** Assume $f$ is non-decreasing on a graph $G = (V,E)$. Let $r_{q,\pm}(m)$ be given by (21) and (22), and $\ell_{\pm}(m)$ by (24). Then it holds for any block estimator $\widehat{\mathcal{f}}_{n}(block)(x)$ in (16) that

$$\mathbb{E} \left\{ \left| \widehat{\mathcal{f}}_{n}(block)(x_i) - f(x_i) \right| \right\}^{q}_{+} \leq 2^q r_{q,+}(m_x), \forall x_i \in V_0,$$

(25)

$$\mathbb{E} \left\{ \left| \widehat{\mathcal{f}}_{n}(block)(x_i) - f(x_i) \right| \right\}^{q}_{-} \leq 2^q r_{q,-}(m_{x,-}), \forall x_i \in V_0.$$

Consequently, for any upper bounds $\ell^\star_{\pm}(m) \geq \ell_{\pm}(m)$ with $\ell^\star_{\pm}(0) = 0$,

$$T_q(V_0) \leq \sum_{m=1}^{\infty} 2^q r_{q,+}(m) \left\{ \ell^\star_{+}(m) - \ell^\star_{+}(m-1) \right\}$$

$$+ \sum_{m=1}^{\infty} 2^q r_{q,-}(m) \left\{ \ell^\star_{-}(m) - \ell^\star_{-}(m-1) \right\}.$$  

Theorem 1 provides risk bound for the block estimator (16) over a subset $V_0$ of design points in terms of upper bound functions $r_{q,\pm}(m)$ and $\ell^\star_{\pm}(m)$. Ideally, we would like to have

$$r_{q,\pm}(m) = C_{q,d} \sigma^q m^{-q/2}$$

in (21) and (22). When the design points in $V_0$ are linear and the $(q \vee 2)$-th moment of the noise variable is uniformly bounded, (21) and (22) hold for the above choice of $r_{q,\pm}(m)$. This choice of $r_{q,\pm}(m)$ is also valid when $V$ is a lattice in $\mathbb{R}^d$ and $\varepsilon_i$ are independent variables with uniformly bounded $(q \vee 2)$-th moment, as we will prove in Subsection 3.3.
3.2. Minimax lower bound in multiple isotonic regression with lattice designs. We study in the rest of this section multiple isotonic regression in $V \subseteq \mathbb{R}^d$ where $a \preceq b$ iff $a \leq b$, i.e. $a_j \leq b_j \forall 1 \leq j \leq d$, for all $a = (a_1, \ldots, a_d)^T$ and $b = (b_1, \ldots, b_d)^T$, and $\mathcal{F}$ is the class of all non-decreasing functions $f(t_1, \ldots, t_d) \uparrow t_j, \forall j = 1, \ldots, d$.

The lattice design we are considering is given by

$$V = \{ x_i : 1 \leq i \leq n \} = [1, n] = \prod_{j=1}^{d} \{1, \ldots, n\},$$

where $n = (n_1, \ldots, n_d)^T$ with positive integers $n_j$ and $n = \prod_{j=1}^{d} n_j$. Here $[1, n]$ is treated as a set of integer-valued vectors in $\mathbb{N}^d$, forming a lattice. Occasionally, we may also use $[u, v]$ to denote a hyper-rectangle of real numbers in continuum. This slight abuse of notation typically would not lead to confusion, for example in $x_i \in [u, v]$, but we would be specific if necessary. Without loss of generality, we assume in this subsection $n_1 \geq n_2 \geq \cdots \geq n_d$. In the above lattice design, we provide a minimax lower bound in multiple isotonic regression as follows.

**Proposition 1.** Suppose $\varepsilon_i \sim N(0, \sigma^2)$. Let $\Delta(f_n/\sigma) = \{ f(n) - f(1) \}/\sigma, n_{d+1} = 1$, $n_s^* = \prod_{j=1}^{s} n_j, t_s = n_s^*/n_s^* t_{d+2} = \infty$ and $s_q = \lfloor 2/(q-1) \rfloor \land (d+1)$. Let $h_0(t) = \Delta_n^* \sqrt{t}$ and define piecewise $H(t) = \min \{ 1, h_0(t)/(n_s^*/t_s^{1/(s\land d)}) \}, t \in [t_s, t_{s+1}], s = 1, \ldots, d+1$. Then,

$$\inf_{f} \sup_{q,d} \sigma^q \max \{ (t \land n)^{-q/2} H(t) : t \land h_0(t) \geq 1 \}$$

$$= \sigma^q \times \begin{cases} 1, & n_1 \leq \Delta_n^*, \\ (\Delta_n^*/(n_s^*))^{q/(2+s)} & n_{s+1}/t_{s+1}^{1/2} \leq \Delta_n^* \leq n_s/t_s^{1/2}, \quad (1 \leq s < s_q) \\ \Delta_n^*/(n_s t_s^{(q-1)/2}) & t_s^{-1/2} \leq \Delta_n^* \leq n_s/t_s^{1/2}, \quad (s_q \leq s \leq d) \\ (\Delta_n^*)^{q-2/s}/(n_s^{1/s}) & t_{s+1}^{-1/2} \leq \Delta_n^* \leq t_s^{-1/2}, \quad (s_q \leq s \leq d) \\ n^{-q/2}, & 0 \leq \Delta_n^* \leq n^{-1/2}, \quad (s = d + 1) \\ \end{cases}$$

In particular, when $n_1 = \cdots = n_d = n_1^{1/d}$ and $\Delta_n^* \geq n^{-1/2}$, the right-hand side of (29) is

$$\sigma^q \times \begin{cases} \min \{ 1, (\Delta_n^*/n_1^{1/d})^{q d/(d+2)} \}, & q \leq 1 + 2/d, \\ \min \{ 1, \Delta_n^*/n_1^{1/d}, (\Delta_n^*)^{q-2/d}/n_1^{1/d} \}, & q \geq 1 + 2/d. \\ \end{cases}$$

On the right-hand side of (29), the breaking points on $[0, \infty)$ for $\Delta_n^*$ are

$$0, n_1^{-1/2} = t_{d+1}^{-1/2}, t_{d+2}^{-1/2}, \ldots, t_{s_q}^{-1/2}, n_{s_q}/t_{s_q}^{1/2}, \ldots, n_1/t_1^{1/2} = n_1.$$
Note that 1 lies in between $t^{-1/2}$ and $n_{s_q}/t^{1/2}$. The above minimax lower bound also depends on the loss function through $q$ and the dimension of the lattice. For $q \geq 3$, we have $s_q = 1$, so that

$$\inf \sup \left\{ R_q(\hat{f}, f_n) : f_n \in F_n, \Delta(f_n/\sigma) \leq \Delta_n^* \right\} \geq \sigma^q \min \left( 1, \Delta_n^*/n_1 \right)$$

for $\Delta_n^* \geq 1$. However for $q = 2$, we have $s_q = 2$, so that (29) yields

$$\inf \sup \left\{ R_2(\hat{f}, f_n) : f_n \in F_n, \Delta(f_n/\sigma) \leq \Delta_n^* \right\} \geq \sigma^q \min \left( 1, \Delta_n^*/n_1 \right)$$

for $\Delta_n^* \geq 1$. However for $q = 2$, we have $s_q = 2$, so that (29) yields

$$\inf \sup \left\{ R_2(\hat{f}, f_n) : f_n \in F_n, \Delta(f_n/\sigma) \leq \Delta_n^* \right\} \geq \sigma^2 \times \begin{cases} 1, & n_1 \leq \Delta_n^*, \\ \left( \Delta_n^*/n_1 \right)^{2/3}, & n_2^{3/2}/n_1^{1/2} \leq \Delta_n^* \leq n_1, \\ \Delta_n^*/(n_1n_2)^{1/2}, & \sqrt{n_2}/n_1 \leq \Delta_n^* \leq n_2^{3/2}/n_1^{1/2}. \end{cases}$$

For $\Delta_n^* > 1$, this matches the lower bound for the $\ell_2$ minimax rate in Chatterjee et al. (2018) for $d = 2$ and Han et al. (2017) for $d \geq 3$. For $5/3 \leq q \leq 2 \leq d$, we have $s_q = 3$.

If (29) is achievable, the integer parameter $s$ can be viewed as the effective dimension of the isotonic regression problem as the rate depends on $n$ only through $n_1, \ldots, n_s$ when $n_{s+1}$ is sufficiently small; the rate would also be achievable by separate $s$-dimensional isotonic regression in the $\prod_{j=s+1}^d n_j = n/n_s^s$ individual $s$-dimensional sheets with fixed $x_{s+1}, \ldots, x_d$. For example, in (31), the minimax rate can be achieved by $\hat{f}_n = y$ for $s = 0$, by the row-by-row univariate isotonic regression for $s = 1$, and by individual bivariate isotonic least squares up to a factor of $(\log n)^4$ for $s = 2$ (Chatterjee et al., 2018). We will prove in the next subsection that the block estimator (16) achieves the rate in (29) for a wide range of $\Delta_n^*$, so that Proposition 1 indeed provides the minimax rate.

In the proof of Proposition 1, we divide $[1, n] \subset V = [1, n]$ into a $K_1 \times \cdots \times K_d$ lattice of hyper-rectangles of size $m_1 \times \cdots \times m_d$, indexed by $k = (k_1, \ldots, k_d)^T$, $k_j = 1, \ldots, K_j$, $j = 1, \ldots, d$, and consider the class of piecewise constant functions $f(x) = g(k)$ satisfying

$$g(k) = \sigma \min \left\{ \Delta_n^*, (m^*)^{-1/2} \left[ \theta(k) + (k_1 + \cdots + k_d - k^*)_+ \right] \right\}, \theta(k) \in \{0, 1\},$$

and $f(x) = \sigma \Delta_n^*$ for $x \in [1, n] \setminus [1, n']$, where $m^* = \prod_{j=1}^d m_j$ is the size of the hyper-rectangle.

As $g(k)$ is non-decreasing in $k_j$ for each $j$ for all $\theta(k) \in \{0, 1\}$, this construction provides a lower bound for the $\ell_q$ risk proportional to the product of $\sigma^{q/(m^*)^{-q/2}}$ and the number of free $\theta(k)$. This is summarized in the following lemma.

**LEMMA 1.** Under the conditions of Proposition 1,

$$\inf \sup \left\{ \mathbb{E}\|\hat{f} - f_n\|_q^q : f_n \in F_n, \Delta(f_n/\sigma) \leq \Delta_n^* \right\} \geq c_q c_d \sigma^{q} n \max_{m \in M} \left\{ \frac{1}{(m^*)^{q/2}} \min \left( \frac{\sqrt{m^*} \Delta_n^*}{\max_j n_j/m_j}, 1 \right) \right\},$$

where $\mathbb{E}$ denotes the expectation operator and $\max_{m \in M}$ denotes the maximum over all $m \in M$. The constants $c_q$ and $c_d$ depend only on $q$ and $d$, respectively.
where \( c_\delta = \inf_{\delta} \mathbb{E}_{\mu \sim \text{Bernoulli}(1/2)} \delta(N(\mu, 1)) - \mu \) is the Bayes risk for estimating \( \mu \) with the Bernoulli(1/2) prior based on a single \( N(\mu, 1) \) observation, \( c_d \) is a constant depending on \( d \) only.

\[
\mathcal{M} = \left\{ \mathbf{m} = (m_1, \cdots, m_d) : m_j \in \mathbb{N}_+, m_j \leq n_j \forall j \leq d, \sqrt{m^* \Delta^*_n} \geq 1 \right\},
\]

and \( m^* = \prod_{j \leq d} m_j \). Moreover, the optimal configuration of \( \mathbf{m} \) in (32) must satisfy either \( m_j = 1 \) or \( [n_j/m_j] = \max_{1 \leq j \leq d} [n_j/m_j] \) for each \( j \).

### 3.3. The block estimator in multiple isotonic regression with lattice designs

We further divide this subsection into three separate sub-sections to study the performance of the block estimator at a single design point \( x_i \), in an arbitrary sub-block \( [a, b] \subset [1, n] \), and on the entire lattice \( [1, n] \).

It is of great interest to show that the block estimator in (16) matches the minimax lower bound given in Proposition 1, which will be done in the third sub-sub-section for general \( q \) and \( d \).

#### 3.3.1. Risk of the block estimator at a single design point

For any given point in the design lattice, the following proposition asserts that the block estimator matches certain one-sided oracle estimators in the rate of one-sided \( L_q \) risks.

**Proposition 2.** Let \( \hat{f}_n^{(\text{block})}(x) \) be the block estimator in (16) with the lattice design \( V = [1, n] \) in (28). Let \( q \geq 1 \) and \( r_q, \pm(m) \) be as in (21) and (22). Assume \( \varepsilon_i \) are independent \( N(0, \sigma^2) \) random variables. Then, for any design point \( x_i \in [1, n] \),

\[
\mathbb{E}\left( \hat{f}_n^{(\text{block})}(x_i) - f(x_i) \right)^q \leq 2^q r_{q,+}(m_{x_i}) \leq C_{q,d} \min_{x_i \leq u, v \leq n} \mathbb{E}\left( \overline{y}_{[u,v]} - f(x_i) \right)^q, \tag{33}
\]

where \( \overline{y}_{[u,v]} = \sum_{u \leq x_i \leq v} y_i / n_{u,v} \), and

\[
\mathbb{E}\left( \hat{f}_n^{(\text{block})}(x_i) - f(x_i) \right)^q \leq 2^q r_{q,-}(m_{x_i}) \leq C_{q,d} \min_{1 \leq u \leq x_i} \mathbb{E}\left( \overline{y}_{[u,x_i]} - f(x_i) \right)^q. \tag{34}
\]

Consequently, with \( \mathbb{E}_g \) being the expectation under which \( y_i = g(x_i) + \varepsilon_i \),

\[
\mathbb{E}\left| \hat{f}_n^{(\text{block})}(x_i) - f(x_i) \right|^q \leq C_{q,d} \min_{u \leq x_i \leq v} \left\{ \mathbb{E}_g \left| \overline{y}_{[u,v]} - g(x_i) \right|^q : g \in \mathcal{F}, g(v) = f(v) \forall v \geq x_i \right\} + C_{q,d} \min_{u \leq x_i \leq v} \left\{ \mathbb{E}_g \left| \overline{y}_{[u,v]} - g(x_i) \right|^q : g \in \mathcal{F}, g(u) = f(u) \forall u \leq x_i \right\}. \tag{35}
\]

Suppose we are confined to consider only block mean estimators \( \overline{y}_{[u,v]} \) with no negative bias in the estimation of \( f(x_i) \) but we also want to control the positive side of the error. As \( f \) is non-decreasing but otherwise unknown, we are thus forced to choose \( u \geq x_i \). As \( \overline{y}_{[u,v]} \) with \( x_i \leq u \leq v \) would have larger bias and variance than \( \overline{y}_{[x_i,v]} \), the optimal \([u, v]\) is given by

\[
\min_{u = x_i, u \leq v \leq n} \mathbb{E}\left( \overline{y}_{[x_i,v]} - f(x_i) \right)^q_+. \tag{36}
\]
The above minimum can be viewed as an oracle benchmark under the no-negative-bias constraint as the solution of the optimal \( v \) still depends on \( f \). Although the block estimator (16) is unlikely to be unbiased, (33) and (34) assert that its one-sided risks match the rates of such oracle benchmarks from both the positive and negative sides. Another interpretation of the performance of the block estimator is (35) in which the oracle expert has to guard against the worst case scenarios in the uncertainty of \( f \) on either sides, but not simultaneously on both.

We prove Proposition 2 with an application of Theorem 1. This requires more explicit variability bounds \( r_{q,\pm}(m) \) in (21) and (22) as in (27). This validity of (27) is a consequence of the following lemma, which extends Doob’s inequality to certain multiple indexed sub-martingales. It plays a key role in removing the normality assumption on the noise \( \varepsilon_1, \ldots, \varepsilon_n \) in our analysis.

**Lemma 2.** Let \( \mathcal{T} = \mathcal{T}_1 \times \cdots \times \mathcal{T}_d \subseteq \mathbb{R}^d \) be an index set with \( \mathcal{T}_j \subseteq \mathbb{R} \). Let \( \{f_t, t \in \mathcal{T}\} \) be a collection of random variables. Suppose for each \( j \) and each \((s_1, \ldots, s_j-1, t_{j+1}, \ldots, t_d)\), \( \{f_{s_1,\ldots,s_j-1, i, t_{j+1},\ldots,t_d}, t \in \mathcal{T}_j\} \) is a sub-martingale with respect to certain filtration \( \{\mathcal{F}_t^{(j)}, t \in \mathcal{T}_j\} \). Then, for all \( q > 1 \) and \( t \in \mathcal{T} \),

\[
E \max_{s \in \mathcal{T}_t, s \leq t} |f_s|^q \leq (q/(q-1))^{qd} E |f_t|^q.
\]

In particular when \( \varepsilon_i \)'s are independent random variables with \( E \varepsilon_i = 0 \),

\[
E \max_{s \leq t} \left| \sum_{x_1 \leq s} \varepsilon_i \right|^q \leq \begin{cases} 
(q/(q-1))^{qd} E \left| \sum_{x_1 \leq t} \varepsilon_i \right|^q, & q \geq 2, \\
(4^d E \left| \sum_{x_1 \leq t} \varepsilon_i \right|^2)^{q/2}, & 1 \leq q < 2.
\end{cases}
\]

3.3.2. **Risk of the block estimator in a sub-block.** To automatically deal with adaptation which gives better risk bound when \( f(\cdot) \) is piecewise constant, we first consider the risk in one of such “piece”, a hyper-rectangle \([a, b] \subseteq V = [1, n]\).

**Theorem 2.** Let \( \tilde{f}_n^{(block)}(x) \) be the block estimator in (16) with the lattice design \( V = [1, n] \) in (28). Assume \( \varepsilon_i \) are independent random variables with \( E \varepsilon_i = 0 \) and \( E \varepsilon_i^{q/2} \leq \sigma^{q/2} \). Let \( a \leq b \) be integer vectors in \( V = [1, n] \) and \( \tilde{n}_j = b_j - a_j + 1 \). Suppose \( \tilde{n}_1 \geq \cdots \geq \tilde{n}_d \). Define \( \tilde{n} = \tilde{n}_a, \tilde{n}_{d+1} = 1, \tilde{n}_i = \prod_{j=1}^{d} \tilde{n}_j \) and \( t_s = \tilde{n}_s/\tilde{n}_a^s \) (with \( 1 \leq t_1 \leq \cdots \leq t_d \leq t_{d+1} = \tilde{n} \)). Then, for \( q \geq 1 \) and any \( f \in \mathcal{T} \) with \( \Delta_{a,b}(f, n, s) = \{ f(b) - f(a) \}/\sigma \leq \Delta_n \),

\[
T_q([a, b]) = \sum_{x_i \in [a, b]} E \left| \hat{f}_n^{(block)}(x_i) - f(x_i) \right|^q \leq C_{q,d}^* n_{a,b} \sigma^q \left( \tilde{H}(1) + \int_1^{n_{a,b}} \frac{\tilde{H}(dt)}{t^{q/2}} + \frac{1}{n_{a,b}} \prod_{j=1}^d \int_0^{\tilde{n}_j} \frac{dt}{(t \vee 1)^{q/2}} \right),
\]

where \( \tilde{H}(t) \) is a non-decreasing and continuous function of \( t \), defined piecewise by \( \tilde{H}(t) = \min \{ 1, \Delta_n^{s/2}(t/\tilde{n}_a^s)^{1/s} \} \) for \( t_s \leq t \leq t_{s+1} \), \( s = 1, \ldots, d \), and \( C_{q,d}^* \) is continuous in \( q \in [1, \infty) \).
and non-decreasing in \( d \). Moreover,

\[
\tilde{H}(t) + \int_1^{n_{a,b}} t^{-q/2} \tilde{H}(dt) \leq q_d \int_0^{b_j - a_j + 1} \frac{dt}{(t+1)^{q/2}} \leq q_d \left( \frac{n_{1-q/2} + \left( \prod_{j=1}^{d} \log_+ (b_j - a_j + 1) \right)}{I(q=2)} \right) \]

where \( q_d = [2/(q-1)] \wedge (d+1) \) is as in Proposition 1 and

\[
\Lambda_s = \left[ \log_+ \left( \min \left\{ \frac{n_{s}}{n_{s+1}}, \frac{n_s/(\bar{n}_s^{*})^{1/(s+2)}}{n_{s}^{*}(e_2/2)^{2/(s+2)}} \right\} \right) \right]^{I(2/(q-1)=s)}.
\]

Remark 1. The last component on the right-hand side of (36) is bounded by

\[
\sigma^q \prod_{j=1}^{d} \int_{j=1}^{b_j - a_j + 1} \frac{dt}{(t+1)^{q/2}} \leq q_d \sigma^q \left[ n_{1-q/2} + \left( \prod_{j=1}^{d} \log_+ (b_j - a_j + 1) \right) \right]^{I(q=2)}.
\]

When \( \Delta_{a,b}(f_n/\sigma) = 0 \), \( \tilde{H}(t) = 0 \) for all \( t \), so that (39) is an upper bound for the rate of the total risk \( T_q(a, b) \) in the block \([a, b]\) by Theorem 2, for any \( a \leq b \). This yields the adaptation rate stated in Subsection 3.4.

Remark 2. The function \( \tilde{H}(t) \) is defined in the same way as \( H(t) \) in Proposition 1 but for the dimensions \( \{n_j = b_j - a_j + 1, j \leq d\} \) of \([a, b]\) and range-to-noise ratio within \([a, b]\). When \([a, b] = [1, n]\), we have \( \tilde{H}(t) = H(t) \) for all \( t \in [1, n] \). Thus, as discussed below (31), the integer parameter \( s \) in (37), completely determined by \( \{n_j\} \), \( \Delta_n^* \) and \( q \), has the interpretation as the effective dimension for the estimation of \( f \) in \([a, b]\) subject to \( \{f(b) - f(a)\} / \sigma \leq \Delta_n^* \). We note that as \( \tilde{H}(t) \) is a smooth fit of pieces proportional to \( t^{1/2+1/s} \) or \( 1 \), the upper limit of the integration is actually \( t_* = \min \{ t \geq 1 : \tilde{H}(t) = 1 \ or \ t = \tilde{n}_{a,b} \} \), which depends on \( \Delta_n^* \) and the effective dimension \( s \) is then determined by the comparison between \( t_* \) and \( t_s \) and the critical \( s_q \).

In addition to the validity of (27) as variability bounds in (21) and (22), which follows from Lemme 2, the proof of Theorem 2 requires the complexity bounds for the \( \ell_\pm(m) \) in (24). We outline here an analysis of the count \( \ell_\pm(m) \) in (24) in the case where \( \tilde{n}_j / \tilde{n}_d \) are integers and \( m \geq t_d = \tilde{n} / \tilde{n}_d^2 \). We note that \( t_d = 1 \) when \( \tilde{n}_j = \tilde{n}_d \) for all \( j \). Upper bounds for both \( \ell_\pm(m) \) in the general setting are given in the proof of Theorem 2 in subsection A3.3 of the supplement.

To find upper bounds for \( \ell_\pm(m) \), we partition \( V_0 = [a, b] \) into an \( \tilde{n}_d \times \cdots \times \tilde{n}_d \) lattice of small “unit blocks” of size \( (\tilde{n}_1 \tilde{n}_d) \times \cdots \times (\tilde{n}_d \tilde{n}_d) \), each composed of \( t_d = \tilde{n} / \tilde{n}_d^2 \) design points. Consider a line of such unit blocks \( L_k \) in the “anti-diagonal” direction and a region \( D_j \) between two contours of the unknown \( f(x) \) at the levels \( c \) and \( c + r_{\tilde{n}_d^2/3}(3^d m) \). In Figure 3, we color in red the unit blocks in \( L_k \) with nonempty intersection with \( D_j \). Due to the monotonicity of the
\( \ell_+(m) \), it suffices to consider \( m = k^d t_d \) for some integer \( k \geq 1 \). If \( x \leq v \) in \( L_k \cap D_j \) are separated by \( k \) unit blocks as depicted in Figure 3, then \( m = k^d t_d < n_{x,v} \leq (k + 2)^d t_d \leq 3^d m \) and \( f(v) - f(x) \leq \frac{1}{q}(3^d m) \leq \frac{1}{q}(n_{x,v}) \), so that \( m_x \geq n_{x,v} \leq m \). Thus, the intersection contains no more than \((k + 1)t_d \leq 2m^{1/d} t_d^{1/d} \) design points \( x_i \) with \( m_{x_i} \leq m \), all within \( k \) unit blocks from the upper contour. Let \( J = \left[ \frac{f(b) - f(a)}{r_{q,+}(3^d m)} \right] \). We divide \( [a, b] \) into \( J \) such regions \( D_j \) between consecutive contours with \( a \in D_1 \) and \( b \in D_J \). The last region \( D_J \) is special. For \( x \in D_j \) with \( n_{x,b} > m \), there must exist \( v \in [x, b] \) such that \( m < n_{x,v} \leq 2m \), so that \( m_x \geq n_{x,v} \leq m \) due to \( f(v) \leq f(x) + \frac{1}{q}(3^d m) \leq f(x) + \frac{1}{q}(n_{x,v}) \). Thus, as there are no more than \( d^d n_{d-1}^d \) such \( L_k \) and \( J - 1 \leq \frac{f(b) - f(a)}{r_{q,+}(3^d m)} \), \( \Delta^*_{\sigma} / r_{q,+}(3^d m) \) regions \( D_j \) not containing \( b \), for \( m = k^d t_d \) with integer \( k \geq 1 \)

\[
\ell_+(m) \leq \min \left\{ \frac{n_{d} n_{d-1}(\Delta^*_\sigma / r_{q,+}(3^d m)) (2m^{1/d} t_d^{1/d})}{\min \left\{ 1, m^{1/d+1/2} (\Delta^*_\sigma / n_{d}^{1/d}) (2d^{3/2} / C_{q,d}^{1/q}) \right\}} + \#\{x_i \in [a, b] : n_{x_i,b} \leq m \} \right\}
\]

with the variability bound \( r_{q,+}(m) = C_{q,d} \sigma^q m^{-q/2} \) in (27). It follows that

\[
\ell_+(m) \leq \ell_+(m) = n n \bar{H}(m) + \#\{x_i \in [a, b] : n_{x_i,b} \leq m \} \quad \forall m \geq t_d
\]

when \( C_{q,d}^{1/q} \geq (2^{1/d+1/2})^{3/2} \). In subsection A3.3 of the supplement, we extend the above inequality to all \( m \geq 1 \) and prove (36) by applying (26) of Theorem 1 with the above \( \ell_+(m) \) and the \( r_{q,\pm}(m) \) in (27).
Theorem 2 is a comprehensive statement which gives rise to many conclusions. In the next sub-subsection, we prove that the block estimator is rate minimax in the $\ell_q$ risk for the entire lattice $[1, n]$ in a wide range of configurations of $n, q$ and $\Delta_n^*$. In the next two subsections, we study the adaptation rate when $f(\cdot)$ is a piecewise constant function, and the variable selection rate when $f(\cdot)$ only depends on a subset of variables.

3.3.3. Risk of the block estimator on the entire lattice and rate minimaxity. We assume without loss of generality in this sub-subsection $n_1 \geq \cdots \geq n_d$. A direct comparison between Proposition 1 and Theorem 2 yields the following Theorem 3.

**Theorem 3.** Let $\tilde{f}_n^{(block)}(x)$ be the block estimator in (16) with the lattice design $V = [1, n]$ as in (28). Assume $\varepsilon_i$ are independent random variables with $\mathbb{E}[\varepsilon_i] = 0$ and $\mathbb{E}[\varepsilon_i^q|\varepsilon_i^2] \leq \sigma^q$. Let $s_q = \lceil 2/(q-1) \rceil \land (q+1)$, $n_q^* = \prod_{j=1}^s n_j$ for $s \leq d + 1$ with $n_{d+1} = 1$, and $\Delta(f_n/\sigma) = \{f(n) - f(1)/\sigma\}$. Then, for $q \geq 1$,

$$
\begin{align*}
\sup \left\{ R_q(\tilde{f}_n^{(block)}, f_n) : f_n \in \mathcal{F}_n, \Delta(f_n/\sigma) \leq \Delta_n^* \right\} \\
\lesssim_{q,d} \Lambda^{(match)} \inf \sup \left\{ R_q(\tilde{f}, f_n) : \Delta(f_n/\sigma) \leq \Delta_n^* \right\} + \frac{\sigma^q}{n} \left( \prod_{j=1}^d \log_2(n_j) \right)^{I\{q=2\}}
\end{align*}
$$

holds when $\Delta_n^* \gtrsim_{q,d} t_{s_q}^{-1/2} = (n_q^*/n_{s_q})^{-1/2}$, where $\Lambda^{(match)} \leq \log n$ is defined by

$$
\Lambda^{(match)} = \left[ \log_+ \left( \min \left\{ \frac{n_{s_q}}{n_{s_q+1}}, \frac{n_{s_q}/(n_{s_q}^{1/2})^{1/(s_q+2)}}{(\Delta_n^*)^{2/(s_q+2)}} \right\} \right) \right]^{I\{q=2\}} = \left\{ \begin{array}{ll} 
1 & \text{if } q = 1; \\
\log_+ \left( \min \left( n \land \left( \frac{n^{1/d}}{\Delta_n^*} \right)^{2d/(d+2)} \right) \right) + \frac{(\log n)^{\delta_2}}{n^{(q/2)^\land 1}} & \text{if } q \geq 2;
\end{array} \right.
$$

Moreover, when $\max_j n_j \lesssim_n n^{1/d}$ and $\Delta(f_n/\sigma) \leq \Delta_n^*$,

$$
\begin{align*}
R_q(\tilde{f}_n^{(block)}, f_n) \\
\lesssim_{q,d} \sigma^q \min \left\{ 1, \left( \frac{\Delta_n^*}{n^{1/d}} \right)^{I\{q=2\}} \left[ \log_+ \left( n \land \left( \frac{n^{1/d}}{\Delta_n^*} \right)^{2d/(d+2)} \right) \right]^{\delta_1} + \frac{(\log n)^{\delta_2}}{n^{(q/2)^\land 1}} \right\},
\end{align*}
$$

holds for all $\Delta_n^* \geq 0$, where $\delta_1 = I\{ q = 2 \} = 1$ and $\delta_2 = I\{ q = 2 \}$.

**Remark 3.** It can be seen in our analysis that the logarithmic term presents for $q = 2$, as the last component on the right-hand side of (36), (41) and (43), due to the lack of data near the extreme points $\{a, b\}$ or $\{1, n\}$ of the domain.

Compared with Proposition 1, Theorem 3 shows that the risk of the block estimator matches the minimax rate when $\Delta_n^* \geq t_{s_q}^{-1/2} = (\prod_{j=1}^s n_j/n_{s_q})^{-1/2}$ (as $\Delta_n^* \geq n^{-1/2}$ if $s_q = d + 1$) possibly up to a logarithmic factor $\Lambda^{(match)} \leq \log(n)$, provided that the minimax rate is no faster than
\[ \sigma^q n^{-1} \left( \prod_{j=1}^d \log_+(n_j) \right)^{\delta_2} \text{ due to the edge effect.} \] The match is always exact when \( 2/(q-1) \neq s_q \leq d, \) i.e., \( 2/(q-1) \) is not an integer or an integer greater than \( d. \) When \( 2/(q-1) = s_q \leq d-1 \) and \( n_{s_q} \approx n_{s_q+1}, \) \( \Lambda^{(\text{match})} = O(1) \) and the match is also exact. However, in the interesting setting where \( q = d = 2 \) and \( n_1 \approx n_2, \) we have \( s_q = 2 \) so that \( \Lambda^{(\text{match})} \approx \log(n) \) when \( \Delta_n^* \ll n_2. \)

The one-dimensional risk bound for all \( q \geq 1 \) can be obtained from (43) as

\[
T_q([1, n]) \lesssim q \sigma^q n \min \left\{ 1, \left( \frac{\Delta^*_n}{n} \right)^{\min(q/3,1)} \left[ \log_+(n) \wedge \left( \frac{n}{\Delta^*_n} \right)^{2/3} \right]^{I(q=3)} + \left( \frac{\log(n)}{n} \right)^{I(q=2)} \right\},
\]

which reproduces (4) for \( 1 \leq q < 3. \) We note that if we view one-dimensional isotonic regression as multi-dimensional on an \( n_1 \times 1 \times \cdots \times 1 \) lattice, the general bound yields this one-dimensional \( n_1^{-1/3} \)-rate. Interestingly, for general \( n, \) we still have the one-dimensional rate as long as the effective dimension \( s \) is 0 or 1, i.e., \( \Delta_n^* \geq n_2/t_2^{1/2} = n_2^{3/2}/n_1^{1/2}. \) For \( q = 2 \) and \( d \geq 2, \) it follows from Theorem 2 that when \( \Delta_n^* \geq n_2/t_2^{1/2} = n_2^{3/2}/n_1^{1/2}, \) we have \( s < s_q = 2 \) and only the first two cases of (37) are effective. This implies

\[
T_2([1, n]) \lesssim_d \sigma^2 n \min \left\{ 1, \left( \frac{\Delta_n^*/n_1}{n} \right)^{2/3} + \prod_{j=1}^d \left( \log_+(n_j)/n_j \right) \right\},
\]

exactly the same as the bound of \( T_2([1, n_1]) \) in univariate case when \((\Delta_n^*/n_1)^{2/3} \) is dominant in both rates. In this case, our theory does not guarantee an advantage of the multiple isotonic regression on the entire lattice in terms of the \( \ell_2 \) risk, compared with the row-by-row univariate isotonic regression of length \( n_1. \) This observation agrees with Chatterjee et al. (2018) where the \( \ell_2 \) minimax rate of two-dimensional isotonic regression, \( \sigma^2 \Delta_n^* n^{-1/2}, \) requires \( n_2^{3/2}/n_1^{1/2} \geq \Delta_n^*. \)

To conclude this subsection, we compare the \( \ell_2 \) risk bound for the block estimator in Theorem 3 with those for the LSE in the existing literature. For \( d = 2, \) Chatterjee et al. (2018) gives an upper bound for the LSE as

\[
R_2(\hat{f}_n^{(\text{lse})}, f_n) \lesssim \sigma^2 \left( \frac{\Delta_n^*}{\sqrt{n}} \log(n) + \frac{1}{n} (\log n)^8 \right),
\]

for any \( n_1 \times n_2 \) lattice and \( f \) satisfying \( \Delta(f_n/\sigma) \leq n_2^{3/2}/n_1^{1/2}, \) in contrast to

\[
R_2(\hat{f}_n^{(\text{block})}, f_n) \lesssim \sigma^2 \left( \frac{\Delta_n^*}{\sqrt{n}} \log(n) + \frac{1}{n} (\log n)^2 \right)
\]

in (43) of Theorem 3 or in the third case of (37) of Theorem 2 with \([a, b] = [1, n]. \) However, for \( n_1 = \cdots = n_d = n^{1/d} \) and \( \Delta_n^* = 1 \) as in Han et al. (2017) for \( d \geq 3, \) (43) is reduced to

\[
R_2(\hat{f}_n^{(\text{block})}, f_n) \lesssim_d n^{-1/d},
\]

which should be compared with the the rate

\[
R_2(\hat{f}_n^{(\text{lse})}, f_n) \lesssim_d n^{-1/d} \log^4(n)
\]

for the LSE (Han et al., 2017).
3.4. Adaptation rate of the block estimator with lattice designs in the piecewise constant case.

We consider here the adaptation behavior of the block estimator in the setting where \( f(\cdot) \) is piecewise constant on a union of rectangles, as a direct consequence of Theorem 2.

**Theorem 4.** Let \( \hat{f}_{n}^{(\text{block})}(x) \) be the block estimator in (16). Assume \( \varepsilon_i \) are independent variables with \( \mathbb{E}\varepsilon_i = 0 \) and \( \mathbb{E}|\varepsilon_i|^{q+2} \leq \sigma^{q+2} \) and \( f \) is non-decreasing and piecewise constant on \( V \) in the sense of \( V = \bigcup_{k=1}^{K} [a_k, b_k] \) with \( K \leq n \) and \( f(a_k) = f(b_k) \) for all \( k \leq K \). Then,

\[
R_q(\hat{f}_{n}^{(\text{block})}, f_n) \lesssim q, d \sigma^q \min \left\{ 1, n^{-1} \sum_{k=1}^{K} n_{a_k, b_k}^{1-q/2} \left( \log^{s_k} (n_{a_k, b_k}) \right)^{I(q=2)} \right\}
\]

with \( s_k = \# \{ j : b_{k,j} > a_{k,j} \} \). Moreover, if in addition \( \{ [a_k, b_k], k = 1, \ldots, K \} \) are disjoint, then

\[
R_q(\hat{f}_{n}^{(\text{block})}, f_n) \lesssim q, d \sigma^q \min \left\{ 1, \left( \frac{K}{n} \right)^{\min\{1, q/2\}} \left( \log^{d_K} (n/K) \right)^{I(q=2)} \right\},
\]

where \( d_K = \max_{1 \leq k \leq K} s_k \) is the largest dimension of \( [a_k, b_k] \) in the partition.

The rate in (44) is consistent with existing results for \( d = 1 \) under which the block estimator is the LSE and the mean squared risk bound is

\[
R_2(\hat{f}_{n}^{(\text{block})}, f_n) \lesssim \sigma^2 \frac{K}{n} \log_+(n/K).
\]

In general, the risk bound in (44) under \( q = 2 \) is reduced to at most

\[
\sigma^2 \frac{K}{n} \log^d_+(n/K),
\]

which should be compared with

\[
\sigma^2 \left( \frac{K}{n} \right)^{2/d} \log^8_+(n/K)
\]

for the LSE as in Chatterjee et al. (2018) for \( d = 2 \) and in Han et al. (2017) for \( d \geq 3 \).

**Remark 4.** Han et al. (2017) proved that even when \( f(\cdot) \) is a constant function, i.e., \( K = 1 \),

\[
R_2(\hat{f}_{n}^{(\text{lse})}, f_n) \gtrsim \sigma^2 n^{-2/d}
\]

so the adaptation rate of the LSE, \( (K/n)^{2/d} \), cannot be further improved, which means the LSE is unable to adapt to parametric rate for \( d \geq 3 \).
The adaptation rate in (44) also implies that when \([a_k, b_k]\) are two-dimensional sheets (i.e. \(|\{j : b_{k,j} \neq a_{k,j}\}| \leq 2\), the upper bound turns out to be

\[
\frac{K}{n} \log^2 (n/K),
\]

which again should be compared with

\[
\frac{K}{n} \log^8 (n/K)
\]

in Han et al. (2017).

3.5. Adaptive estimation to variable selection with lattice designs. In this subsection, we consider the case where the true function of interest, \(f(\cdot)\), depends only on a subset \(S\) of \(s\) variables, i.e., \(f(x) = f_S(x_S)\). We study the adaptive estimation when \(\max_{j \leq d} n_j \leq d n^{1/d}\), i.e., \(n_j \asymp n^{1/d}\) for all \(1 \leq j \leq d\).

**Theorem 5.** Assume \(f(\cdot)\) is non-decreasing and dependent only on an unknown set \(S\) of \(s < d\) variables. Let \(\hat{f}_n^{\text{(block)}}(x)\) be the block estimator in (16) on the lattice design \(V = [1, n]\). Assume \(\max_{1 \leq j \leq d} n_j \leq d n^{1/d}\) and \(\varepsilon_i\)'s are independent and satisfies \(E \varepsilon_i = 0\) and \(E |\varepsilon_i|^{q/2} \leq \sigma^{q/2}\). Let

\[
\Delta(f_n/\sigma) = \{f(n) - f(1)/\sigma\}.
\]

Then,

\[
\sup \left\{ R_q(f_n^{\text{(block)}}, f_n) : f_n \in F_n, f(x) = f_S(x_S), \Delta(f_n/\sigma_S) \leq \Delta^*_n, S \right\}
\]

\[
\leq d \sigma_S \min \left\{ \Lambda_{s,1}^{(\text{select})}, \Lambda_{s,2}^{(\text{select})}(\Delta^*_n/\sigma_S)^{1/d} \right\}
\]

\[
= \min \left\{ \frac{(\log n)^{q/2}}{(n^{1/d}(1-q/2))^{d-s}}, \frac{1}{(n^{1/d}(1-q/2) + 1)^{d-s}} \right\},
\]

for all \(1 \leq s \leq d\), where \(\sigma_S = \sigma/(\prod_{j \notin S} n_j)^{1/2} \leq c_d \sigma/n^{(1-s/d)/2}\) and

\[
\Lambda_{s,1}^{(\text{select})} = \left( \sum_{j=1}^{n^{1/d}} j^{-q/2} \right)(n^{1/d}(1-q/2))^{d-s},
\]

\[
\Lambda_{s,2}^{(\text{select})} = \left( \sum_{j=1}^{n^{1/d}} j^{-q/2} \right)(n^{1/d}(1-q/2) + 1)^{d-s} \log n \Gamma\left(\frac{q}{q+2}\right).
\]

In particular,

\[
R_2(f_n^{\text{(block)}}, f_n)
\]

\[
\leq d \left\{ \sigma^2 n^{s/d-1} \min \left\{ (\log n)^{d-s}, \Delta_n^{*} n^{-1/d} (\log n)^{I(s=2)} + n^{-s/d} (\log n)^d \right\}, \quad s \geq 2, 
\right.
\]

\[
\sigma^2 n^{s/d-1} \min \left\{ (\log n)^{d-1}, (\Delta_n^{*} n^{1/d})^{2/3} + n^{-1/d} (\log n)^d \right\}, \quad s = 1.
\]
In the proof of Theorem 5, the key observation is that in the sheet of $x$ with fixed $x_{S^c}$, the risk bound is identical to that of model $S$ with $\sigma^2$ reduced by a factor of $n^{-q/2}x_{S^c,n_{S^c}}^{-q/2}$. The above rate would then become clear after the summation of risk bounds over $x_{S^c}$.

Let $n_j = n^{1/d}$ for all $j$. Consider an oracle expert with the extra knowledge of the subset $S$. Suppose the oracle expert first computes the average of the $n^{1-s/d}$ values of $y_i$ holding $x_S$ fixed and then solves the $s$-dimensional isotropic regression problem at the noise level $\sigma_S = \sigma n^{(s/d-1)/2}$. For this oracle expert, the sample size becomes $n^{s/d}$ and the condition on the range-to-noise ratio becomes $(f(n) - f(1))/\sigma_S \leq \Delta^*_n$, equivalent to $(f(n) - f(1))/\sigma \leq \Delta^*_n$ with $\Delta^*_n,S = \Delta^*_n(n^{1-s/d}/2)$. It follows from (30) in Proposition 1 that for $\varepsilon_i \sim N(0, \sigma^2)$ and $\Delta^*_n,S \geq (n^{-s/d}/2) \lor (I\{q > 1 + 2/s\})$, the $\ell_q$ minimax lower bound for the oracle expert is

\[
\inf f \sup \{ R_q(\hat{f}, f_n) : f_n \in \mathcal{F}_n, f(x) = f_S(x_S), \Delta(f_n/\sigma_S) \leq \Delta^*_n \} \geq \sigma^*_n \min \left\{ 1, (\Delta^*_n,S/n^{1/d})^{\min\{1, q/(s+2)\}} \right\}.
\]

Hence the variable-selection adaptation rate in (45) matches the oracle minimax lower bound up to some constant or logarithmic factors $\Lambda^{(select)}_{s,1}, \Lambda^{(select)}_{s,2}$ and $\Lambda^{(select)}_{s,1}(\sqrt{n}\log n)^{s/I_q=2}$, provided that

\[
\Delta^*_n,S \geq \max \left( n^{-s/(2d)}, I\{q > 1 + 2/s\} \right),
\]

or equivalently $\Delta(f_n/\sigma) \leq \Delta^*_n$ with $\Delta^*_n \geq \max \left( n^{-1/2}, n^{-(1-s/d)/2} I\{q > 1 + 2/s\} \right)$. The match to the oracle minimax rate is always exact for $q = 1$ and any $s$ as both $\Lambda^{(select)}_{s,1}$ and $\Lambda^{(select)}_{s,2}$ are bounded by a constant. When $q = 2$, the match is also exact but up to some logarithmic factors as $\Lambda^{(select)}_{s,1} \prec_d (\log n)^{d-s}$ and $\Lambda^{(select)}_{s,2} \prec_d (\log n)^{I_q=s=2}$.

3.6. Multiple isotropic regression with random designs. In this subsection we consider $V = [0, 1]$ in continuum and, same as before, $a \preceq b$ iff $a \leq b$. Different from fixed designs, here $x_1, \ldots, x_n$ are i.i.d. random vectors from a distribution $\mathbb{P}$ supported on $[0, 1]$. For simplicity we assume the distribution of the design points has a Lebesgue density bounded both from above and below; for $\mu_{u,v} = \mathbb{P}\{u \leq x_i \leq v\}$ and the Lebesgue $\mu^L_{u,v} = \mu^L([u, v]) = \int_{[u,v]} d\mathcal{X}$,

\[
(47) \quad \rho_1 \mu^L_{u,v} \leq \mu_{u,v} \leq \rho_2 \mu^L_{u,v},
\]

with certain fixed constants $0 < \rho_1 \leq \rho_2 < \infty$. We consider the integrated $L_q$ risk in (3), i.e.,

\[
R_q^*(\hat{f}_n^{(block)}, f) = \int_{x \in [0,1]} \mathbb{E} |f_n^{(block)}(x) - f(x)|^q dx,
\]

and partial integrated $L_q$ risk on block $[a, b]$ as

\[
R_q^*([a, b]) = \int_{[a,b]} \mathbb{E} |f_n^{(block)}(x) - f(x)|^q dx.
\]
Theorem 6. Let $\hat{f}_n^{\text{block}}(x)$ be the block estimator in (16) with $V = [0,1]$. Assume $\mathbf{x}_1, \ldots, \mathbf{x}_n \in [0,1]$ are i.i.d. random vectors drawn from a distribution satisfying (47). Assume $f$ is non-decreasing and $\varepsilon_i$ are independent random variables with $\mathbb{E}\varepsilon_i = 0$ and $\mathbb{E}|\varepsilon_i|^{q/2} \leq \sigma^{q/2}$. Let $\{a, b\} \subset V$ with $a \leq b$. Then, for $q \geq 1$,

$$R_q^*(a, b) = \int_{[a, b]} \mathbb{E}|\hat{f}_n^{\text{block}}(x) - f(x)|^q dx$$

$$\leq C_{q,d,\rho_1,\rho_2} \sigma q \left[ \int_0^{n\mu_{a,b}} \left( (t \vee 1)^{-q/2} + \Delta_{a,b}^q e^{-t} \right) H^*(dt) \right]^2 + \int_{x \in [a, b]} \left[ \{ \{n\mu_{x,b} \vee 1 \}^{-q/2} + \Delta_{0,1}^q e^{-n\mu_{x,b}} \} dx \right],$$

where $\Delta_{a,v} = (f(v) - f(u))/\sigma$ and $\mu_{a,v} = \mathbb{P}\{ \mathbf{x}_i \in [u, v] \} \text{ for all } u \leq v \text{ and } H^*(t) = \min \{ 1, \Delta_{a,b}(n\mu_{a,b})^{-1/d \log q} + 1 \}$. Specifically, (48) is no greater than

$$\sigma q \min \left\{ \left( \Delta_{0,1}^q + 1 \right) \mu_{a,b}, \left( \frac{\Delta_{a,b}}{(n\mu_{a,b})^{1/d}} \right)^{\min \{ 1, \frac{\log q}{d} \}} \Lambda_{1}^{(\text{random})} \right\}$$

$$+ \frac{\Delta_{a,b}^{q+1}}{(n\mu_{a,b})^{1/d}} + \left( \Delta_{0,1}^q + 1 \right) \mu_{a,b} \Lambda_{2}^{(\text{random})} \left[ \log_+ \left( \frac{n\mu_{a,b} \vee \left( (n\mu_{a,b})^{2d/(d+2)} / \Delta_{a,b}^{2/(d+2)} \right) }{\Delta_{a,b}^{2/(d+2)}} \right) \right]^{I\{ \frac{\log q}{d} = 1 \}},$$

up to a constant depending on $q, d, \rho_1, \rho_2$ only, where

$$\Lambda_{1}^{(\text{random})} = \left[ \log_+ \left( (n\mu_{a,b} \vee \left( (n\mu_{a,b})^{2d/(d+2)} / \Delta_{a,b}^{2/(d+2)} \right) \right) \right]^{I\{ \frac{\log q}{d} = 1 \}},$$

and $\Lambda_{2}^{(\text{random})} = (\log_+ (n\mu_{a,b}))^{d(I\{q = 2\} + (d-1)I\{q > 2\})}.$

The $H^*(t)$ here is identical to the $\tilde{H}(t)$ in Theorem 2 in $t \in [t_d, n]$, effectively taking $t_d = 1$. This reveals an intrinsic difference between lattice design and random design: the effective dimension of the random design over $[a, b] \subseteq [0,1]$ is always $d$ — any hyper-rectangle $[a, b]$ with positive measure behaves similarly to a hyper-cube. The above rate in (49) is therefore comparable to the rate in (43) for the lattice design with $n_j = n_1^{1/d}$ for all $j$. In fact, the rate in (49) can be derived from a scale change of the upper bound for $R_q^*([0,1])$.

The study of the integrated $L_q$ risk in isotonic regression is relatively new. Fokianos et al. (2017) gives an asymptotic bound, $O(n^{-1/(d+2)})$, for the $L_1$ risk with $[a, b] = [0,1]$. The $L_1$ error bound in Theorem 6 is consistent with their result.

To fit in with random design, we now define $r_{q,+}(m)$ as a non-increasing function of $m \in [0, n]$ in continuum satisfying

$$r_{q,+}(m) \geq \max \left\{ \mathbb{E}\left( \max_{u \leq x} \sum_{x_i \in [u,v]} \frac{\varepsilon_i}{n_{u,v} \vee 1} \right)^q : \mathbb{E}[n_{x,v}] = m, x \preceq v \text{ and } v \in V_0 \right\},$$
and modify the definition of \( m_x = m_{x,+} \) in (23) to

\[
(51) \quad m_x = n_{\mu_x, v_x}, \text{ where } v_x = \arg \sup_{x \leq v \leq b} \{ n_{\mu_x, v} : f(v) \leq f(x) + r_{q,\pm}(n_{\mu_x, v}) \}.
\]

Note \( n_{x,v} \), the number of design points in \([x, v]\), becomes a Binomial\((n, \mu_{x,v})\) random variable. Here we omit \( m_{x,-} \) as it can be analyzed by symmetry. Nevertheless, Theorem 6 is still proved in a similar way to Theorem 2. However, different from (25) in Theorem 1, the point risk bound is given by the following proposition.

**PROPOSITION 3.** Assume the conditions of Theorem 6. Then, (50) holds for

\[
(52) \quad r_{q,+}(n_{\mu_x, v}) = C_{q,d, \rho, \rho_2}^q (n_{\mu_x, v} \vee 1)^{-q/2}
\]

with \( C_{q,d, \rho, \rho_2} \) continuous in \( q \in [1, \infty) \) and for all \( x \in [a, b] \)

\[
(53) \quad \mathbb{E} (\tilde{h}_n^{\text{(block)}}(x) - f(x))^q_+ \\
\leq 2^q r_{q,+}(m_x) + 2^{q-1} \sigma_q C_{q,d, \rho, \rho_2} \left( (\Delta_{a,b}^q + 1) e^{-m_x} + (\Delta_{0,1}^q + 1) e^{-n_{\mu_x, v}} \right).
\]

As we discussed below (23), the positive part of the bias of \( \tilde{f}_n^{\text{(block)}}(x) \) is of no greater order than the variability of the noise as measured by \( r_{q,+}(n_{x,v_x}) \approx r_{q,+}(m_x) \) provided the presence of at least one design point in \([x, v_x]\). The first term on the right-hand side of (53) thus comes from the case of \( n_{x,v_x} > 0 \). However, \([x, v_x]\) might be an empty cell with no design points. We then have to consider points in \([x, b]\) when \( n_{x,v_x} = 0 \) and in \([x, 1]\) when \( n_{x,b} = 0 \), leading to terms with \( \Delta_{a,b} \) and \( \Delta_{0,1} \) respectively.

Corresponding to Theorem 3 and 4, the following two theorems give the risk bounds for random designs under the general case and the piecewise constant case for the entire \([0, 1]\). Due to space limitations, the minimax rate and the adaptation rate to variable selection in random design are not discussed.

**THEOREM 7.** Let \( \tilde{h}_n^{\text{(block)}}(x) \), \( f \) and \( \{x_i, \varepsilon_i, i \leq n\} \) be as in Theorem 6. Suppose \( \Delta_{0,1} = (f(1) - f(0))/\sigma \) is bounded by a constant. Then

\[
R^*_q(\tilde{h}_n^{\text{(block)}}, f) \leq_{q,d, \rho, \rho_2} \sigma_q \left( \frac{\Delta_{0,1}}{n^{1/d}} \right) \min \{ 1, \frac{n^{d/p}}{\Delta_{0,1}} \} \left( \log n \right) I\left( \frac{n^{p/d}}{\Delta_{0,1}} = 1 \right)\]

\[
+ \frac{\left( \log n \right)^d I\{q=2\} + (d-1) I\{q>2\}}{n^{(q/2)\wedge 1}}.
\]

In particular when \( q = 2 \) and \( d \geq 2 \),

\[
(54) \quad R^*_q(\tilde{h}_n^{\text{(block)}}, f) \leq_{d, \rho, \rho_2} \sigma^2 \min \left\{ 1, \frac{\Delta_{0,1}}{n^{1/d}} \left( \log n \right)^d I\{d=2\} + \frac{\left( \log n \right)^d}{n} \right\}.
\]
Remark 5. For simplicity, we here consider the case of bounded $\Delta_{0,1}$. Theorem 6 also directly yields error bounds for general $\Delta_{0,1}$ by setting $[a, b] = [0, 1]$ in (48) and (49).

Theorem 8. Let $\hat{f}_{n}(\text{block}) (x), f$ and $\{x_i, \varepsilon_i, i \leq n\}$ be as in Theorem 6. Suppose $V$ has disjoint partition $V = \cup_{k=1}^{K} [a_k, b_k]$ with $K \leq n$ and $f(a_k) = f(b_k)$ for all $k \leq K$. Then

\[
R_{q}^{*}(\hat{f}_{n}(\text{block}), f) \preceq_{q, d, p_1, p_2} \sigma^{q} (\Delta_{0,1}^{q} + 1) \left(\frac{K}{n}\right)^{\min\{1, q/2\}} \left(\frac{\log (n/K)}{n}\right)^{d I\{q = 2\} + (d-1) I\{q > 2\}},
\]

where $\Delta_{0,1} = (f(1) - f(0))/\sigma$. In particular, when $q = 2$,

\[
R_{2}^{*}(\hat{f}_{n}(\text{block}), f) \preceq_{d, p_1, p_2} \sigma^{2} (\Delta_{0,1}^{2} + 1) \frac{K}{n} \log^{d}(n/K).
\]

We can also derive risk bounds for the empirical $\ell_{q}$ risk. As $[x_i, v_{x_i}]$ always has the design point $x_i$, there is no “empty cell” problem as in Proposition 3 when bounding the empirical risk. It follows that

\[
\mathbb{E} \left[ (\hat{f}_{n}(\text{block})(x_i) - f(x_i))^{q} \mid x_i = x \right] \preceq_{q, d, p_1, p_2} \sigma^{q} \min \left\{ \mu_{a,b}, \left(\frac{\Delta_{a,b}}{(n\mu_{a,b})^{1/d}}\right)^{\min\{1, q/2\}} \Lambda_{1}(\text{random}), \mu_{a,b} \frac{\Lambda_{1}(\text{random})}{(n\mu_{a,b})(q/2)^{1/d}} \right\}
\]

by an almost identical proof. It follows that under the conditions of Theorem 6 and $\Delta_{0,1} = 1$, the worst case upper bound of the mean squared risk is

\[
R_{2}(\hat{f}_{n}(\text{block}), f) \preceq_{d, p_1, p_2} \sigma^{2} n^{-1/d} (\log n)^{I\{d=2\}},
\]

and under the conditions of Theorem 8, the mean squared risk bound in piecewise constant case is

\[
R_{2}(\hat{f}_{n}(\text{block}), f) \preceq_{d, p_1, p_2} \sigma^{2} \frac{K}{n} \log^{d}(n/K).
\]

We shall compare the above two rates with the results for the LSE in Han et al. (2017) respectively, i.e.,

\[
\sigma^{2} n^{-1/d} \log^{\gamma_{d}}(n)
\]

and

\[
\sigma^{2} \left(\frac{K}{n}\right)^{2/d} \log^{2\gamma_{d}}(\epsilon n/K),
\]

where $\gamma_{2} = 9/2$ and $\gamma_{d} = (d^2 + d + 1)/2$ when $d \geq 3$. It is worth mentioning that Han et al. (2017) also proved the piecewise constant rate for the LSE, $(K/n)^{2/d}$, is not improvable as when $K = 1$,

\[
R_{2}(\hat{f}_{n}(\text{LSE})(x), f) \preceq_{d, p_1, p_2} \sigma^{2} n^{-2/d}.
\]
3.7. Model misspecification. We consider in this subsection properties of the block estimator in the nonparametric regression model

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

for general \( f \). When the true regression function \( f \) fails to be non-decreasing, the isotonic regression model (1) is misspecified, so that the block estimators actually estimate their noiseless versions, say \( \mathcal{F}_n^*(x) \), instead of the true \( f \). For the block max-min and min-max estimator in (10),

\[ \mathcal{F}_n^*(x) = \mathcal{F}_n^{(\text{max-min})}(x) = \max_{u \leq x, n_{u,v} > 0} \min_{x \leq v, n_{u,v} > 0} \mathcal{T}_{u,v} \quad \forall x \in V, \]

\[ \mathcal{F}_n^*(x) = \mathcal{F}_n^{(\text{min-max})}(x) = \min_{x \leq v, n_{u,v} > 0} \max_{u \leq x, n_{u,v} > 0} \mathcal{T}_{u,v} \quad \forall x \in V, \]

are their noiseless versions, where \( \mathcal{T}_A \) denotes the average of \( \{f(x_i) : 1 \leq i \leq n, x_i \in A\} \). For the average (17) of the two estimators, the noiseless version is

\[ \mathcal{F}_n^*(x) = \frac{1}{2} \left( \mathcal{F}_n^{(\text{max-min})}(x) + \mathcal{F}_n^{(\text{min-max})}(x) \right), \quad \forall x \in V. \]

The functions in (57) and (58) can be viewed as estimation targets.

Our results can be summarized as follows. If we treat \( \mathcal{F}_{n_0}^{(\text{block})}(x) - \mathcal{F}_n^*(x) \) as the estimation error and use \( \frac{\mathcal{F}_{n_0}}{\sigma} \) to measure the range-to-noise ratio, all the theoretical results we have presented so far hold in the nonparametric regression model (56) for general \( f \) with the following adjustments of the error bounds \( r_{q,\pm}(m) \) in (21) and (22),

\[ r_{q,+}(m) \geq \max \left\{ \mathbb{E} \left[ \max_{u \leq x, v > 0} \left( \sum_{x_i \in [u, v]} \frac{\varepsilon_i}{n_{u',v'}} \right)^q \right] : n_{x,v} = m, x \leq v \text{ and } v \in V_0 \right\}, \]

\[ r_{q,-}(m) \geq \max \left\{ \mathbb{E} \left[ \min_{v \leq u} \left( \sum_{x_i \in [u, v]} \frac{\varepsilon_i}{n_{u',v'}} \right)^q \right] : n_{u,x} = m, u \leq x \text{ and } u \in V_0 \right\}, \]

without changing the notation. Both \( r_{q,\pm}(m) \) are still required to be non-increasing functions of \( m \in \mathbb{N}^+ \). Accordingly, this leads to the following adjustment of the functions in (23),

\[ m_{x,-} = \max \left\{ n_{u,x} : \mathcal{F}_n^*(u) \geq \mathcal{F}_n^*(x) - r_{q,-}^{1/q}(n_{u,x}), u \leq x \text{ and } u \in V_0 \right\}, \]

\[ u_x = \arg \max_{u \in V_0} \left\{ n_{u,x} : \mathcal{F}_n^*(u) \geq \mathcal{F}_n^*(x) - r_{q,-}^{1/q}(n_{u,x}) \right\}, \]

\[ m_{x,=} = m_{x,+} = \max \left\{ n_{x,v} : \mathcal{F}_n^*(v) \leq \mathcal{F}_n^*(x) + r_{q,+}^{1/q}(n_{x,v}), x \leq v \text{ and } v \in V_0 \right\}, \]

\[ v_x = \arg \max_{v \in V_0} \left\{ n_{x,v} : \mathcal{F}_n^*(v) \leq \mathcal{F}_n^*(x) + r_{q,+}^{1/q}(n_{x,v}) \right\}, \]

with the error bounds \( r_{q,\pm}(m) \) in (59) and the estimation target \( \mathcal{F}_n^*(x) \) in (57) or (58).
Theorem 9. Let \( \hat{f}_n^{(\text{block})} \) be as in (17), \( \hat{f}_n^* \) as in (58), \( r_{q, \pm}(m) \) as in (59), and \( \ell_{\pm}(m) \) as in (24) with the \( m_{a_\pm, \pm} \) in (60). Then, the error bounds (25) and (26) of Theorem 1 hold with \( f \) replaced by \( \hat{f}_n^* \). Consequently, for the lattice design and under the \( q \sqrt{2} \) moment assumption on the noise \( \{ \varepsilon_i \} \), the error bounds in Theorems 2, 3, 4 and 5 hold with the same substitution. In particular, with \( f \) replaced by \( \hat{f}_n^* \) and \( f_n \) by \( \hat{f}_n = (\hat{f}_n^*(x_1), \ldots, \hat{f}_n^*(x_n))^T \), (36) holds with the same function \( H(t) \) when \( \{ \hat{f}_n^*(b) - \hat{f}_n^*(a) \}/\sigma \leq \Delta_n^*, \) (41) and (43) hold when \( \Delta(\hat{f}_n^*/n) \leq \Delta_n^* \), (44) holds when \( \hat{f}_n^*(a_k) = \hat{f}_n^*(b_k) \) with \( V = \bigcup_{k=1}^{K} \{ a_k, b_k \} \), and (45) and (46) hold when \( \hat{f}_n^*(x) \) depends on only \( s \) of the \( d \) variables and \( n_j \asymp n^{1/d} \) for all \( j \). The above results also hold when \( \{ \hat{f}_n^{(\text{block})}, \hat{f}_n^* \} = \{ \hat{f}_n^{(\text{max-min})}, \hat{f}_n^{(\text{max-min})} \} \) or \( \{ \hat{f}_n^{(\text{block})}, \hat{f}_n^* \} = \{ \hat{f}_n^{(\text{min-max})}, \hat{f}_n^{(\text{min-max})} \} \).

Theorem 9 asserts that \( \hat{f}_n \) is close to \( \hat{f}_n^* \) in many ways when the isotonic condition on the unknown \( f \) is misspecified. However, the interpretation of this result is not as clear as the existing oracle inequality for the LSE as \( \hat{f}_n^* \) is not based on an optimality criteria.

4. Simulation results. In this section, we report the results of several experiments in \( d = 2 \) and \( d = 3 \) to demonstrate the feasibility of the block estimators and to compare its estimation performance with the LSE. Among potentially many choices of the block estimator, we simply use the block max-min estimator as in (10). In six simulation settings, the block max-min estimator yields smaller average \( \ell_2 \) losses than the LSE, with very small \( p \)-values in piecewise constant and variable selection settings. In a seventh setting, the LSE slightly outperforms the block max-min estimator but the difference is insignificant.

To compare the LSE and the block estimator, we carry out our experiments as follows. In each experiment, we generate one unknown \( f \), 5000 replications of \( y \) with standard Gaussian noise, find the LSE and the block max-min estimator for each \( y \), and compute the mean squared losses \( \| \hat{f}_n - f_n \|_2^2/n \) for both estimators. We therefore obtain 5000 simulated losses for each estimator and take the averages to approximate their mean squared risks.

We use quadratic programming to compute the LSE in our experiments. We’d like to mention that fast algorithms for the LSE have been developed in the literature: Dykstra (1983), Kyung et al. (2015), Stout (2015), to name a few. We stick to quadratic programming as it provides somewhat more accurate results, although the difference seems small. The purpose of our experiment is to compare the risk of estimators, not the computational complexity of different algorithms. For the block max-min estimator, we use brute force which exhaustively calculates means over all blocks and finds the max-min value for each lattice point \( x \). We note again that the computation cost via brute force is of order \( n^3 \).

In \( d = 2 \), we consider isotonic regression with the \( n_1 \times n_2 \) lattice design \( [1, n] \) with \( n_1 = 50 \) and \( n_2 = 20 \), so that the number of design points in total is \( n = 1000 \). In Experiment I, we consider the function \( f(x) = c(x_1 + x_2)^{2/3} \) (here and in the sequel, \( c \) is a constant such that \( f(n) = 10 \) so that the range of \( f \) is about 10 on the lattice). As the region between two contours of this \( f \) cannot be efficiently represented by rectangular bocks, this example is not expected to favor the block estimator. In Experiment II, we split the lattice into \( 5 \times 5 \) small blocks of size \( 10 \times 4 \), randomly assign \( 1, \ldots, 10 \) to each small block, conditionally on the realizations satisfying...
the isotonic constraint. The adaptation of the LSE and the block max-min estimator to piecewise constant $f$ is compared in this experiment. Lastly, we compare the adaptation of the two estimators to variable selection in Experiment III by setting $f(x) = f_1(x_1) = c \log(x_1)$. See Figure 4, 5 and 6 for heat maps in Experiment I, II and III respectively; each figure contains heat maps for the unknown $f$, one example of observed $y$, the LSE and the block max-min estimator for this $y$. Figure 7 provides boxplots of mean squared losses of both estimators in Experiment I, II and III.

In $d = 3$, we consider isotonic regression with $n_1 \times n_2 \times n_3$ lattice designs where $n_1 = n_2 = n_3 = 10$, so that the number of design points in total is also $n = 1000$. We choose the true mean functions in a similar manner to $d = 2$. In Experiment IV, we consider $f(x) = c(x_1 + x_2 + x_3)^{2/3}$. In Experiment V, we randomly assign $1, \ldots, 10$ to $2 \times 2 \times 5$ small blocks of size $5 \times 5 \times 2$ conditionally on the isotonic constraint. Lastly, the true mean function is $f(x) = f_1(x_1) = c \log(x_1)$ in Experiment VI. See Figure 8 for boxplots of mean squared losses of both estimators in Experiment IV, V and VI.

Two basic statistics, mean and standard deviation of the losses of the LSE and the block max-min estimator and the loss difference of the two estimators are listed in Table 1, along with the two-sided $p$-value for the difference. In Experiment I and IV which are less favorable to the block estimator, the block estimator still yields slightly smaller risk, although the risk difference is insignificant (with $p$-values 0.6190 and 0.1600 respectively) in all other four experiments the block max-min estimator significantly outperforms the LSE with $p$-values 0.0062 or smaller, supporting...
FIG 5. Heatmaps for the true piecewise-constant $f$, an observed $y$, and its LSE and max-min estimate in Experiment II.

FIG 6. Heatmaps for the true $f$, an observed $y$, and its LSE and max-min estimate in Experiment III.
(a) Experiment I

(b) Experiment II

(c) Experiment III

Fig 7. Boxplots for the losses of LSE and block estimator in $d = 2$.

(a) Experiment IV

(b) Experiment V

(c) Experiment VI

Fig 8. Boxplots for the losses of LSE and block estimator in $d = 3$. 
Experiment I  Experiment II  Experiment III
LSE block diff  LSE block diff  LSE block diff
mean 0.0822 0.0807 0.0016 0.1029 0.0918 0.0111 0.0713 0.0603 0.0110
s.d. 0.0096 0.0095 0.0031 0.0156 0.0149 0.0041 0.0115 0.0109 0.0033
p-value 0.6190 0.0062 0.0007

(d = 2)

Experiment IV  Experiment V  Experiment VI
LSE block diff  LSE block diff  LSE block diff
mean 0.1412 0.1353 0.0059 0.1316 0.1096 0.0220 0.0917 0.0746 0.0170
s.d. 0.0119 0.0117 0.0042 0.0178 0.0169 0.0059 0.0160 0.0147 0.0045
p-value 0.1600 0.0002 0.0002

Table 1

The mean and standard deviation (s.d.) of the mean squared losses for the LSE and the block max-min estimator (block), and the mean, s.d. and two-sided p-value for the loss differences (diff = loss of LSE - loss of block estimator).

Our theoretical analysis. It is worthwhile to mention that, although the risk values are incomparable due to different dimension $d$, we observe more significant difference in the mean squared losses between the LSE and the block max-min estimator in $d = 3$ than in $d = 2$, in view of the $p$-values and box plots. This observation coincide with Theorem 4 and its comparison to the existing risk bounds for the LSE.

We end this section with an example in which the LSE actually yields slightly smaller mean squared risk than the block max-min estimator. In Experiment VII, we consider the two-piece function $f(x_1, x_2) = I\{x_1/n_1 + x_2/n_2 \geq 1\}$ on an $n_1 \times n_2$ lattice. Same as in Experiment I, II and III, we take $(n_1, n_2) = (50, 20)$ and add standard gaussian noises to $f(x_1, x_2)$. See the heat maps in Figure 9.

We shall recall $\widehat{f}_n^{(lse)}(x) = \mathcal{U}_{U\cap L}$ for some upper set $U$ and lower set $L$. Suppose $x_1/n_1 + x_2/n_2 \geq 1$ so that $f(x) = 1$, then the best level set $U \cap L$ for this design point is the upper red triangle in Figure 9(a). In contrast, as $\widehat{f}_n^{(block)}(x) = \mathcal{U}_{[u,v]}$ for some $u$ and $v$, the best possible block contains at most half design points of the upper triangle (when $u = (n_1/2, n_2/2)$ and $v = (n_1, n_2)$). Therefore, the variability of the block estimator at each design point may be larger than the LSE, resulting in a greater risk. Indeed, when we compare them on 5000 replications of $y$ as in Experiments I-VI, the mean squared losses for the LSE has mean 0.0420 and standard deviation 0.0090, while for the block max-min estimator the mean is 0.0440 and the standard deviation is 0.0087. However, the difference is not significant as the mean and standard deviation for the loss difference are $-0.0020$ and $0.0040$, and the two-sided $p$-value is 0.6163.

It would be difficult to characterize settings or general examples in which the LSE outperforms the block estimator. When we set $f(x) = 0.5I\{x_1/n_1 + x_2/n_2 \geq 1\}$, the average normalized $\ell_2$ loss for the LSE is 0.0298, slightly greater than 0.0280 for the block max-min estimator, but the difference is insignificant as the two-sided $p$-value is 0.5568.
FIG 9. Heatmaps for the true two-piece function $f$, an observed $y$, and its LSE and max-min estimate.

**SUPPLEMENTARY MATERIAL**

**Supplement to “Isotonic Regression in Multi-Dimensional Spaces and Graphs”**

This supplement contains proofs of all the theoretical results stated in the main body of the paper.
References.


