A nonparametric regression approach to asymptotically optimal estimation of normal means

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Abstract

Simultaneous estimation of multiple parameters has received a great deal of recent interest, with applications in multiple testing, causal inference, and large-scale data analysis. Most approaches to simultaneous estimation use empirical Bayes methodology. Here we propose an alternative, completely frequentist approach based on nonparametric regression. We show that simultaneous estimation can be viewed as a constrained and penalized least-squares regression problem, so that empirical risk minimization can be used to estimate the optimal estimator within a certain class. We show that under mild conditions, our data-driven decision rules have asymptotically optimal risk that can match the best known convergence rates for this compound estimation problem. Our approach provides another perspective to understand sufficient conditions for asymptotic optimality of simultaneous estimation. Our proposed estimators demonstrate comparable performance to state-of-the-art empirical Bayes methods in a variety of simulation settings and our methodology can be extended to apply to many practically interesting settings.

1 Introduction

The need to simultaneously estimate many parameters is common across many areas of modern applied statistics such as small area estimation, computational biology, econometrics, and signal processing. In this paper we study a canonical simultaneous estimation problem, known as the compound estimation of normal means, that serves as a foundational model in many areas of theoretical statistics such as empirical Bayes [17, 28], admissibility [45], multiple testing [1], variable selection [20], and deconvolution [37]. Here the goal is to simultaneously estimate \( \theta_1, \ldots, \theta_n \) given \( X_i \sim N(\theta_i, \sigma^2) \), where \( \sigma > 0 \) is known. The performance of our estimates is judged using the expected average squared error. Early results [40, 45] established that the naive estimator \( X_i \) is inadmissible, and that estimation of \( \theta_i \) can be improved by including other indices \( j \neq i \) in the estimation procedure. These estimators are often called shrinkage estimators because an early approach to developing them scaled the naive estimator towards zero [18]. Recent advances in computation and the prevalence of big data problems in areas such as genomics have led to a resurgence of interest in this problem [16, 32].

Most work on this problem focuses on a class of estimators called separable estimators, sometimes also called simple symmetric estimators. Separable estimators were first introduced by Robbins [40] and have the form \( \hat{\theta}_i = \delta_i(X_1, \ldots, X_n) = d(X_i) \) for some fixed, deterministic function \( d : \mathbb{R} \rightarrow \mathbb{R} \). This class is attractive because it contains the naive estimator, \( d(X_i) = X_i \), so the optimal separable estimator always matches or improves the performance of the naive estimator. Furthermore, the optimal separable estimator is also essentially asymptotically optimal within the much larger class of all permutation invariant estimators [22]. The main difficulty is that the optimal separable estimator cannot be directly computed. Robbins [40] showed that it equals

\[
d^*(x) = \frac{\sum_{i=1}^{n} \theta_i \phi_{\sigma}(\theta_i - x)}{\sum_{i=1}^{n} \phi_{\sigma}(\theta_i - x)},
\]
where \( \phi_x(\cdot) \) denotes the density function of a \( N(0, \sigma^2) \) random variable. In other words, \( d^*(x) \) depends on the unknown \( \theta_i \). A major goal of research in simultaneous estimation problems is to develop approaches for estimating \( d^*(x) \), and to show that the resulting data-driven estimators provides good simultaneous estimates of \( \theta_1, \ldots, \theta_n \).

In recent years, the dominant strategy for simultaneous estimation has been to take an empirical Bayesian approach \[18\]. This approach pretends that the true means \( \theta_1, \ldots, \theta_n \) are independent and identically distributed samples from some prior distribution \( G \). It is thus natural to estimate \( \theta_i \) using its posterior mean, which can also be expressed using Tweedie’s formula as

\[
E(\theta | X = x) = \frac{\int_{-\infty}^{\infty} \phi_x(t-x) dG(t)}{\int_{-\infty}^{\infty} \phi_x(t-x) dG(t)} = x + \sigma^2 \frac{f_G(x)}{f_G(x)},
\]

with \( f_G(x) \) denoting the marginal distribution of \( X \) \[14\]. The connection between this Bayesian formulation and the original frequentist simultaneous estimation problem is given by the fundamental theorem of compound decision theory \[27\], which states that for any separable estimator, the frequentist average expected squared error is equal to the Bayes risk under the Bayesian formulation when the prior equals \( G_n(t) = n^{-1} \sum_{i=1}^{n} 1(\theta_i \leq t) \). Indeed, letting \( G(t) = G_n(t) \) in the expected squared error rule \( d^*(x) \) \[1\]. Thus the fundamental approach of most empirical Bayesian methods is to construct plug-in estimators of \( E(\theta | X = x) \). Efron \[15\] divides empirical Bayesian methods into two classes: \( f \)-modeling and \( g \)-modeling, based on whether the marginal or prior distribution is estimated and plugged into \( d^*(x) \), respectively. A classical result is that the James-Stein estimator \[46\] can be recovered as an empirical Bayesian estimator by modeling the prior as a normal distribution \[17\]. For other parametric models of the marginal density or prior distribution the resulting estimators can also be very simple \[49, 59\].

A major reason for the popularity of the empirical Bayesian approach is that it has produced the best known estimators of \( d^* \) to date, in terms of asymptotic risk and practical implementation. Specifically, Jiang and Zhang (2009) \[27\] proposed a nonparametric \( g \)-modeling procedure that estimates the prior \( G \) using nonparametric maximum likelihood \[53\], which can be efficiently calculated using modern convex optimization techniques \[32\]. They showed that the resulting plug-in estimate \( \hat{d}_{JZ} \) of the posterior mean enjoys asymptotic ratio optimality, in other words,

\[
\limsup_{n \to \infty} \frac{E \sum_{i=1}^{n} \left[ (\hat{\theta}_i - \theta_i)^2 \right]}{E \sum_{i=1}^{n} \left[ (\hat{\theta}_i - d^*(X_i))^2 \right]} = 1
\]

under mild conditions. Similarly, Brown and Greenshtein (2009) \[11\] proposed a nonparametric \( f \)-modeling procedure that estimates the marginal \( f_G \) using a simple kernel density estimator and showed that the resulting plug-in estimate \( \hat{d}_{BG} \) of the posterior mean is also asymptotically ratio optimal.

However, the success of empirical Bayesian methods may be somewhat unexpected because the simultaneous estimation problem is fundamentally frequentist in nature. Indeed, Efron \[16\] recently described empirical Bayes in this context as suffering from a “philosophical identity problem.” There are other non-Bayesian approaches to the simultaneous estimation problem, including for example Stein’s \[45\] original geometric explanation for the inadmissibility of the naive estimator \( X_i \). Yet these other approaches have not yet to date produced estimators able to achieve the same asymptotic optimality that the nonparametric empirical Bayesian methods described above enjoy. This gap is surprising because in many instances, the empirical Bayesian and non-Bayesian approaches to the simultaneous estimation problem all lead to mathematically equivalent formulations \[17, 48, 52\].

A natural question is therefore whether any of these other approaches can be generalized to produce asymptotically optimal estimators, or whether there is something uniquely special about the empirical Bayes framework. We study this question in this paper and demonstrate that a purely frequentist nonparametric regression-type approach can also produce asymptotically optimal estimators for the compound estimation of normal means. In simulations across a variety of settings, we demonstrate performance comparable to that of the nonparametric empirical Bayes methods described above. We also provide convergence rates for the excess risk of the nonparametric regression estimators that match the rate of the state-of-the-art empirical Bayes estimator \( \hat{d}_{JZ} \) \[27\]. The key to our approach is to combine the regression modeling strategy with empirical risk minimization to write the compound estimation problem as a constrained and penalized nonparametric least-squares regression problem. The use of regression regularization strategies, such as shape
constraints, allows us to derive asymptotically optimal estimators without appealing to Bayesian arguments. We hope that our results will serve as a foundation for the development of the regression approach in settings where empirical Bayes methods struggle, such as the designing of non-separable estimators [21, 61] and the incorporation of side information [1, 60]. We also hope that our approach can lead to novel estimators with distinct advantages for frequentist questions such as confidence intervals and inference.

2 A Penalized Regression Framework

Our regression framework is motivated by the observation that finding a good estimate of the optimal separable estimator, Equation (1), in order to estimate each \( \theta_i \) from \( X_i \) closely resembles least-squares regression [48]. If we had the oracle coordinate pairs \( (X_i, \theta_i) \), we could model and estimate the optimal separable estimator, \( d^*(x) \), by minimizing the oracle loss,

\[
R_n(d) = n^{-1} \sum_{i=1}^{n} \{\theta_i - d(X_i)\}^2,
\]

using standard least-squares regression methods.

Minimizing \( R_n(d) \) is generally a difficult task; however, by sticking to the class of simple linear models, \( d_{a,b}(x) = a + bx \), Stigler [48] solved this problem by first finding the oracle regression coefficients based on \( (X_i, \theta_i) \) and then developing method-of-moments type estimates of the oracle coefficients. This class of linear functions results in a James-Stein type estimator that dominates the naive estimator, but fails to be asymptotically optimal for general \( \theta_1, \ldots, \theta_n \). The main shortcoming of Sigler’s approach is its reliance on a simple, parametric form of the estimator. Equation (1) demonstrates that optimal separable estimator, \( d^*(x) \), is generally a highly complex function that need not be well approximated by any simple, parametric model. Furthermore, as we increase the number of parameters in our model, the method-of-moments type estimation procedure may become more difficult to specify and study.

The main insight of this paper is that the use of empirical risk minimization [50] imbues the regression framework with the ability to fit nonparametric regression models that can capture the complexity of \( d^*(x) \). Here, instead of estimating the unknown minimizer of \( R_n(d) \) as in [48], our approach is to estimate unknown loss, \( R_n(d) \), so that the loss estimate can be directly minimized. The empirical risk minimization framework offers many useful tools such as the easy implementation of shape constraints and a well established set of tools for theoretical analysis from the M-estimation literature [55].

Our main task is to develop a computable estimate of \( R_n(d) \) that can be directly minimized. A natural approach is to plug in \( X_i \) for each \( \theta_i \) to produce the loss estimate \( \hat{R}_{\text{naive}}(d) = n^{-1} \sum_{i=1}^{n} \{X_i - d(X_i)\}^2 \); however, this estimate of \( R_n(d) \) is biased. Our use of “biased” here is a slight abuse of terminology since \( R_n(d) \) is a random quantity, what we mean is that \( R(d; \theta) = E\{R_n(d)\} \neq E\{\hat{R}_{\text{naive}}(d)\} \). Furthermore, we observe that \( \hat{R}_{\text{naive}}(d) \) can be exactly minimized by many functions such as the identity function. This is a problem because the identity function corresponds to the naive estimator, so we know that the minimizer of \( \hat{R}_{\text{naive}}(d) \) will never produce asymptotically optimal estimators.

The following risk decomposition, due to Stein’s lemma [47], suggests an unbiased estimate of \( R_n(d) \) for a large class of \( d(x) \). Let \( d(x) \) be an absolutely continuous function, then by Stein’s lemma we have:

\[
R(d; \theta) = \frac{1}{n} \sum_{i=1}^{n} E\{\theta_i - d(X_i)\}^2
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} E\{X_i - d(X_i)\}^2 + \frac{2}{n} \sum_{i=1}^{n} E\{(X_i - \theta_i)d(X_i)\} - \sigma^2
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} E\{X_i - d(X_i)\}^2 + \frac{2\sigma^2}{n} \sum_{i=1}^{n} E\{d'(X_i)\} - \sigma^2.
\]

We note that it is actually sufficient for \( d(x) \) to be weakly differentiable; however, we will stick to absolute continuity for consistency with our later discussion. With this risk decomposition, an unbiased estimate of
$R_n(d)$ is:

$$\hat{R}_1(d) = \frac{1}{n} \sum_{i=1}^{n} (X_i - d(X_i))^2 + \frac{2\sigma^2}{n} \sum_{i=1}^{n} d'(X_i) - \sigma^2. \quad (6)$$

The risk estimate $\hat{R}_1(d)$ is readily interpreted as a penalized least-squares loss in our regression framework where the penalty $2\sigma^2 n^{-1} \sum_{i=1}^{n} d'(X_i) - \sigma^2$ is added to our least-squares loss estimate $\hat{R}_{naive}(d)$ $\mathbf{[7]}$. The inclusion of the additive $\sigma^2$ term in the penalty does not affect the estimation procedure, but we include it to maintain the unbiased interpretation. We note that in contrast to most penalized least-squares regression problems, $\hat{R}_1(d)$ does not have a tuning parameter that governs the trade-off between the goodness-of-fit and parsimony of the fitted function.

The penalized loss $\mathbf{[6]}$, often called Stein’s unbiased risk estimate (SURE), has two important connections to existing methodology. First, since Stein’s lemma is used to compute the covariance between $X_i$ and parsimony of the fitted function, the penalty term can be thought of as a covariance penalty similar to Akaike’s information criterion and Mallow’s $C_p$ criterion $\mathbf{[13, 2, 35]}$. In contrast to most uses of these information criteria, here we include the information criteria in fitting procedure rather than use it for model evaluation after fitting the model. Secondly, if we restrict $d(x)$ to be monotone non-decreasing, the penalty term can be seen as an $\ell_1$-type penalty; this suggests many connections to existing $\ell_1$-penalized least-squares regression problems. For example, if we parameterize $d(x)$ to be a continuous, piecewise linear function with knots at each $X_i$, then for monotone non-decreasing $d(x)$ the penalized least-squares problem becomes an irregularly spaced, degree-one trend-filter $\mathbf{[50]}$. Furthermore, for any monotone non-decreasing $d(x)$, the penalty can be interpreted as a weighted total variation penalty. To see this, let $F_n(t)$ denote the empirical distribution of $X_i$, then $n^{-1} \sum_{i=1}^{n} d'(X_i) = \int_{-\infty}^{\infty} |d'(t)| dF_n(t)$, where the usual total variation is an integral with respect to the Lebesgue measure instead of the empirical measure. The usual total variation is used as a penalty for adaptive regression splines $\mathbf{[36]}$ and a constraint for saturating splines $\mathbf{[9]}$. Based on this interpretation, our approach is to estimate the optimal separable estimator by casting the problem as a self-supervised, $\ell_1$-penalized, monotone non-decreasing, least-squares regression problem.

To illustrate the simplest nontrivial application of the penalized regression framework, we return to the class of simple linear estimators used by $\mathbf{[43]}$: $d_{a,b}(x) = a + bx$. Since estimators in this class have a constant slope, our estimator is given by:

$$\hat{d}_{a,b}(x) = \arg\min_{a,b \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} (X_i - a - bX_i)^2 + 2\sigma^2 b - \sigma^2. \quad (7)$$

Our resulting estimates are $\hat{a} = (1 - \hat{b})\bar{X}_n$ and $\hat{b} = 1 - na^2 S^{-2}$, where $S^2 = \sum_{i=1}^{n} (X_i - \bar{X}_n)^2$ and $\bar{X}_n$ is the sample mean. These estimates are very close to the Efron-Morris estimator $\mathbf{[17]}$ and Stigler’s the method-of-moments type estimator $\mathbf{[18]}$ which use $n - 3$ and $n - 1$, respectively, rather than $n$ in $\hat{b}$.

We develop the penalized regression framework for large, nonparametric function classes that contain or closely approximate the optimal separable estimator $\mathbf{[1]}$. In doing so, we handle the step of estimating the risk when the class of estimators may not have a constant slope. In Section $\mathbf{[6]}$ we provide an additional shape constraint that allows for the easy development and theoretical analysis of an asymptotically optimal estimator. In Section $\mathbf{[4]}$ we develop a second asymptotically optimal estimator that trades theoretical performance for ease of implementation.

Related approaches have been considered for this problem before. Many empirical Bayesian methods such as $\mathbf{[59, 58, 60, 4]}$ use empirical risk estimation to fit their estimators. These methods get their parameterization from Tweedie’s formula $\mathbf{[2]}$ and often utilize a secondary metric, such as marginal likelihood, as their fitting criteria. In contrast our approach directly targets the risk of interest and does not utilize a parameterization based on Tweedie’s formula. Koenker and Mizera $\mathbf{[32]}$ show that within the empirical Bayes framework, shape constraints, such as monotonicity, can improve the performance of the estimation procedure; we extend this idea by illustrating the utility of additional shape constraints. Finally, Zhao and Biscarri $\mathbf{[61]}$ use the same penalized regression framework; however, their methods are limited to parametric models and may not achieve asymptotic optimality with respect to the optimal separable estimator.

By directly modeling the optimal separable estimator, the penalized regression framework can produce estimators that have no natural Bayesian interpretation. For this reason, we propose referring to the regression estimators as “$\ell$-modeling” estimators, in analogy to Efron’s decomposition of empirical Bayes methods.
into $f$- and $g$-modeling estimators \cite{15}. Our proposed name comes from the standard interpretation of regression as modeling a conditional mean. As Stigler \cite{18} points out, the standard regression approach would model the wrong expectation: $E(X \mid \theta)$; Bayesian arguments are required to make sense of the regression line we are actually interested in: $E(\theta \mid X)$.

### 3 Regression via Constrained SURE Minimization

A natural approach to developing an asymptotically optimal estimator based on the discussion above is to minimize $R$ over a suitable function class. The main challenge is that the optimal separable estimator, $d^*(x)$, depends on the unknown means $\theta_i$, so specifying a useful function class that contains $d^*(x)$ a priori is challenging. Instead, we focus on developing a data-dependent function class that contains a good approximation to $d^*(x)$. Our approach focuses on absolutely continuous functions so that $\hat{R}_1(d)$ is an unbiased estimate of the risk. We show that the penalty in $\hat{R}_1(d)$ provides insufficient regularization for minimizing over all absolutely continuous functions; however, we propose an additional shape constraint that helps to produce asymptotically optimal estimators. Once a function class is fixed, we use empirical risk minimization to estimate $d^*(x)$.

The reason $\hat{R}_1(d)$ provides insufficient regularization for absolutely continuous estimators is that there exist absolutely continuous functions that can over-fit this risk estimate. We say that a function $\hat{d}(x)$ over-fits $\hat{R}_1(d)$ if $d(x_i) = X_i$ and $d(x_i) \leq 0$ for each $i = 1, \ldots, n$; this condition describes the event where an estimator can simultaneously minimize the squared error while having a penalty that may be arbitrarily small. For example, we can construct an absolutely continuous estimator as a continuous, piecewise linear function that has two knots evenly spaced between each consecutive pair of observations so that $d_{\text{sawtooth},a}(X_i) = X_i$ and $d_{\text{sawtooth},a}(X_i) = a$ for every $i = 1, \ldots, n$ and some $a \in \mathbb{R}$. When $a \leq 0$, $d_{\text{sawtooth},a}(x)$ over-fits $\hat{R}_1(d)$.

Further, because $\hat{R}_1(d_{\text{sawtooth},a}) = 2\sigma^2 a - \sigma^2$, we can make the risk estimate $\hat{R}_1(d_{\text{sawtooth},a})$ arbitrarily small by decreasing $a$. Notice that $d_{\text{sawtooth},a}(x)$ is monotone non-decreasing, so the addition of a monotonicity constraint is not sufficient to prevent over-fitting. Figure 1 illustrates two of these curves.

Figure 1 suggests a total variation-based shape constraint on the derivative of our estimators that makes it almost surely impossible for absolutely continuous functions to over-fit $\hat{R}_1(d)$. The use of total variation is based on the examples of $d_{\text{sawtooth},a}(x)$ in Plot B of Figure 1 which exhibit too much flexibility. Moreover, we note that the absolute continuity constraint imposes no restriction on the derivative other than Lebesgue integrability; this suggests that further smoothness constraints are required if we wish to control the flexibility of the derivative. Proposition 1 provides an exact characterization of the total variation of the derivatives of functions that do not over-fit $\hat{R}_1(d)$.

**Proposition 1.** Let $x_1 < \cdots < x_n$ and $g : \mathbb{R} \to \mathbb{R}$ be an absolutely continuous function. If $TV(g') < 2(n-1)$, then there exists an $i \in \{1, \ldots, n\}$ such that either $g(x_i) \neq x_i$ or $g'(x_i) \geq 0$.

Proposition 2 characterizes $d^*(x)$ so that we can determine if it satisfies the total variation constraint proposed in Proposition 1. The characterization of $d^*(x)$ in Proposition 2 is further used to help design a function class for our empirical risk minimization fitting procedure. In particular, Proposition 2 implies that $d^*(x)$ is always bound, absolutely continuous, and monotone non-decreasing.

**Proposition 2.** The optimal separable estimator \cite{11}, $d^*(x)$, is bounded, monotone non-decreasing, and Lipschitz continuous; its derivative has bound total variation and is also Lipschitz continuous. Let $r(\theta) = \max_{i=1}^n \theta_i - \min_{i=1}^n \theta_i$ denote the range of $\theta_1, \ldots, \theta_n$. These bounds are summarized as:

1. $\min_{i=1}^n \theta_i \leq d^*(x) \leq \max_{i=1}^n \theta_i$
2. $0 \leq d'^*(x) \leq \sigma^2 r(\theta)^2$
3. $TV(d'^{*}) \leq \sigma^2 r(\theta)^2$
4. $|d''^*(x)| \leq \sigma^4 r(\theta)^3$.

Using Propositions 1 and 2, we can now choose a suitable function class for estimating $d^*(x)$. Observe that if $TV(d'^{*}) < 2(n-1)$, then we can choose an upper bound on $TV(d'^*)$ that simultaneously prevents over-fitting.
Figure 1: Two examples of absolutely continuous functions that satisfy $d_{\text{sawtooth},a}(X_i) = X_i$ and $d_{\text{sawtooth},a}'(X_i) = a$ for every $i = 1, \ldots, n$ and some $a \in \mathbb{R}$. Plot A shows $d_{\text{sawtooth},a}(x)$ functions and plot B shows their derivatives. The lines are labeled with their slopes, $a$, at each $X_i$. The dashed line is monotone non-decreasing.

of $\hat{R}_1(d)$ and ensures that $d^*(x)$ is in our function class. Since neither $TV(d'^*)$ nor $r(\theta) = \max_{i=1}^n \theta_i - \min_{i=1}^n \theta_i$ are known when defining our function class, we specify data-dependent estimates for these quantities so that both of our desired properties hold simultaneously with high probability. We find a high probability upper bound on the range of $\theta_1, \ldots, \theta_n$ by expanding the range of $X_1, \ldots, X_n$ by a non-random quantity, $b_n > 0$. We propose the following data-dependent function class:

$$D_{1,n} = \left\{ d : \mathbb{R} \to \left[ \min_i X_i - b_n, \max_i X_i + b_n \right] \mid d \text{ monotone non-decreasing, } TV(d') \leq \tau_n \right\}, \quad (8)$$

where $b_n$ and $\tau_n = \sigma^{-2}(\max_{i=1}^n X_i - \min_{i=1}^n X_i + 2b_n)^2$ are constants that can depend on $X_i$, $\sigma$, and $n$. Theorem 5 suggests that $b_n = \{3\sigma^2 \log(n)\}^{1/2}$ be used in $D_{1,n}$. The inclusion of the monotonicity constraint is advantageous because the optimal separable estimator is always monotone non-decreasing. Furthermore, we note that while all bounded functions satisfying $TV(d') \leq 1$ have finite total variation, the total variation of these functions is not uniformly bound; the combination of bounded and monotonicity constraints provide this uniform bound on the total variation. Note that the constraint $TV(d') \leq \tau_n < \infty$ ensures that all of the functions in $D_{1,n}$ are absolutely continuous.

Lemma 3 enables us to develop an estimator that asymptotically obtains the optimal risk among all separable estimators using empirical risk minimization. This is because a properly chosen $b_n$ ensures that the risk minimizer over $D_{1,n}$ is the optimal separable estimator with high probability while simultaneously...
ensuring that functions in $\mathcal{D}$ cannot over-fit $\hat{R}_1(d)$.

**Lemma 3.** Let $b_n \geq 0$ be a non-random value that may depend on $\sigma$ and $n$ and let $\mathcal{D}_{1,n}$ be defined as in [8] and $d^*(x)$ be the optimal separable estimator $\theta$, then

$$P(d^* \notin \mathcal{D}_{1,n}) \leq 6n \exp \left( -\frac{b_n^2}{2\sigma^2} \right).$$

In particular, when $b_n = (K\sigma^2 \log n)^{1/2}$ for some $K \in \mathbb{R}$, the bound becomes $6n^{1 - \frac{K}{2}}$, which can be made to converge to zero at an arbitrarily quick polynomial rate by selecting the correct $K > 2$.

We therefore define the following estimate of $d^*(x)$ using the function class using our data-dependent function class $\mathcal{D}_{1,n}$:

$$\hat{d} = \arg \min_{d \in \mathcal{D}_{1,n}} \hat{R}_1(d). \quad (9)$$

Theorem 4 shows that $\hat{d}(x)$ can be characterized as a piecewise linear function. The proof of Theorem 4 uses Carathéodory’s theorem for convex hulls [12] to reduce the infinite dimensional optimization problem over $\mathcal{D}_{1,n}$ to a finite dimensional optimization problem, similar to the proof of Theorem 1 in [9]. Notice that the range of $\hat{d}(x)$ always lies within $[\min_{i=1}^n X_i, \max_{i=1}^n X_i]$, so in practice the role of $b_n$ is only needed for defining the high probability bound $TV(d^*) \leq \tau_n$.

**Theorem 5.** For every $g \in \mathcal{D}_{1,n}$ [8], there exists a continuous, piecewise linear function, $\hat{g} \in \mathcal{D}_{1,n}$ with at most $n + 3$ knots, such that $\hat{g}(X_i) = g(X_i)$ for $i = 1, \ldots, n$, $\sum_{i=1}^n \hat{g}'(X_i) = \sum_{i=1}^n g'(X_i)$, and $\hat{g}'(x) = 0$ for $x < \min_{i=1}^n X_i$ and $x > \max_{i=1}^n X_i$.

Based on Theorem 4, we implement $\hat{d}(x)$ as a piecewise linear function: $\hat{d}(x) = \beta_0 + \sum_{j=1}^M \beta_j(x - t_j)_+$, where $(y)_+ = \max\{y, 0\}$ and $t_1 < t_2 < \cdots < t_M$ are a finite collection of fixed knots. The minimization of $\hat{R}_1(d)$ over $\beta_i$ and $t_j$ is non-convex, so in practice we fix a regular grid of knots and only optimizing over $\beta_i$, similar to [52]. We note that for fixed knots $t_1 < t_2 < \cdots < t_M$, minimizing $\hat{R}_1(d)$ over $\beta_i$ is a convex problem that can be readily solved by many off-the-shelf convex optimizers. Other potentially viable strategies for rapidly finding a good set of knots include placing knots at each of the observations or their quantiles and iterative approaches that slowly accumulate knots, similar to [9, 10]. The performance of various knot placement strategies are compared in the appendix.

Once the knots are fixed, we approximate $d(x)$ as:

$$\hat{d}(x) \approx \arg \min_{\beta_0, \beta_1, \ldots, \beta_M \in \mathbb{R}} n^{-1} \sum_{i=1}^n \left\{ X_i - \beta_0 - \sum_{j=1}^M \beta_j (X_i - t_j)_+ \right\}^2 + 2\sigma^2 n^{-1} \sum_{i=1}^n \sum_{j=1}^M \beta_j 1(X_i \geq t_j) - \sigma^2$$

subject to: $\sum_{j=1}^M \beta_j = 0$, $\sum_{j=1}^k \beta_j \geq 0$ for $k = 1, \ldots, M - 1$, $\sum_{j=1}^M |\beta_j| \leq \tau_n$,

where the constraints correspond to our bounded, monotone non-decreasing, and total variation constraints, respectively. We note that there are two interesting interpretations of this parameterization. First, when we place the knots at each of the observations, this estimator is a constrained, irregularly-spaced, degree-one trend-filter [50]; the function constraints can be easily translated into the trend-filter parameterization. Second, this parameterization resembles a degree-one locally adaptive regression spines [46] and one-dimensional MARS [19]; however, our minimization problem includes constraints and a slightly different penalty. We stick to the more general model described above for flexibility and ease of implementation.

Theorem 5 demonstrates that the conservative, high probability upper bounds on $TV(d^*)$ and $r(\theta)$ that we pursued in [8] produce an asymptotically optimal estimator. In practice, however, $\tau_n$ is usually too large and a smaller estimate may be more efficient. This follows from the observation that when our total variation constraint is active, $TV(\hat{d}) = \tau_n$, so it is very likely that $TV(d^*) < TV(\hat{d})$. We further note that because $\tau_n$ can be thought of as a tuning parameter used to regulate the size of $\mathcal{D}_{1,n}$, the optimal value of $\tau_n$ often lies in $(0, TV(d^*))$. 

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Theorem 5. Let \( X_i \sim N(\theta_i, \sigma^2) \) for \( i = 1, \ldots, n \) be independent such that \( \sigma^2 > 0 \) is known and assume \( \max_{i=1}^n |\theta_i| < C_n \). Further, let \( b_n = (3\sigma^2 \log n)^{1/2} \) and \( \tau_n = \sigma^{-2}(\max_{i=1}^n X_i - \min_{i=1}^n X_i + 2b_n)^2 \). Define \( \hat{d}(x) \) as in (9) and let \( \hat{d}^*(x) \) be the optimal separable estimator (1), then

\[
R(\hat{d}; \theta) - R(\hat{d}^*; \theta) = \mathcal{O} \left( n^{-1/2} \left( C_n + \log^{1/2} n \right)^2 \right).
\]

Theorem 5 demonstrates that our constrained and penalized regression estimator can achieve asymptotically optimal risk whenever \( C_n = o(n^{1/4}) \). The excess risk bounded in Theorem 5 is sometimes referred to as the compound regret [10, 38], and the regret rate in our result reveals an interesting connection between the Gaussian noise and range of the unknown means, \( C_n \). When \( C_n = \mathcal{O}(\log^{1/2} n) \), \( C_n \) does not affect the asymptotic regret rate and the Gaussian noise dominates the range of \( X_i \); when \( C_n \) is larger than \( \mathcal{O}(\log^{1/2} n) \) but still \( o(n^{1/4}) \), the range of the unobserved means dominates the range of \( X_i \) and the regret rate convergence is slower, but still asymptotically optimal. Intuitively this makes sense because \( E(\max_{i=1}^n |X_i - \theta_i|) \leq 2\sigma \log^{1/2} n \) [8], so when the range of \( \theta_i \) grows too quickly, the information cannot be shared as efficiently. Finally, Theorem 5 demonstrates that when \( C_n = o(n^\epsilon) \) for every \( \epsilon > 0 \), the regret of our constrained and penalized regression estimator is essentially of order \( n^{-1/2} \). This matches the best known rate for this compound estimation problem, achieved by the nonparametric g-modeling estimator \( \hat{d}_{jz} \) of Jiang and Zhang [27], whose asymptotic ratio optimality result [3] can be translated to a regret that also scales like \( n^{-1/2} \) [38].

Our proof of Theorem 5 leverages standard techniques for studying M-estimators. We use symmetrization and metric entropy bounds based on the size of \( D_{1,n} \) and the function class of its derivatives. It turns out that our total variation bound, based on Proposition 1, provides the needed control over the function class of derivatives and that the bounded and monotone non-decreasing constraints are used to bound the size of \( D_{1,n} \). We note that the monotonicity constraint is not necessary for the proof and other function classes such as bound total variation or Lipschitz over a finite domain, may be used instead; however, these alternative function classes may increase the size of the function class, introduce additional tuning parameters, or slow the rate of excess risk convergence.

Our proof techniques lead naturally to bounds on the excess risk, which is why we study regret in Theorem 5. An alternative quantity of interest would be the ratio of the two risks, as in (3). Bounding the ratio is more meaningful in settings where the optimal separable estimator may perform very well, such as when \( \theta \) is sparse and \( R(d^*; \theta) \) already tends quickly toward zero. Studying the ratio optimality of our \( \hat{d} \) would be an interesting direction for future work, and simulations in Section 5 already show that our estimator is comparable to the nonparametric empirical Bayes methods when estimating sparse \( \theta \).

4 Removing Constraints with Biased Risk Minimization

In this section we explore whether monotonicity alone, rather than monotonicity plus our total variation constraint, is sufficient for developing an asymptotically optimal estimator. We are motivated by the fact that standard isotonic least-squares regression methods do not require tuning parameters and can be implemented in linear time and memory [10]; both of these properties are very desirable for large-scale simultaneous estimation problems.

In order to avoid adding shape constraints beyond monotonicity, we revisit the discussion of over-fitting that lead to the introduction of our total variation constraint in Section 3. Because monotonicity, alone, provides sufficient regularization for standard least-squares regression [54], it is likely that our use of the empirical distribution to estimate the penalty is the reason monotone functions can over-fit \( R_1(d) \) [6]. A close decomposition of the out-of-sample risk [5] reveals that:

\[
R(d; \theta) = \frac{1}{n} \sum_{i=1}^n E(\{X_i - \hat{d}(X_i)\})^2 + 2\sigma^2 \int_{-\infty}^\infty \hat{d}'(t) \left\{ \frac{1}{n} \sum_{i=1}^n \phi_{\sigma}(t - \theta_i) \right\} dt - \sigma^2
\]

\[
= \frac{1}{n} \sum_{i=1}^n E(\{X_i - \hat{d}(X_i)\})^2 + 2\sigma^2 \int_{-\infty}^\infty \hat{d}'(t) f_{\theta}(t) dt - \sigma^2,
\]

(10)
In the Bayesian setting, when connection we sometimes refer to $h$ of $X$ is:

empirical Bayes estimator. Based on (11), our new, biased risk estimate for weakly differentiable estimators $h > 0$ is:

where $\sigma^2$ is a constant depending on $\sigma$ and $n$. As in Lemma 3, $b_n$ is used to ensure that $D_{0,n}$ contains the optimal separable estimator with high probability. This result can be established by noting that $D_{1,n} \subset D_{0,n}$ when the range of $D_{0,n}$ is at least as large as range of $D_{1,n}$. We would like to use (12) to fit functions in $D_{0,n}$; unfortunately, (12) is not well justified for this function class because not all monotone functions are weakly differentiable. In order to justify a risk estimate for all functions in $D_{0,n}$, Proposition 6 extends Stein’s lemma to apply to every bounded, monotone non-decreasing function. The proof of Proposition 6 draws heavily on a Corollary 1 in [11]. Rather than extend Stein’s lemma to apply to all of $D_{0,n}$, we could instead study a smoother function class that is a subset of $D_{0,n} \cap \{d \mid d \text{ weakly differentiable}\}$; however, this smoother function classes may introduce additional tuning parameters or make it difficult to establish a parameterization for the optimal estimator.

**Proposition 6.** Let $Z \sim N(\mu, \sigma^2)$. Let $g : \mathbb{R} \to \mathbb{R}$ have finite total variation and let $\mathcal{J}(g) = \{t_1, t_2, \ldots\}$ be the countable set of locations where $g$ has a discontinuity. Let $g'$ be the derivative of $g$ almost everywhere and assume that $E|g'(Z)| < \infty$. Then

\[
\frac{1}{\sigma^2} E[(Z - \mu)g(Z - \mu)] = E[g'(Z - \mu)] + \sum_{t_k \in \mathcal{J}(g)} \phi_\sigma(t_k - \mu) \left\{ \lim_{x \uparrow t_k} g(x) - \lim_{x \downarrow t_k} g(x) \right\}.
\]
Using Proposition 6 we can find a decomposition of \( R(d; \theta) \) that holds for every \( d \in \mathcal{D}_{0,n} \). Since every bounded, monotone non-decreasing function has finite total variation:

\[
R(d; \theta) = \frac{1}{n} \sum_{i=1}^{n} E\{X_i - d(X_i)\}^2 + 2\sigma^2 \int_{-\infty}^{\infty} d'(t) f_0(t) dt + 2\sigma^2 \sum_{t_k \in \mathcal{J}(d)} f_0(t_k) \left\{ \lim_{x \uparrow t_k} d(x) - \lim_{x \downarrow t_k} d(x) \right\} - \sigma^2,
\]

holds for every \( d(x) \in \mathcal{D}_{0,n} \), where \( \mathcal{J}(d) \) is the countable set of discontinuities of \( d(x) \), as defined in Proposition 6. Based on this risk decomposition and our plug-in estimate (11), a natural risk estimate is:

\[
\hat{R}_0(d; h) = \frac{1}{n} \sum_{i=1}^{n} \{X_i - d(X_i)\}^2 + 2\sigma^2 \int_{-\infty}^{\infty} d'(t) \hat{f}_0(t) dt + 2\sigma^2 \sum_{t_k \in \mathcal{J}(d)} \hat{f}_0(t_k) \left\{ \lim_{x \uparrow t_k} d(x) - \lim_{x \downarrow t_k} d(x) \right\} - \sigma^2. (14)
\]

As previously noted, the use of \( \hat{f}_0(t) \) makes \( \hat{R}_0(d; h) \) a biased risk estimate and some care will be needed to select the proper \( h > 0 \). Notice that because \( \hat{f}_0(t) \) is positive for all of \( \mathbb{R} \) and because only constant functions minimize both the penalty terms, \( \hat{R}_0(d; h) \) almost surely cannot be over-fit by functions in \( \mathcal{D}_{0,n} \). We propose the following estimator using this new risk estimate:

\[
\hat{d}_h = \arg \min_{d \in \mathcal{D}_{0,n}} \hat{R}_0(d; h).
\]

Theorem 7 exactly characterizes \( \hat{d}_h(x) \) for any fixed value of \( h > 0 \). This theorem is similar to Proposition 1 in Mammen and van der Geer [36] except they study the standard total variation penalty and place knots at the data, while we study a weighted total variation penalty and place knots according to the weight function. In practice, the penalized least-squares regression formulation ensures that we can ignore \( b_n \) because \( \hat{d}_h(x) \) always has a range within \([\min_{i=1}^{n} X_i, \max_{i=1}^{n} X_i]\), hence \( \mathcal{D}_{0,n} \) is free of tuning parameters in practice; however, \( b_n \) is still required to ensure that \( \mathcal{D}_{0,n} \) contains the optimal separable estimator with high probability.

**Theorem 7.** Let \( h > 0 \). For every \( g \in \mathcal{D}_{0,n} \) that is right continuous at \( X_1, \ldots, X_n \), there exists a piecewise constant function, \( \hat{g} \in \mathcal{D}_{0,n} \), that has at most \( n - 1 \) knots and satisfies \( \hat{g}(X_i) = g(X_i) \) from the right and \( \hat{R}_0(\hat{g}; h) \leq \hat{R}_0(g; h) \). The knots of \( \hat{g}(x) \) lie at the minimum of \( \hat{f}_0(t) \) between each consecutive order statistics of \( X_1, \ldots, X_n \).

Theorem 7 provides both the existence and the finite parameterization of \( \hat{d}_h(x) \). This makes exactly finding \( \hat{d}_h(x) \) a convex optimization problem for any fixed \( h > 0 \), unlike \( \hat{d}(x) \) in the previous section. For a fixed \( h > 0 \), finding the true knots can still be a somewhat time-intensive procedure and in practice placing the knots at the average of each consecutive pair of \( X_i \) provides a good approximation and alleviates much of the computational burden. We further note that the true knots may not be worth finding because they minimize \( \hat{R}_0(d; h) \), so they are random and may not be the best knots for minimizing the out-of-sample risk. Simulations comparing knot placement strategies are in the appendix. Once the knots are fixed, computing \( \hat{d}_h(x) \) can be performed using off-the-shelf convex optimization software.

We efficiently compute \( \hat{d}_h(x) \) using a tailored algorithm that builds on Theorem 7 and leverages the pool adjacent violators algorithm [11, 15]. The goal is to transform minimization of \( \hat{R}_0(d; h) \) into an unpenalized, isotonic regression problem. We assume that \( X_1 < \cdots < X_n \) without loss of generality. We first note that \( \hat{d}_h(x) \) is a piecewise constant function, by Theorem 7, so the integral term in \( \hat{R}_0(\hat{d}_h; h) \) is zero and our penalty is linear. Rather than parameterizing \( \hat{d}_h(x) \) based on the size of the step like \( \hat{d}_h(x) = \beta_0 + \sum_{i=1}^{n} \beta_i 1(x \geq t_i) \), we adopt a degree-zero trend-filter parameterization [34] for \( \hat{d}_h(x) \) allowing us to directly estimate \( \hat{d}_h(X_i) \) for each \( i = 1, \ldots, n \); this parameterization is equivalent to setting \( \beta_0 = d(X_1) \) and \( \beta_i = d(X_{i+1}) - d(X_i) \). Now, for a fixed \( h > 0 \) and knots \( t_1 < \cdots < t_{n-1} \) from Theorem 7 we define the following quantities for the matrix form of the \( \hat{R}_0(d; h) \):

\[
x = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix}, \quad d = \begin{bmatrix} d(X_1) \\ \vdots \\ d(X_n) \end{bmatrix}, \quad f_h = \begin{bmatrix} \hat{f}_h(t_1) \\ \vdots \\ \hat{f}_h(t_{n-1}) \end{bmatrix}, \quad D = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -1 \end{bmatrix}, \quad w_h = D^T f_h.
\]
Inspired by [57], we observe that the linear penalty can be absorbed into the least-squares loss as:

\[
\left( \hat{d}_h(X_1), \ldots, \hat{d}_h(X_n) \right)' = \arg \min_{d \in D_{0,n}} \| x - d \|_2^2 + 2n\sigma^2 w'd - n\sigma^2 = \arg \min_{d \in D_{0,n}} \| (x - n\sigma^2 w) - d \|_2^2. \tag{16}
\]

Since our minimization is now a monotone, least-squares regression problem, the pooled adjacent violators algorithm can be used to efficiently compute \( \hat{d}_h(X_i) \) for each \( i = 1, \ldots, n \). We do not use this trick in the previous section because of the total variation shape constraint. The use of the matrix \( D \) illustrates that this penalized regression problem is indeed a special case of a constrained and weighted degree-zero trend filter [50]. This least-squares regression problem (16) demonstrates that the introduction of a penalty is not necessary to estimate (4) if we use a better plug-in estimate of \( \theta_i \) than \( X_i \).

Corollary 8.1. Let \( X_i \sim N(\theta_i, \sigma^2) \) be independent such that \( \sigma^2 \) is known and \( \max_{i=1}^n |\theta_i| < C_n \). Further, let \( b_n = \{(8/3)\sigma^2 \log(n)\}^{1/2} \) and \( h_n > 0 \) such that \( h_n \approx \sigma n^{-1/6} \). Define \( \hat{d}_{h_n}(x) \) as in (15) and let \( d^*(x) \) be the optimal separable estimator \( \hat{d} \), then

\[
R(\hat{d}_{h_n}; \theta) - R(d^*; \theta) = O \left\{ n^{-1/3} \left( C_n + \log^{1/2} n \right)^2 \right\}.
\]

This result demonstrates that monotonicity alone can produce an asymptotically optimal estimator; however, the use of a larger function class results in a slower convergence of excess risk. The slower convergence of excess risk in Theorem 8 compared to Theorem 3 is due to the bias in the risk estimate (14). We note that while using monotonicity alone results in a slower theoretical regret rate, for a given \( h > 0 \), \( \hat{d}_h(x) \) can be approximately computed in \( O(n \log n) \) time by placing knots at the average of consecutive order statistics and using the fast Fourier transformation to approximate \( \hat{f}_h(t) \). This suggests that \( \hat{d}_h(x) \) is a good estimator for very large simultaneous estimation problems because when \( n \) is large, \( \hat{d}(x) \) remains easy to approximately compute and produces nearly optimal risk.

Corollary 8.1 continues the trend of removing constraints on the function class by demonstrating that the class of bounded functions with bounded total variation is sufficient for deriving an asymptotically optimal estimator. Increasing the size of the function class introduces an additional tuning parameter which can be estimated using a conservative, high probability upper bound, as we did in Section 3. We have no practical reason to suggest this function class; however, we conjecture that bound total variation is a necessary property for achieving asymptotically optimal risk using our penalized regression framework and analysis methods because of the interpretation of the penalty as a weighted total variation. We note that weakening the monotonicity constraint means that more general convex optimization software is required to fit the estimator; however, Theorem 7 still applies to this larger function class.

Corollary 8.1. Let \( X_i \sim N(\theta_i, \sigma^2) \) be independent such that \( \sigma^2 \) is known and \( \max_{i=1}^n |\theta_i| < C_n \). Further, let \( b_n = \{(8/3)\sigma^2 \log(n)\}^{1/2} \), \( \lambda_n = \max_{i=1}^n X_i - \min_{i=1}^n X_i + 2b_n \), and \( h_n > 0 \) such that \( h_n \approx \sigma n^{-1/6} \). Define the new function class:

\[
C_{0,n} = \left\{ d : \mathbb{R} \to \left[ \min_i X_i - b_n, \max_i X_i + b_n \right] \mid TV(d) \leq \lambda_n \right\},
\]

and the corresponding estimator \( \hat{d}_{h_n} = \arg \min_{d \in C_{1,n}} \hat{R}_0(d; h_n) \). Let \( d^*(x) \) be the optimal separable estimator \( \hat{d} \), then

\[
R(\hat{d}_{h_n}; \theta) - R(d^*; \theta) = O \left\{ n^{-1/3} \left( C_n + \log^{1/2} n \right)^2 \right\}.
\]
The estimators \( \tilde{d}(x) \) and \( \hat{d}_h(x) \) exhibit two interesting connections with empirical Bayes \( f \)-estimators. Firstly, as demonstrated in [11, 32], the monotonicity constraint is not necessary but it can improve the efficiency of the estimator in practice and replaces a tuning parameter. Secondly, the monotone \( f \)-estimator proposed by Koenker and Mizera [32] is a piecewise constant estimator, just like \( \hat{d}_h(x) \); however, because \( f_h(t) \) is not necessarily a log-concave density, there is no guarantee that the two estimators are equal for any value of \( h > 0 \). In contrast to the log-concave density estimate, we avoid justifying a secondary metric for fitting \( f_h(t) \) such as marginal maximum likelihood, by using a tuning parameter and directly targeting the risk of interest.

5 Simulations

5.1 Methods

This section compares the performance of our constrained SURE estimator [6, \( \hat{d}(x) \), and monotone-only estimator [15, \( \hat{d}_h(x) \), to state-of-the-art, asymptotically optimal, empirical Bayes estimators for the compound estimation of homoscedastic normal means. The alternative methods we consider are Jiang and Zhang’s nonparametric \( g \)-estimator, \( \hat{d}_{BG}(x) \), [27] using 300 regularly spaced knots along \( \{\min_{i=1}^n X_i, \max_{i=1}^n X_i\} \) and Brown and Greenshtein’s nonparametric \( f \)-estimator, \( \hat{d}_{BG}(x) \), [11] using their recommended bandwidth: \( h = \sigma(\log n)^{-1/2} \). All four of these estimators asymptotically achieve optimal risk, we now investigate their finite sample empirical performance using a variety of simulation settings. For computational efficiency, we fit the \( \hat{d}(x) \) using 30 regularly spaced knots along \( \{\min_{i=1}^n X_i, \max_{i=1}^n X_i\} \) and we fit \( \hat{d}_h(x) \) using knots at the average of each consecutive order statistic of \( X_1, \ldots, X_n \); further knot placement strategies are explored in the Appendix. Figure 2 visualizes each of these separable estimators applied to the same data using the optimal separable estimator as a common reference. All four of the estimators obtain asymptotically optimal risk, so they should be similar to the optimal separable estimator, \( d^*(x) \); however, they exhibit different shapes because of their estimation methods.

We pursue three distinct methods for selecting the total-variation constraint \( TV(\hat{d}) \leq \tau_n \) when fitting \( \hat{d}(x) \): a high-probability upper bound, a plug-in estimate of \( TV(d^*) \), and 5-fold cross-validation over a grid of possible \( \tau_n \). The first method is to use the high-probability upper bound \( \tau_n = \sigma^{-2}\{\max_{i=1}^n X_i - \min_{i=1}^n X_i + (3\sigma^2 \log n)^{1/2}\}^2 \) studied in Theorem 5. The second method is to develop a plug-in estimate of \( TV(d^*) \); as discussed in Section 3 we expect this bound to produce a smaller function class than the high-probability upper bound that still contains the optimal separable estimator. To develop the plug-in estimate of \( TV(d^*) \) we first estimate

\[
d^{**}(x) = \sigma^2 \frac{f^{(3)}(x)}{f_\theta(x)} - 3\sigma^2 \frac{f''(x)f'(x)}{f_\theta(x)^2} + 2\sigma^2 \left\{ \frac{f'(x)}{f_\theta(x)} \right\}^3
\]

by plugging-in \( X_i \) for \( \theta_i \) to estimate each of the \( f^{(k)}(x) \) for each \( k \in \{0, 1, 2, 3\} \), then we use use numerical integration to approximate \( TV(d^{**}) = \int_{-\infty}^{\infty} |d^{**}(x)| dx \). Because we avoid introducing a bandwidth parameter, this plug-in estimator is likely biased; however in practice it often out-performs the conservative high-probability bound. The final method to tune \( \tau_n \) is to use cross-validation. This approach draws on standard regression methodology [24]; however, we have not fully justify its use in this setting. For leave-one-out cross-validation (LOOCV), we fit \( \hat{d}^{(-i)}(x) \) using all samples \( i \neq j \), then estimate the out-of-sample risk as:

\[
\hat{R}_{1,LOOCV}(\hat{d}) = \frac{1}{n} \sum_{j=1}^{n} \{X_j - \hat{d}^{(-i)}(x_j)\}^2 + \frac{2\sigma^2}{n} \sum_{j=1}^{n} \hat{d}^{(-i)}(x_j) - \sigma^2.
\]

The development of \( k \)-fold cross-validation follows analogously to leave-one-out cross-validation by partitioning \( \{1, \ldots, n\} \) into \( k \) sets. Because the cross-validation approach ignores \( d^*(x) \) in favor of estimating and minimizing the out-of-sample risk, it is likely that the resulting \( \tau_n \) will be small enough that \( d^*(x) \notin D_{1,n} \).

The monotone-only estimator, \( \hat{d}_h(x) \), uses our asymptotic bandwidth rate: \( h = \sigma n^{-1/6} \); further bandwidth choices are explored in the Appendix. We provide \( R \) implementations of our methods in the cole package (https://github.com/sdzhao/cole).
5.2 Sparse Setting

The first set of simulations investigates the performance of estimators for various sparse, binary models. In this model we fix $n = 1000$ and $\sigma^2 = 1$, then for each simulation we set $k \in \{5, 50, 500\}$ of the $\theta_i = \mu$ for $\mu \in \{3, 4, 5, 7\}$ and set the remaining $\theta_i$ to zero; we observe independent $X_i \sim N(\theta_i, \sigma^2)$.

This sparse simulation setting is popular for studying the compound estimation of normal means because many shrinkage methods utilize sparsity structure to improve their performance [27]. Johnstone and Silverman [29] introduced this simulation setting to compare their posterior median method to many false discovery rate methods and various thresholding methods. Many other papers including [27, 11, 32, 60, 31] have extended this Johnstone and Silverman’s Table 1 to study their estimators, making this simulation setting a standard performance metric for this simultaneous estimation problem. In Table 1 we continue the pattern of using the sparse model setting to study our estimators. We provide the performance of $\hat{d}_{JZ}$ and $\hat{d}_{BG}$ in this setting from their original papers [27, 11] as a benchmark for state-of-the-art, asymptotically optimal, empirical Bayes estimators.

Table 1 demonstrates that our nonparameteric regression estimators perform comparably to the nonparametric empirical Bayes estimators over a range of sparse settings. In most settings, $\hat{d}_{JZ}$ has the best average performance of all the estimators considered followed closely by $\hat{d}(x)$, then $\hat{d}_h(x)$, and finally $\hat{d}_{BG}$. We attribute the dominance of $\hat{d}_{JZ}$ to its full use of the Gaussian noise and fast rate of compound regret convergence, see the discussion for more details. We further connect the relative performance of $\hat{d}_h(x)$ to it’s
Table 1: Table values are the total squared errors $\sum_{i=1}^{n}(\theta_i - \hat{\theta}_i)^2$ averaged across 50 replications. Our proposed monotone-only estimator \cite{15} with our default bandwidth is denoted $\hat{d}_h(x)$. Our proposed constrained SURE estimator \cite{9} with high-probability upper bound on $TV(d^*)$, plug-in estimate of $TV(d^*)$, and cross-validated $\tau_n$ are denoted $\hat{d}_{UB}(x)$, $\hat{d}_{PI}(x)$, and $\hat{d}_{CV}(x)$, respectively. The performance of the estimators $\hat{d}_{BG}$ and $\hat{d}_{JZ}$ are taken from Table 1 in \cite{11} and Table 1 in \cite{27}, respectively.

5.3 Dense Setting

The second set of simulations compares the performance of our proposed estimators to $\hat{d}_{JZ}$ and $\hat{d}_{BG}$ when the unknown means are dense. This setting is particularly interesting to us because our methodology and theory in Sections 3 and 4 make no assumptions of sparse or discrete $\theta_i$; furthermore, there are many problems of interest, such as the denoising of gene expression levels from single-cell RNA-sequencing data or the estimation of certain demographic statistics for small areas or sub-populations from limited data, that are not well captured by the sparse model.

For these simulations we fix $n = 1000$ and $\sigma^2 = 1$, then sample $\theta_1, \ldots, \theta_n \sim iid \ G$ and independently sample $X_i | \theta_i \sim N(\theta_i, 1)$. We choose a diverse collection of $G$ to represent various tail bounds and problem complexities; we note that in this sampling scheme, the tail bound $E \max_{i=1}^{n} |\theta_i|$ plays the role similar to $C_n$ in our excess risk rate theorems.

In Table 2, we consider four choices of $G$: 1) the uniform distribution on $[0, 5]$; 2) the Normal distribution with mean zero and variance of one; 3) the Laplace distribution with mean zero and variance of one; and 4) an asymmetric two-component Gaussian mixture with means at -3 and 3 and variances of 1 and 2. The first three choices of $G$ look at increasing rates of $C_n$ while the final choice of $G$ looks at asymmetry. Table 2 also introduces the James-Stein estimator \cite{46}, $\hat{d}_{JS}$, as an additional benchmark because it is optimal when $G$ is Normal.

Table 2 demonstrates a similar ranking of estimator performance to Table 1; however, we observe that our estimators perform relatively better in the denser, more complicated settings. Additionally, because Table
includes the James-Stein estimator and the Normal means setting, we observe that the nonparametric estimators adapt well to various dense settings and perform favorably to methods tailored to the specific problem.

6 Discussion

In this work we re-framed the compound estimation of normal means as a penalized, self-supervised, least-squares regression problem [2]. We showed that using nonparametric regression modeling and empirical risk minimization fitting led to the construction of entirely frequentist estimators that asymptotically achieve optimal risk. Our nonparametric regression modeling focused on finding shape constraints that simultaneously provided enough structure to avoid over-fitting the empirical risk, enabled the development of consistent estimators, and contained the oracle separable estimator with high probability.

We conjecture that the performance of our estimators in simulation can be improved to be competitive with the nonparametric $g$-modeling methods by incorporating additional shape constraints. Even when using the oracle tuned parameter, constrained SURE estimator (9) fails to consistently match the simulation performance of $d_{fZ}$ [27], even though both estimators achieve the same asymptotic compound regret rate [35] up to log-factors. We suspect that this is because our methodology targets the minimally sufficient conditions for optimally, rather than maximally utilizing the problem’s structure. For example, because both the optimal separable estimator (1), $d^*(x)$, and the nonparametric $g$-modeling estimators can be thought of as Gaussian posterior means, they have infinite, continuous, bounded derivatives; however, this property is not satisfied by all functions in the two function classes we studied. It is likely that estimating $d^*(x)$ using a smaller function class of smoother functions would improve the performance of our methodology; this is supported by the performance of the use of empirical risk minimization to estimate $d^*(x)$ directly [60].

One potential benefit of the regression approach is that it allows for the development and study of non-separable estimators. We can incorporate covariates and structural information that are useful for estimating the unknown means by including additional inputs in the estimator. The need to include covariates and structural information is prevalent in settings where there are replications that can be used as covariates [25], where there are results from auxiliary experiments [2], where there is a regular dependence structure, similar to AR($q$) [21] or pixel neighborhoods [34], and where the heteroskedastic variances are known [61]. In the general problem, we want to estimate $\theta_i$ using $X_i$, $p$ fixed covariates $C_{i1}, \ldots, C_{ip}$, and $q$ of the other observations $X_{i1}, \ldots, X_{iq}$, the regression problem becomes one of modeling and fitting the function $d(X_i, C_{i1}, \ldots, C_{ip}, X_{i1}, \ldots, X_{iq})$. A multi-dimensional version of Stein’s lemma can be used derive risk estimates that can be used to fit such non-separable estimators. A natural approach to modeling this general estimator is to use the generalized additive model: $g(X_i) + f(C_{i1}, \ldots, C_{ip}, X_{i1}, \ldots, X_{iq})$ [23, 24].

This additive model decomposition breaks the modeling and the fitting steps into separate problems so that any penalties and shape constraints can be specified separately for each function. This decomposition is closely related to the hierarchical Bayesian model studied in [20]. In this model, $f(\cdot)$ can be interpreted as an estimate of the unknown mean and $g(\cdot)$ is a shrinkage estimator adjusting for additional noise.

Finally, another implication of our work is to offer two additional explanations for why the naive estimator, $d(X_i) = X_i$, is not the best estimate of $\theta_i$. Using Stein’s lemma, we observe that our estimated penalty is a covariance penalty $\sum_{i=1}^{n} E\{d'(X_i)\} = \sum_{i=1}^{n} cov(X_i, d(X_i))$ [13]: this suggests that is we explicitly penalizing estimators for depending too much on any individual estimate. Thus, for smooth estimators, such as those in Section [2], the estimator minimizing the risk estimate must have a smaller penalty than the naive estimator, so we observe shrinkage away from the naive estimator. Furthermore, by framing the compound decision problem as a penalized regression problem we introduce the notion of over-fitting to further explain why the naive estimator is not the best estimate of $\theta_i$. The penalized regression framework additionally allows us to connect prediction in statistical learning with the estimation of empirical Bayes decision rules.

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7 Appendix

7.1 Additional Simulations

7.1.1 Knots for the Constrained SURE Estimator, \( \hat{d}(x) \)

Table 3 investigates knot placement for our constrained SURE estimator \( \hat{d}(x) \), across a selection of the simulation settings from Section 5. Throughout these simulations \( n = 1000 \) and \( \sigma^2 = 1 \). The Uniform setting draws \( \theta_i \sim iid \) Uniform\((0,5)\); the Normal setting draws \( \theta_i \sim iid \) \( N(0,1) \); the Laplace setting draws \( \theta_i \sim iid \) Laplace with a mean of zero and a variance of one; and the “Sparse k” settings refer to the settings in Table 1 where there \( k \) of the \( \theta_i = 5 \) and the rest are zero. The “M Regular” methods set \( M \) evenly spaced knots along the range of \( X_1, \ldots, X_n \); the “Order Statistics” method places knots at each observation; and the “Percentiles” places knots at the first, second, \ldots, ninety-ninth percentiles of \( X_1, \ldots, X_n \).

| method          | Uniform | Normal | Laplace | Sparse 5 | Sparse 50 | Sparse 500 |
|-----------------|---------|--------|---------|----------|-----------|------------|
| 1000 Regular    | 646     | 519    | 489     | 42       | 76        | 165        |
| 300 Regular     | 646     | 517    | 489     | 41       | 74        | 164        |
| 30 Regular      | 646     | 519    | 490     | 44       | 77        | 165        |
| Order Statistics| 646     | 521    | 505     | 118      | 76        | 165        |
| Percentiles     | 646     | 521    | 505     | 118      | 76        | 165        |

Table 3: Table values are the total squared errors \( \sum_{i=1}^{n}(\theta_i - \hat{\theta}_i)^2 \) averaged across 50 replications. In each simulation, \( \tau_n \) is first estimated using the plug-in estimator of \( \tau_n \), discussed in Section 5, then \( \hat{d}(x) \) is fit with each of the knot placements and the performance is measured.

We see that in general the knots placement makes very little difference to the efficiency of \( \hat{d}(x) \). In fact, we observe that reducing the number of knots can sometimes have a regularizing effect on the estimator. The only example in Table 3 where knot placement has a significant negative impact on the performance of \( \hat{d}(x) \) is when percentiles are used as knots in the “Sparse 5” setting. Here, there are five non-zero \( \theta_i \) but because the knots are placed every ten observations, \( \hat{d}(x) \) cannot adapt to the very sparse means. Because fitting \( \hat{d}(x) \) takes longer with more knots, we use 30 regular knots for our simulations in Section 5 to provide good performance and fast computation.

7.1.2 Knots and Density Computation for the Monotone-Only Estimator Knots, \( \hat{d}_h(x) \)

Table 4 compares various knot placement and density computation methods for our monotone-only estimator (15), \( \hat{d}_h(x) \). Specifically we look at the two knot placement strategies discussed in Section 4: the optimal knots, “Opt.” given by Theorem 7 and the approximate knots, “Approx.” placed at the average of consecutive order statistics of \( X_1, \ldots, X_n \). Additionally, we look at the performance of the two methods of computing \( \hat{f}_h(t) \): the exact method, “Exact”, and the Fast Fourier Transform, “FFT”, approximate method. The simulation settings are exactly the same as those described before Table 3.

| Knots      | Density | Uniform | Normal | Laplace | Sparse 5 | Sparse 50 | Sparse 500 |
|------------|---------|---------|--------|---------|----------|-----------|------------|
| Approx.    | FFT     | 669     | 531    | 506     | 32       | 70        | 150        |
| Approx.    | Exact   | 669     | 531    | 506     | 32       | 70        | 151        |
| Opt.       | FFT     | 671     | 531    | 506     | 33       | 71        | 153        |
| Opt.       | Exact   | 671     | 531    | 506     | 33       | 71        | 153        |

Table 4: Table values are the total squared errors \( \sum_{i=1}^{n}(\theta_i - \hat{\theta}_i)^2 \) averaged across 50 replications. In each simulation, we use the asymptotic rate for bandwidth: \( h = \sigma n^{-1/6} \).

We observe that the approximate knots seem to slightly out-perform the optimal knots. This is slightly surprising; however, we recall that the optimal knots are chosen to be optimal for the risk estimate, not the out-of-sample risk. Furthermore, we observe that because the FFT method is so accurate, there is virtually no difference in efficiency between the two methods of computing \( \hat{f}_h(t) \). Based on these observations, we
recommend and use the approximate knots and FFT approximation of \( \hat{f}_h(t) \), for fast computations and good simulation performance.

### 7.1.3 Bandwidth for the Monotone-Only Estimator, \( \hat{d}_h(x) \)

Table 5 compares various bandwidth selection methods for our monotone-only estimator (15), \( \hat{d}_h(x) \). We use a fixed grid of bandwidths to study how the optimal bandwidth may vary across simulation settings and how robust \( \hat{d}_h(x) \) is to bandwidth choice. We compare our asymptotic bandwidth rate, \( h = \sigma_n^{-1/6} \), to common bandwidth estimation methods that are included in the stats package in R [39]. The simulation settings are exactly the same as those described before Table 3.

| bw    | Uniform | Normal | Laplace | Sparse 5 | Sparse 50 | Sparse 500 |
|-------|---------|--------|---------|----------|-----------|------------|
| 0.2   | 689     | 541    | 515     | 38       | 80        | 164        |
| 0.3   | 671     | 532    | 507     | 32       | 71        | 151        |
| 0.4   | 659     | 526    | 502     | 30       | 67        | 148        |
| 0.5   | 653     | 524    | 501     | 32       | 71        | 151        |
| 0.6   | 650     | 526    | 505     | 40       | 82        | 161        |
| 0.7   | 649     | 530    | 512     | 52       | 99        | 177        |
| 0.8   | 649     | 536    | 523     | 68       | 121       | 200        |
| SJ    | 655     | 528    | 504     | 34       | 73        | 150        |
| Silverman | 659 | 530 | 507 | 36 | 75 | 162 |
| UCV   | 659     | 530    | 505     | 37       | 75        | 153        |
| \( \sigma_n^{-1/6} \) | 669     | 531    | 506     | 32       | 70        | 150        |

Table 5: Table values are the total squared errors \( \sum_{i=1}^{n} (\theta_i - \hat{\theta}_i)^2 \) averaged across 50 replications. The “SJ” bandwidth is the Sheather & Jones bandwidth [43]; the “Silverman” bandwidth is Silverman’s rule-of-thumb bandwidth [44]; the “UCV” is the unbiased mean integral squared error cross-validation estimate [52]. We use the approximate knots for each of the simulations.

Table 5 demonstrates that all of the bandwidth selection methods we consider result in nearly optimal estimators across our simulation settings. Moreover, \( \hat{d}_h(x) \) appears to be somewhat robust to bandwidth choice as good estimators can be found over a usefully wide interval, usually around 0.2-0.3 wide. This wide interval of good bandwidths suggests that many heuristic bandwidths may result in efficient estimators. Based on these results, we use our asymptotic bandwidth rate for all of our other simulations because of its theoretical support, computational speed, and overall good performance.

### 7.2 Proof of Proposition 1

**Proposition.** Let \( x_1 < \cdots < x_n \) and \( g : \mathbb{R} \to \mathbb{R} \) be an absolutely continuous function. If \( TV(g') < 2(n-1) \), then there exists an \( i \in \{1, \ldots, n\} \) such that either \( g(x_i) \neq x_i \) or \( g'(x_i) \geq 0 \).

**Proof.** We proceed by proving the contrapositive. Let \( x_1 < x_2 < \cdots < x_n \) be fixed and let \( g : \mathbb{R} \to \mathbb{R} \) be an absolutely continuous function such that \( g(x_i) = x_i \) and \( g'(x_i) \leq 0 \) for each \( i = 1, \ldots, n \).

Assume for contradiction that for every \( t \in [x_1, x_2] \), \( g'(t) < 1 \). Then by our definition of \( g \) and its absolute continuity we have:

\[
x_2 - x_1 = g(x_2) - g(x_1) \\
= \int_{x_1}^{x_2} g'(t) dt \\
< \int_{x_1}^{x_2} 1 dt \\
= x_2 - x_1.
\]
Since this is a strict inequality, we arrive at a contradiction, and thus there exists \( t_1 \in [x_1, x_2] \) such that \( g'(t_1) \geq 1 \). By analogous arguments, there exists \( t_2, \ldots, t_{n-1} \) such that \( t_i \in [x_i, x_{i+1}] \) and \( g'(t_i) \geq 1 \) for \( i = 2, \ldots, n - 1 \).

Let \( \mathcal{P} \) denote the set of all partitions of \( \mathbb{R} \) and \( n_p \) denote the number of intervals in \( \mathcal{P} \), then by the definition of supremum and our definition of \( g \), we have:

\[
TV(g') = \sup_{P \in \mathcal{P}} \sum_{i=1}^{n_p-1} |g'(z_{i+1}) - g'(z_i)|
\]

\[
\geq |g'(t_1) - g'(x_1)| + |g'(x_2) - g'(t_1)| + \cdots + |g'(t_{n-1}) - g'(x_{n-1})| + |g'(x_n) - g'(t_{n-1})|
\]

\[
= \sum_{i=1}^{n-1} |g'(t_i) - g'(x_i)| + \sum_{i=1}^{n-1} |g'(x_{i+1}) - g'(t_i)|
\]

\[
= \sum_{i=1}^{n-1} \{g'(t_i) - g'(x_i)\} + \sum_{i=1}^{n-1} \{g'(x_i) - g'(x_{i+1})\}
\]

\[
= 2 \sum_{i=1}^{n-1} g'(t_i) - \left\{g'(x_1) + g'(x_{n}) + 2 \sum_{i=2}^{n-1} g'(x_i)\right\}
\]

\[
\geq 2 \sum_{i=1}^{n-1} 1 - \left\{0 + 0 + 2 \sum_{i=2}^{n-1} 0\right\}
\]

\[
= 2(n - 1).
\]

\[\square\]

### 7.3 Proof of Proposition 2

**Proposition.** The optimal separable estimator \([1], d^*(x)\), is bounded, monotone non-decreasing, and Lipschitz continuous; its derivative has bound total variation and is also Lipschitz continuous. Let \( r(\theta) = \max_{i=1}^n \theta_i - \min_{i=1}^n \theta_i \) denote the range of \( \theta_1, \ldots, \theta_n \). These bounds are summarized as:

1. \( \min_{i=1}^n \theta_i \leq d^*(x) \leq \max_{i=1}^n \theta_i \)
2. \( 0 \leq d''(x) \leq \sigma^{-2} r(\theta)^2 \)
3. \( TV(d^*) \leq \sigma^{-2} r(\theta)^2 \)
4. \( |d'''(x)| \leq \sigma^{-4} r(\theta)^3 \).

**Proof.** We start by showing that \( d^*(x) \) is bound:

\[
d^*(x) = \sum_i \frac{\theta_i \phi(\theta_i - x)}{\sum_i \phi(\theta_i - x)}
\]

\[
\leq \sum_i \max_{i=1}^n \frac{\theta_i \phi(\theta_i - x)}{\sum_i \phi(\theta_i - x)}
\]

\[
= \max_{i=1}^n \theta_i
\]

and

\[
d^*(x) = \sum_i \frac{\theta_i \phi(\theta_i - x)}{\sum_i \phi(\theta_i - x)}
\]

\[
\geq \sum_i \min_{i=1}^n \frac{\theta_i \phi(\theta_i - x)}{\sum_i \phi(\theta_i - x)}
\]

\[
= \min_{i=1}^n \theta_i.
\]

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Next, we will show that \( d^*(x) \) is monotone and Lipschitz, this amounts to showing that its derivatives are non-negative and bound. Start by recalling the definition of \( f_\theta(x) \) and its derivatives:

\[
f_\theta(x) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\sigma} \phi \left( \frac{x - \theta_i}{\sigma} \right)
\]

\[
f'_\theta(x) = \frac{1}{n} \sum_{i=1}^{n} \phi \left( \frac{\theta_i - x}{\sigma^2} \right) \frac{1}{\sigma} \left( \frac{x - \theta_i}{\sigma} \right)
\]

\[
f''_\theta(x) = \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{(\theta_i - x)^2 - \sigma^2}{\sigma^4} \right\} \frac{1}{\sigma} \phi \left( \frac{x - \theta_i}{\sigma} \right),
\]

and define:

\[
w_i(x) = \frac{\frac{1}{n} \phi \left( \frac{x - \theta_i}{\sigma} \right)}{\sum_{j=1}^{n} \frac{1}{n} \phi \left( \frac{x - \theta_j}{\sigma} \right)}.
\]

We notice that these \( w_i(x) \) are non-negative and \( \sum_{i=1}^{n} w_i(x) = 1 \) for every \( x \). These \( w_i(x) \) happen to be the Bayesian posterior distribution weights when our prior is \( G_n(t) = n^{-1} \sum_{i=1}^{n} 1(\theta_i \leq x) \).

Following from Tweedie’s formula \([2]\), we can easily find the derivative of \( d^*(x) \) in terms of \( f_\theta(x) \):

\[
\frac{d}{dx} d^*(x) = \frac{d}{dx} \left\{ x + \sigma^2 \frac{f'_\theta(x)}{f_\theta(x)} \right\}
\]

\[
= 1 + \sigma^2 \frac{f''_\theta(x)}{f_\theta(x)} - \sigma^2 \left( \frac{f'_\theta(x)}{f_\theta(x)} \right)^2.
\]

Then using \( w_i(x) \) we can simplify \( d^*(x) \):

\[
d^*(x) = 1 + \sigma^2 \frac{f''_\theta(x)}{f_\theta(x)} - \sigma^2 \left( \frac{f'_\theta(x)}{f_\theta(x)} \right)^2
\]

\[
= 1 + \sigma^2 \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{(\theta_i - x)^2 - \sigma^2}{\sigma^4} \right\} \frac{1}{\sigma} \phi \left( \frac{x - \theta_i}{\sigma} \right) - \sigma^2 \left\{ \frac{1}{n} \sum_{i=1}^{n} \frac{(\theta_i - x)}{\sigma} \right\} - \sigma^2 \left\{ \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\sigma} \phi \left( \frac{x - \theta_i}{\sigma} \right) \right\}^2
\]

\[
= \sum_{i=1}^{n} w_i(x) \left( \frac{\theta_i - x}{\sigma} \right)^2 - \sum_{i=1}^{n} w_i(x) \left( \frac{\theta_i - x}{\sigma} \right)
\]

\[
= \sum_{i=1}^{n} w_i(x) \left\{ \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right\}^2
\]

Since \( w_i(x) \) are positive and sum to one, we can easily see that

\[
d^*(x) \geq 0
\]

\[
d^*(x) \leq \sigma^{-2} \left( \max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i \right)^2
\]

where \( r(\theta) = \max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i \).

Now, we will show that \( d^*(x) \) has finite total variation. Continuing with the definitions in the previous proof, observe that:

\[
f^{(3)}_\theta(x) = \frac{1}{n \sigma} \sum_{i=1}^{n} \left\{ \frac{(\theta_i - x)^3 - 3 \sigma^2 (\theta_i - x)}{\sigma^6} \right\} \phi \left( \frac{x - \theta_i}{\sigma} \right).
\]
and so

\[ d''''(x) = \sigma^2 f''(x) f_0(x) - 3\sigma^2 f'(x) f_0(x) + 2\sigma^2 \left( \frac{f_0''(x)}{f_0(x)} \right)^3 \]

\[ = \sigma^{-4} \sum_{i=1}^{n} w_i(x) \left\{ \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right\}^3. \]

Now we can bound \( TV(d'') \):

\[ TV(d'') = \int_{-\infty}^{\infty} |d''''(x)| \, dx \]

\[ = \int_{-\infty}^{\infty} \left| \frac{1}{\sigma^4} \sum_{i=1}^{n} w_i(x) \left\{ \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right\} \right|^3 \, dx \]

\[ \overset{(1)}{\leq} \int_{-\infty}^{\infty} \frac{1}{\sigma^4} \sum_{i=1}^{n} w_i(x) \left| \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right|^3 \, dx \]

\[ \overset{(2)}{\leq} \int_{-\infty}^{\infty} \frac{1}{\sigma^4} \sum_{i=1}^{n} w_i(x) \left\{ \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right\}^2 \left( \max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i \right) \, dx \]

\[ = \frac{\max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i}{\sigma^2} \int_{-\infty}^{\infty} \frac{1}{\sigma^2} \sum_{i=1}^{n} w_i(x) \left\{ \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right\}^2 \, dx \]

\[ = \frac{\max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i}{\sigma^2} \int_{-\infty}^{\infty} d''(x) \, dx \]

\[ \overset{(3)}{=} \frac{\max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i}{\sigma^2} \int_{-\infty}^{\infty} |d''(x)| \, dx \]

\[ = \frac{\max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i}{\sigma^2} TV(d'') \]

\[ \overset{(4)}{\leq} \frac{\max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i}{\sigma^2} \]

\[ = \sigma^{-2} r(\theta)^2 \]

Here (1) is Jensen’s inequality (noting that the \( w_i(x) \) sum to one and are non-negative); (2) bounds a single \( \theta_i - \sum_{j=1}^{n} \theta_j w_j(x) \) term by the range of \( \theta_i \), this is easy to see by remembering that \( d''(x) = \sum_{j=1}^{n} \theta_j w_j(x) \) which is bound in the range of \( \theta_i \); (3) is simply using the fact that \( d''''(x) \geq 0 \) for every \( x \in \mathbb{R} \); finally, (4) uses the bound on the total variation of \( d'''(x) \) that follows from it being bounded and monotone.

Finally, we show that \( d''''(x) \) is Lipschitz by again bounding derivatives. Continuing from the previous proof:

\[ |d''''(x)| = \left| \sigma^{-4} \sum_{i=1}^{n} w_i(x) \left\{ \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right\} \right| \]

\[ \leq \sigma^{-4} \sum_{i=1}^{n} w_i(x) \left| \theta_i - \sum_{j=1}^{n} w_j(x) \theta_j \right|^3 \]

\[ \leq \sigma^{-4} \left( \max_{i=1}^{n} \theta_i - \min_{i=1}^{n} \theta_i \right)^3 \]

\[ = \sigma^{-4} r(\theta)^3. \]
This bound is an application of Jensen’s inequality and our previous arguments using the range of \( \theta_i \) to bound the summation.

### 7.4 Proof of Lemma \[\text{Lemma. Let } b_n \geq 0 \text{ be a non-random value that may depend on } \sigma \text{ and } n \text{ and let } D_{1,n} \text{ be defined as in [8] and } d^*(x) \text{ be the optimal separable estimator [1], then}

\[
P(d^* \notin D_{1,n}) \leq 6n \exp \left\{ -\frac{\|\theta\|^2}{8\sigma^2} \right\}.
\]

In particular, when \( b_n = (K\sigma^2 \log n)^{1/2} \) for some \( K \in \mathbb{R} \), the bound becomes \( 6n^{1-\frac{K}{2}} \), which can be made to converge to zero at an arbitrarily quick polynomial rate by selecting the correct \( K > 2 \).

**Proof.** Because \( X_i - \theta_i \sim N(0, \sigma^2) \) are independent we have:

\[
P\{\min_i X_i - b_n \leq \min_i \theta_i, \max_i X_i + b_n \leq \max_i \theta_i\} = P\{\max_i (X_i - b_n) \geq \max_i (-\theta_i), \max_i X_i + b_n \leq \max_i \theta_i\}
\]

\[
= P\{\max_i (X_i - \theta_i) \geq -b_n, \max_i X_i \geq b_n\}
\]

\[
\leq P\{\max_i ((X_i - \theta_i) - (-\theta_i)) \geq -b_n, \max_i (\theta_i - X_i) \geq b_n\}
\]

\[
= P\{\max_i (\theta_i - X_i) \geq -b_n, \max_i (\theta_i - X_i) \geq b_n\}
\]

\[
= P\{\max_i (\theta_i - X_i) \geq b_n\}
\]

\[
\leq n \exp \left\{ -\frac{b_n^2}{2\sigma^2} \right\},
\]

where the first inequality is a property of the max operator and the second inequality is a standard Gaussian tail bound [8]. Similarly we have

\[
P\{\min_i \theta_i \leq \min_i X_i - b_n, \max_i \theta_i \leq \max_i X_i + b_n\} \leq n \exp \left\{ -\frac{b_n^2}{2\sigma^2} \right\}
\]

and

\[
P\{\min_i \theta_i \leq \min_i X_i - b_n, \max_i X_i + b_n \leq \max_i \theta_i\} \leq 2n \exp \left\{ -\frac{b_n^2}{2\sigma^2} \right\}.
\]

The leading factor of 2 in the above result comes from the need to bound \( P\{\max_i |X_i - \theta_i| \geq b_n\} \) rather than \( P\{\max_i (X_i - \theta_i) \geq b_n\} \). Finally, by a union bound we have:

\[
P\left(|\min_i \theta_i, \max_i \theta_i| \leq |\min_i X_i - b_n, \max_i X_i + b_n|\right) \leq P\{\min_i X_i - b_n \leq \min_i \theta_i, \max_i X_i + b_n \leq \max_i \theta_i\}
\]

\[
+ P\{\min_i \theta_i \leq \min_i X_i - b_n, \max_i \theta_i \leq \max_i X_i + b_n\}
\]

\[
+ P\{\min_i \theta_i \leq \min_i X_i - b_n, \max_i X_i + b_n \leq \max_i \theta_i\}
\]

\[
\leq 4n \exp \left\{ -\frac{b_n^2}{2\sigma^2} \right\}.
\]
Now, utilizing Proposition 2 and the definition of $\tau_n = \sigma^{-2}(\max_{i=1}^{n} X_i - \min_{i=1}^{n} X_i + 2b_n)$, we have:

$$P \{TV(d^*) > \tau_n\} = P \left\{ \sigma^{-2}(\max_i \theta_i - \min_i \theta_i)^2 > \sigma^{-2}(\max_i X_i - \min_i X_i + 2b_n)^2 \right\}$$

$$= P \left\{ \max_i \theta_i - \min_i \theta_i > \max_i X_i - \min_i X_i + 2b_n \right\}$$

$$= P \left\{ (\max_i \theta_i - \max_i X_i) + (\min_i \theta_i - \min_i X_i) > 2b_n \right\}$$

$$\leq P \left\{ \max_i (\theta_i - X_i) - \min_i (\theta_i - X_i) > 2b_n \right\}$$

$$\leq P \left\{ \max_i |\theta_i - X_i| > b_n \right\}$$

$$\leq 2n \exp \left( \frac{-b_n^2}{2\sigma^2} \right)$$

And so by applying a final union bound, noting that $d^*(x)$ is always monotone non-decreasing, we get that:

$$P (d^* \notin D_{1,n}) = P \left\{ ([\min_i \theta_i, \max_i \theta_i] \notin [\min_i X_i - b_n, \max_i X_i + b_n]) \cup \{TV(d^*) > \tau_n\} \right\}$$

$$\leq P \left\{ ([\min_i \theta_i, \max_i \theta_i] \notin [\min_i X_i - b_n, \max_i X_i + b_n]) \right\} + P \{TV(d^*) > \tau_n\}$$

$$\leq 6n \exp \left( \frac{-b_n^2}{2\sigma^2} \right).$$

Directly plugging in $b_n = (K\sigma^2 \log n)^{1/2}$ gives the bound $P (d^* \notin D_{1,n}) \leq 6n^{1-K/2}$ which converges to zero for any $K > 2$.  

7.5 Proof of Theorem 4

**Theorem.** For every $g \in D_{1,n}$ [8], there exists a continuous, piecewise linear function, $\tilde{g} \in D_{1,n}$ with at most $n + 3$ knots, such that $\tilde{g}(X_i) = g(X_i)$ for $i = 1, \ldots, n$, $\sum_{i=1}^{n} \tilde{g}'(X_i) = \sum_{i=1}^{n} g'(X_i)$, and $\tilde{g}'(x) = 0$ for $x < \min_{i=1}^{n} X_i$ and $x > \max_{i=1}^{n} X_i$.

**Proof.** This proof is based heavily on the proof of Theorem 1 in Boyd et al. [9]. Fix $x_1 < \cdots < x_n$. Our goal is to characterize the minimizer of the risk estimate (8):

$$\hat{R}_1(d) = \frac{1}{n} \sum_{i=1}^{n} (\tilde{d}(x_i) - d(x_i))^2 + 2\sigma^2 \frac{1}{n} \sum_{i=1}^{n} d'(x_i) - \sigma^2$$

over $D_{1,n} = \{ d : \mathbb{R} \to [\min_i X_i - b_n, \max_i X_i + b_n] \mid d \text{ monotone non-decreasing}, TV(d') \leq \tau_n \}$.

Fix an $g \in D_{n,1}$ such that $TV(g') = \tau$. Following from [9], we know that there is a signed measure $\mu(t)$ such that

$$g'(x) = \int_{-\infty}^{\infty} 1(t \leq x) d\mu(t)$$

$$g(x) = g(0) + \int_{-\infty}^{x - t} d\mu(t).$$

First notice that our risk estimate $\hat{R}_1(d)$ only depends on the function’s behavior at $\{x_1, \ldots, x_n\}$. This means that we can restrict $\mu(t)$ to $[x_1, x_n]$ without loss of generality, as changes made outside of that range are not relevant to our risk estimate.

Further notice that since $g(x)$ is monotone non-decreasing, it is either constant for large $|x|$ or asymptotically approaches a constant as $x \to \pm \infty$. In light of the prior observation, we can assume $g(x)$ is constant outside of $[x_1, x_n]$ without loss of generality. This implies that $\int_{-\infty}^{\infty} d\mu(t) = \int_{x_1}^{x_n} d\mu(t) = 0$. We notice that this argument generalizes to any $g(x)$ with finite total variation.
Finally notice that \( g(0) \) affects the calculation of \( \hat{R}_1(g) \) but does not depend on \( \mu(t) \) so we will ignore it (set it to zero) for the rest of this proof. This is equivalent to absorbing it into the observations in the squared error term or simply minimizing it out of the problem.

Our goal now is to show that there is a discrete, signed measure \( \omega(t) \) such that the corresponding function: 
\[
\tilde{g}(x) = \int_{x_1}^{x_n} (x - t) \, d\omega(t)
\]
matches \( g(x) \) on each \( x_i \) and has the same penalty value. We will further ensure that the function is constant outside of \([x_1, x_n]\) and has a derivative with the same total variation as \( g'(x) \).

Observe that
\[
\frac{1}{n} \sum_{i=1}^{n} g'(x_i) = \frac{1}{n} \sum_{i=1}^{n} \int_{x_1}^{x_n} 1(x_i \geq t) \, d\mu(t)
\]
\[
= \int_{x_1}^{x_n} \left\{ \frac{1}{n} \sum_{i=1}^{n} 1(x_i \geq t) \right\} \, d\mu(t)
\]
\[
0 = \int_{x_1}^{x_n} d\mu(t)
\]

Now, define the vector \( v \) as
\[
v = \left( g(x_1), \ldots, g(x_n), \frac{1}{n} \sum_{i=1}^{n} g'(x_i), 0 \right)
\]
\[
= \left( \int_{x_1}^{x_n} (x_1 - t) \, d\mu(t), \ldots, \int_{x_1}^{x_n} (x_n - t) \, d\mu(t), \int_{x_1}^{x_n} \left( \frac{1}{n} \sum_{i=1}^{n} 1(x_i \geq t) \right) \, d\mu(t), \int_{x_1}^{x_n} d\mu(t) \right)
\]
\[
= \int_{x_1}^{x_n} \left( (x_1 - t), \ldots, (x_n - t), \frac{1}{n} \sum_{i=1}^{n} 1(x_i \geq t), 1 \right) \, d\mu(t)
\]

Notice that \( n^{-1} \sum_{i=1}^{n} 1(x_i \geq t) \in [0, 1] \) for every \( t \in [x_1, x_n] \). Now define the convex set \( C \subset \mathbb{R}^{n+2} \) as:
\[
C = \left\{ \pm \left( \tau(x_1 - t), \ldots, \tau(x_n - t), \frac{1}{n} \sum_{i=1}^{n} 1(x_i \geq t), \tau \right) : t \in [x_1, x_n] \right\}.
\]

We do not need \( C \) to be convex, so long as we can say that it is in the convex hull of \( C \); however, we can see that since each components is convex \( C \) is an intersection of finitely many convex sets, and so it is convex. Notice that because \( TV(g') = TV(\mu) = \int_{-\infty}^{\infty} d\mu(t) = \tau \), we have \( v \in C \subset \mathbb{R}^{n+2} \). Since \( C \) is convex, \( v \) is also in the convex hull of \( C \), i.e. \( v \in \text{conv}(C) \).

Now by Caratheodory’s theorem for convex hulls we can represent \( v \) as the linear combination of at most \( n+3 \) points from \( \text{conv}(C) \). The standard statement of Caratheodory’s theorem for convex hulls ensures that this linear combination is a convex combination, i.e the coefficients satisfy \( \alpha_j \geq 0 \) and \( \sum_{j=1}^{n+3} \alpha_j = 1 \). It will be convenient to recognize that this implies there is at least one linear combination where the coefficients simply satisfy \( \sum_{j=1}^{M} |\alpha_j| = 1 \). Observe that there are more of these linear combinations than the convex combinations due to the loosening of the non-negativity constraint. Denote the points ensured by our extension of the Caratheodory’s theorem for convex hulls with their indices \( t_1, \ldots, t_{n+3} \in [x_1, x_n] \) and assume the corresponding coefficients satisfy \( \sum_{j=1}^{n+3} |\alpha_j| = 1 \).

Using this representation we have a new signed measure defined as \( \omega(x) = \sum_{j=1}^{n+3} \omega_j \delta_{t_j}(x) \), where \( \delta_{t_j} \) is a
Kronecker delta function placing a mass of one at $t_j$ and $\omega_j = \tau \alpha_j$. Finally, we have:

$$g(x_i) = \sum_{j=1}^{n+3} \alpha_j \tau (x_i - t_j)_+ = \sum_{j=1}^{n+3} \omega_j (x_i - t_j)_+ = \tilde{g}(x_i)$$

$$\frac{1}{n} \sum_{i=1}^{n} g'(x_i) = \sum_{j=1}^{n+3} \alpha_j \tau \frac{1}{n} \sum_{i=1}^{n} 1(x_i \geq t_j) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n+3} \omega_j 1(x_i \geq t_j) = \frac{1}{n} \sum_{i=1}^{n} \tilde{g}'(x_i) = 0 = \sum_{j=1}^{n+3} \alpha_j \tau = \sum_{j=1}^{n+3} \omega_j$$

Further notice that $\sum_{j=1}^{n+3} |\omega_j| = \sum_{j=1}^{n+3} |\alpha_j \tau| = \tau \sum_{j=1}^{n+3} |\alpha_j| = \tau$ so that $TV(\tilde{g}') = TV(g')$.

This means that we have found a new, discrete, signed measure $\omega$ such that the corresponding function $\tilde{g}(x) = \sum_{j=1}^{n+3} \omega_j (x - t_j)_+$ matches $g$ on each $x_1, \ldots, x_n$, has the same penalty value, and satisfies $TV(\tilde{g}') = TV(g')$. Further 1) since $\sum_{j=1}^{n+3} \omega_j = 0$, we have that $\tilde{g}$ saturates, and 2) because $\tilde{g}(x_i) = g(x_i)$, if $g$ is monotone non-decreasing, $\tilde{g}$ must be, too. Thus we can assume the minimizer of $\hat{R}_1(d)$ over $D_{n,1}$ is a piecewise linear function with at most $n + 3$ knots without loss of generality.

We notice that similar to Proposition [1], this argument requires $2n + 2$ knots if we want to match specific derivatives at each $x_i$, the reduction in required knots is because we are only matching the total penalty rather than each term in the summation. 

\[ \square \]

7.6 Proof of Theorem 5

7.6.1 Supporting Lemmas

Lemma 9. Let $X_i \sim N(\theta_i, \sigma^2)$ for $i = 1, \ldots, n$ be independent and $\sigma > 0$ known, then

$$E \left| \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i)^2 - \sigma^2 \right| \leq \sigma^2 (2/n)^{1/2}.$$
Proof. First observe that by independence of $X_i$, $\sigma^{-2}(X_i - \theta)^2$ are independent $\chi^2_1$ random variables, so

$$E \left\{ \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta)^2 - \sigma^2 \right\}^2 = \frac{\sigma^4}{n^2} E \left\{ \sum_{i=1}^{n} \left( \frac{X_i - \theta}{\sigma} \right)^2 - n \right\}^2$$

$$= \frac{\sigma^4}{n^2} \text{Var} \left\{ \sum_{i=1}^{n} \left( \frac{X_i - \theta}{\sigma} \right)^2 \right\}$$

$$= \frac{\sigma^4}{n^2} \cdot 2n$$

$$= \frac{2\sigma^4}{n}.$$

Our result now follows from Jensen’s inequality:

$$E \left| \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i) \right| \leq \left[ E \left\{ \left( \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i)^2 \right)^2 \right\} \right]^{1/2}$$

$$= \frac{\sigma^2 (2/n)^{1/2}}{n}.$$

\[\square\]

**Lemma 10.** Let $X_i \sim N(\theta_i, \sigma^2)$ for $i = 1, \ldots, n$ be independent with $|\theta_i| \leq C_n$ where $\sigma > 0$ and $C_n$ are known, then

$$E \left| \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i) \theta_i \right| \leq \sigma C_n n^{-1/2}.$$

Proof. First observe that for all $i = 1, \ldots, n$ $(X_i - \theta_i) \theta_i$ are independent, mean zero random variables, then

$$E \left\{ \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i) \theta_i \right\}^2 = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} E\{(X_i - \theta_i) \theta_i \cdot (X_j - \theta_j) \theta_j\}$$

$$= \frac{1}{n^2} \sum_{i=1}^{n} E\{(X_i - \theta_i) \theta_i\}^2$$

$$= \frac{1}{n^2} \sum_{i=1}^{n} \sigma^2 \theta_i^2$$

$$\leq \frac{\sigma^2}{n^2} \sum_{i=1}^{n} C_n^2$$

$$= \frac{\sigma^2 C_n^2}{n}.$$

Our result now follows from Jensen’s inequality:

$$E \left| \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i) \theta_i \right| \leq \left[ E \left\{ \left( \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i) \theta_i \right)^2 \right\} \right]^{1/2}$$

$$\leq \left( \frac{\sigma^2 C_n^2}{n} \right)^{1/2}$$

$$= \sigma C_n n^{-1/2}.$$

\[\square\]
Lemma 11. Let \( F \) denote a uniformly bounded, separable function class and fix \( x_1, \ldots, x_n \in \mathbb{R} \). Define the mean-zero random variable \( Z_f = n^{-1/2} \sum_{i=1}^{n} \epsilon_i f(x_i) \) where \( \epsilon_i \) are independent, identically distributed Rademacher random variables. Also define the empirical \( L_2 \) norm as \( \|f\|_{L_n}^2 = n^{-1} \sum_{i=1}^{n} f(x_i)^2 \). Then

\[
E \sup_{f \in F} |Z_f| \leq C \int_{0}^{2b} \{ \log N(F; L_n; t) \}^{1/2} dt,
\]

where \( C > 0 \) is a universal constant and \( \log N(F; L_n; t) \) denotes the metric entropy of the function class \( F \) with respect to the metric \( L_n \).

Proof. The proof follows from the observation that \( Z_f \) has sub-Gaussian increments with parameter \( \|f - g\|_{L_n} \). Further, we observe that if \( F \) is uniformly bound by \( b \), then \( \sup_{f,g \in F} \|f - g\|_{L_n} \leq 2b \). Now we apply a chaining argument and Dudley’s integral bound to get our desired result. More details and definitions can be found in \([25, 50]\) for much more details.

Lemma 12. Let \( R_n(d; \theta) = n^{-1} \sum_{i=1}^{n} \{ \theta_i - d(X_i) \}^2 \) and \( R(d; \theta) = ER_n(d; \theta) \). Let \( D_n \) denote one of \( D_{1,n} \) \([8]\), \( D_{o,n} \) \([13]\), or \( C_{o,n} \) (from Corollary 8.1), we note these function classes have the same data-dependent range in terms of \( X_i \) and \( b_n \). Let \( d^*(x) \) be the optimal separable estimator \([1]\) and \( d^* = \arg\min_{d \in D_n} R_n(d; \theta) \). Then for \( n \geq 3 \),

\[
E \left\{ R_n(d^*; \theta) - R_n(d^*; \theta) | d^* \notin D_n \right\} \leq 5\sigma^2 \log(n) + 4\sigma(4C_n + b_n) \log^{1/2}(n) + (b_n^2 + 8b_n C_n + 12C_n^2).
\]

Proof. Recall that \( \max_{i=1}^{n} |\theta_i| \leq C_n \). First use the triangle inequality and the range bounds on \( d^*(x) \) from Proposition 2 and \( D_n \) to see that:

\[
\max_{i=1}^{n} |d^*(X_i) - \hat{d}_n(X_i)| \leq \max_{i=1}^{n} |d^*(X_i)| + \max_{i=1}^{n} |\hat{d}(X_i)| \\
\leq \max_{i=1}^{n} |\theta_i| + \left( \max_{i=1}^{n} |X_i| + b_n \right) \\
\leq \max_{i=1}^{n} |\theta_i| + \left( \max_{i=1}^{n} |X_i - \theta_i| + \max_{i=1}^{n} |\theta_i| + b_n \right) \\
= \max_{i=1}^{n} |X_i - \theta_i| + 2\max_{i=1}^{n} |\theta_i| + b_n \\
\leq \max_{i=1}^{n} |X_i - \theta_i| + 2C_n + b_n.
\]

Now, we can bound the difference in oracle loss as:

\[
R_n(d^*; \theta) - R_n(d^*; \theta) = \frac{1}{n} \sum_{i=1}^{n} \{ \theta_i - d^*(X_i) \}^2 - \frac{1}{n} \sum_{i=1}^{n} \{ \theta_i - d^*(X_i) \}^2 \\
= \frac{1}{n} \sum_{i=1}^{n} \left[ \{ d^*(X_i) - \hat{d}_n(X_i) \}^2 + 2(\theta_i - d^*(X_i)) \{ d^*(X_i) - \hat{d}_n(X_i) \} \right] \\
\leq \frac{1}{n} \sum_{i=1}^{n} \left[ \{ d^*(X_i) - \hat{d}_n(X_i) \}^2 + 2 \{ d^*(X_i) - \hat{d}_n(X_i) \} \cdot \max_{i=1}^{n} |\theta_i - d^*(X_i)| \right] \\
\leq \frac{1}{n} \sum_{i=1}^{n} \left[ \{ d^*(X_i) - \hat{d}_n(X_i) \}^2 + 2 \{ d^*(X_i) - \hat{d}_n(X_i) \} C_n + C_n \right] \\
= \frac{1}{n} \sum_{i=1}^{n} \left[ \{ d^*(X_i) - \hat{d}_n(X_i) \}^2 + 4C_n \{ d^*(X_i) - \hat{d}_n(X_i) \} \right] \\
\leq \frac{1}{n} \sum_{i=1}^{n} \left[ \max_{i=1}^{n} \{ d^*(X_i) - \hat{d}_n(X_i) \}^2 + 4C_n \max_{i=1}^{n} \{ d^*(X_i) - \hat{d}_n(X_i) \} \right] \\
= \left\{ \max_{i=1}^{n} \{ d^*(X_i) - \hat{d}_n(X_i) \}^2 + 4C_n \max_{i=1}^{n} \{ d^*(X_i) - \hat{d}_n(X_i) \} \right\}.
\]
The first inequality in the above bound is a Hölder 1-infinity bound; the second inequality is another instance of the triangle inequality and range bounds; and, the third inequality uses the fact that the max is larger than the average.

Finally, we can plug these results into the main bound we are interested in. Below we use maximal inequalities for both Gaussian random variables and chi-squared random variables. Let \( n \geq 3 \), then

\[
E\left\{ R_n(\theta, \hat{d}_n) - R_n(\theta, d^*) \mid d^* \notin D_n \right\} 
\leq E \left\{ \left[ \max_{i=1}^n \left| d^*(X_i) - \hat{d}^*(X_i) \right| \right]^2 + 4C_n \max_{i=1}^n \left| d^*(X_i) - \hat{d}^*(X_i) \right| \mid D \subseteq D_n \right\} 
\leq E \left\{ \left( \max_{i=1}^n |X_i - \theta_i| + 2C_n + b_n \right)^2 \right\} + 4C_n \left( \max_{i=1}^n |X_i - \theta_i| + 2C_n + b_n \right) 
= E \left\{ \left( \max_{i=1}^n |X_i - \theta_i| \right)^2 + (8C_n + 2b_n) \max_{i=1}^n |X_i - \theta_i| + (b_n^2 + 8b_n C_n + 12C_n^2) \right\} 
\leq \sigma^2 \left\{ 1 + 2(\log(n))^{1/2} + 2 \log(n) \right\} + (8C_n + 2b_n) \sigma \left\{ 2 \log(2n) \right\}^{1/2} + (b_n^2 + 8b_n C_n + 12C_n^2) 
\leq 5\sigma^2 \log(n) + 4\sigma (4C_n + b_n) \log(n) \right\}^{1/2} + (b_n^2 + 8b_n C_n + 12C_n^2) 

\]

\[ \square \]

### 7.6.2 Theorem \[5\]

**Theorem.** Let \( X_i \sim N(\theta_i, \sigma^2) \) for \( i = 1, \ldots, n \) be independent such that \( \sigma^2 > 0 \) is known and assume \( \max_{i=1}^n |\theta_i| < C_n \). Further, let \( b_n = \sigma(3 \log n)^{1/2} \) and \( r_n = \sigma^{-2}(\max_{i=1}^n X_i - \min_{i=1}^n X_i + 2b_n)^2 \). Define \( d(x) \) as in \[9\] and let \( d^*(x) \) be the optimal separable estimator \[1\], then

\[
R(\hat{d}; \theta) - R(d^*; \theta) = \mathcal{O} \left\{ n^{-1/2} \left( C_n + \log^{1/2} n \right)^2 \right\}.
\]

**Proof.** Recall or define the following estimators:

\[
d^*(x) = \arg \min_{d : \mathbb{R} \to \mathbb{R}} R(d; \theta) \\
\hat{d}^*(x) = \arg \min_{d \in D_1, n} R_n(d; \theta) \\
\hat{d}(x) = \arg \min_{d \in D_1, n} \hat{R}_1(d).
\]

We break the excess risk into two terms:

\[
R(\hat{d}; \theta) - R(d^*; \theta) = \left\{ R(\hat{d}; \theta) - R(d^*; \theta) \right\} + \left\{ R(d^*; \theta) - R(d^*; \theta) \right\}.
\]

We refer to these terms as estimation error and an approximation error, respectively. We start by bounding the approximation error.

First observe that we can bound the approximation error using the law of total expectation (tower rule), Lemma \[ 5 \] and Lemma \[ 12 \]

\[
R(d^*; \theta) - R(d^*; \theta) = E R_n(\hat{d}^*; \theta) - E R_n(d^*; \theta) 
= E \left\{ R_n(\theta, \hat{d}^*) - R_n(\theta, \hat{d}^*) \mid d^* \in D_1, n \right\} \mathbb{P} \left\{ d^* \in D_1, n \right\} 
+ E \left\{ R_n(\theta, \hat{d}^*) - R_n(\theta, \hat{d}^*) \mid d^* \notin D_1, n \right\} \mathbb{P} \left\{ d^* \notin D_1, n \right\} 
\leq 0 \cdot \mathbb{P} \left\{ d^* \in D_1, n \right\} + E \left\{ R_n(\theta, \hat{d}^*) - R_n(\theta, d^*) \mid d^* \notin D_1, n \right\} \mathbb{P} \left\{ d^* \notin D_1, n \right\} 
= E \left\{ R_n(\theta, \hat{d}^*) - R_n(\theta, d^*) \mid d^* \notin D_1, n \right\} \mathbb{P} \left\{ d^* \notin D_1, n \right\} 
\leq \left\{ 5\sigma^2 \log(n) + 4\sigma (4C_n + b_n) \log^{1/2}(n) + (b_n^2 + 8b_n C_n + 12C_n^2) \right\} \cdot 6n \exp \left( \frac{-b_n^2}{2\sigma^2} \right)
\]

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Now, letting \( b_n = \sigma(K \log n)^{1/2} \), we get:

\[
R(d^*; \theta) - R(d^*; \theta) = \mathcal{O} \left\{ n^{1-\frac{K}{2}} \left( C_n + \sigma \log^{1/2} n \right)^2 \right\}
\]

We will plug-in \( K = 3 \) later to minimize the total excess risk bound.

Now we bound the estimation error using M-estimation techniques (symmeterization and metric entropy bounds) [53,56]. When necessary, we will use subscripts to denote which random variables an expectation is being taken over. Let \( X'_i \) be an independent copy of \( X_i \) and \( \epsilon_i \) be independent Rademacher random variables. Then observe by a symmeterization argument and Theorem 2.2 in [53]:

\[
E \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \left( (X_i - \theta_i) d(X_i) - E_{X_i}(X_i - \theta_i) d(X_i) \right) \right|
\]

\[
= E_X \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \left( (X_i - \theta_i) d(X_i) - E_{X_i}(X'_i - \theta_i) d(X'_i) \right) \right|
\]

\[
= E_X \sup_{d \in \mathcal{D}_n} \left| E_{X',X} \frac{1}{n} \sum_{i=1}^n \left( (X_i - \theta_i) d(X_i) - (X'_i - \theta_i) d(X'_i) \right) \right|
\]

\[
\leq E_{X,X'} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \left( (X_i - \theta_i) d(X_i) - (X'_i - \theta_i) d(X'_i) \right) \right|
\]

\[
= E_{X,X'} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i \left( (X_i - \theta_i) d(X_i) - (X'_i - \theta_i) d(X'_i) \right) \right|
\]

\[
\leq 2E_{X_i} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i (X_i - \theta_i) d(X_i) \right|
\]

\[
= 2E_{X_i} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i X_i - \theta_i d(X_i) \right|
\]

\[
= 2E_{X_i} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i X_i - \theta_i d(X_i) \right| \frac{\max_{i=1}^n |X_i - \theta_i|}{\max_{i=1}^n |X_i - \theta_i|}
\]

\[
= 2E_{X_i} \left\{ \max_{i=1}^n |X_i - \theta_i| \cdot \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i \frac{|X_i - \theta_i|}{\max_{i=1}^n |X_i - \theta_i|} d(X_i) \right| \right\}
\]

\[
= 2E \left\{ \max_{i=1}^n |X_i - \theta_i| \cdot \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i \frac{|X_i - \theta_i|}{\max_{i=1}^n |X_i - \theta_i|} d(X_i) \right| \right\}
\]

\[
\leq 2E \left\{ \max_{i=1}^n |X_i - \theta_i| \cdot \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i d(X_i) \right| \right\}
\]

Now we can bound the inner expectation using Lemma [11] Van der Geer [54] uses [5] and [53] to establish that

\[
\log N(D_{1,n}; L; t) \leq A \frac{B_n}{t}
\]

for some universal constant \( A > 0 \) and \( B_n = \max_{i=1}^n X_i - \min_{i=1}^n X_i + 2b_n \). The numerator of the entropy bound comes from scaling the class of all monotone functions whose range is \([0, 1]\) to have the range of \( D_{1,n} \). Notice that \( B_n \leq 2\max_{i=1}^n |X_i - \theta_i| + 2C_n + 2b_n \), so applying Lemma [11] and standard maximal inequalities.
for \( n \geq 3 \) we have:

\[
E \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \{(X_i - \theta_i)d(X_i) - E_{\tau_i}(X_i - \theta_i)d(X_i)\} \right|
\]

\[
\leq 2E \left[ \max_{i=1}^{n} |X_i - \theta_i| \cdot \sup_{d \in \mathcal{D}_n} \left\{ \frac{1}{n} \sum_{i=1}^{n} \epsilon_i d(X_i) \right\} \right]
\]

\[
\leq 2E \left[ \max_{i=1}^{n} |X_i - \theta_i| \cdot n^{-1/2} C \int_0^{2B_n} \{ \log N(F; L_n; t) \}^{1/2} dt \right]
\]

\[
\leq 2E \left\{ \max_{i=1}^{n} |X_i - \theta_i| \cdot n^{-1/2} C \int_0^{2B_n} (AB_n/t)^{1/2} dt \right\}
\]

\[
= 2E \left\{ \max_{i=1}^{n} |X_i - \theta_i| \cdot n^{-1/2} 2\sqrt{2C\sqrt{AB_n}} \right\}
\]

\[
\leq \frac{4C(2A)^{1/2}}{n^{1/2}} E \left\{ \max_{i=1}^{n} |X_i - \theta_i| \cdot 2 \left( \max_{i=1}^{n} |X_i - \theta_i| + C_n + b_n \right) \right\}
\]

\[
= C_1 n^{-1/2} E \left\{ \left( \max_{i=1}^{n} |X_i - \theta_i| \right)^2 + (C_n + b_n) \max_{i=1}^{n} |X_i - \theta_i| \right\}
\]

\[
\leq C_1 n^{-1/2} E \left\{ \max_{i=1}^{n} |X_i - \theta_i|^2 + (C_n + b_n) \max_{i=1}^{n} |X_i - \theta_i| \right\}
\]

\[
\leq C_1 n^{-1/2} \left[ \sigma^2 \left\{ 1 + 2(\log n)^{1/2} + 2\log(n) \right\} + (C_n + b_n)\sigma \left\{ 2\log(2n) \right\}^{1/2} \right]
\]

\[
\leq C_1 n^{-1/2} \left\{ 5\sigma^2 \log n + 2\sigma(C_n + b_n)(\log n)^{1/2} \right\}
\]

\[
= O \left[ n^{-1/2} \left\{ \log n + C_n(\log n)^{1/2} \right\} \right],
\]

where \( C_1 = 4C(2A)^{1/2} > 0 \) is a constant and the final big-O notation is simplified by plugging in \( b_n = \sigma(K \log n)^{1/2} \) with \( K > 0 \).

A similar bound, but with simpler symmetrization, can be used to bound the final component of our proof. First, we need to make a few observations about the class of derivatives in \( \mathcal{D}_{1,n} \). Fix an arbitrary \( d \in \mathcal{D}_{1,n} \), then because \( d \) is bounded and monotone, we have \( d'(x) \to 0 \) as \( x \to \pm \infty \). Since \( TV(d') \leq \tau_n = \sigma^{-2}B_n^2 \) we know that the class of derivatives is bound in \([-0.5\tau_n, 0.5\tau_n]\), hence the function class, \( \{d'|d \in \mathcal{D}_{1,n}\} \) has a range uniformly bound by \( \tau_n/2 \) and a total variation less than \( \tau_n \). This implies the following metric entropy bound on the class of derivatives \([54]\):

\[
\log N(\{d'|d \in \mathcal{D}_{1,n}\}; L_n; t) \leq A_2 \frac{\tau_n^2}{t},
\]

where \( A_2 > 0 \) is fixed. Recall that \( \tau_n = \sigma^{-2}(\max_{i=1}^{n} X_i - \min_{i=1}^{n} X_i + 2b_n)^2 \) and let \( n \geq 3 \), then by
symmetrization, a chaining bound (Lemma 11), and standard maximal inequalities [8], we have:

\[ E_X \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \{d'(X_i) - E_X d'(X_i)\} \right| \]

\[ = E_X \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \{d'(X_i) - E_X d'(X_i')\} \right| \]

\[ = E_X \sup_{d \in \mathcal{D}_n} E_{X'} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \{d'(X_i) - d'(X_i')\} \right| \]

\[ \leq E_{XX'} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \{d'(X_i) - d'(X_i')\} \right| \]

\[ = E_{XX'} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i \{d'(X_i) - d'(X_i')\} \right| \]

\[ \leq 2E_{X'} \sup_{d \in \mathcal{D}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i d'(X_i) \right| \]

\[ \leq 2E_X \left[ n^{-1/2} C \int_0^{\tau_n} \{ \log N(\{d'|d \in \mathcal{D}_{1,n}\}; L_n; t)\}^{1/2} dt \right] \]

\[ \leq 2E_X \left\{ n^{-1/2} C \int_0^{\tau_n} (A_2 \tau_n/t)^{1/2} dt \right\} \]

\[ = 4CA_2^{1/2} n^{-1/2} E_X (\tau_n) \]

\[ \leq 16CA_2^{1/2} \sigma^{-2} n^{-1/2} E_X \left\{ \left( \max_{i=1}^{n} |X_i - \theta_i| + C_n + b_n \right)^2 \right\} \]

\[ = C_2 n^{-1/2} E_X \left\{ \max_{i=1}^{n} (X_i - \theta_i)^2 + 2(C_n + b_n) \max_{i=1}^{n} |X_i - \theta_i| + (C_n + b_n)^2 \right\} \]

\[ \leq C_2 n^{-1/2} \sigma^2 \left\{ 1 + 2(\log n)^{1/2} + 2 \log(n) \right\} \]

\[ + 2(C_n + b_n) \sigma^2 \left( 2 \log(2n) \right)^{1/2} + (C_n + b_n)^2 \]

\[ \leq C_2 n^{-1/2} \left[ 5 \sigma^2 \log(n) + 4(C_n + b_n) \sigma (\log n)^{1/2} + (C_n + b_n)^2 \right] \]

\[ = n^{-1/2} \left\{ (C_n + b_n) + \sigma (\log n)^{1/2} \right\}^2 \]

\[ = O \left[ n^{-1/2} \left\{ C_n + \sigma (\log n)^{1/2} \right\}^2 \right], \]

where \( C_2 = 16CA_2^{1/2} \sigma^{-2} > 0 \) is a constant and the final big-O notation is simplified by plugging in \( b_n = \sigma(K \log n)^{1/2} \) with \( K > 0 \).

Thus our final bound on the estimation error can be found by a global supremum approach and combining
the above results with Lemma 9 and Lemma 10. We start with the basic inequality:

\[
R(\hat{d}; \theta) - R(d^*; \theta)
\]

\[
= E \left\{ R_n(\hat{d}; \theta) - R_n(d^*; \theta) \right\}
\]

\[
= E \left\{ R_n(\hat{d}; \theta) - \hat{R}_1(\hat{d}) + \hat{R}_1(\hat{d}) - \hat{R}_1(d^*) + \hat{R}_1(d^*) - R_n(d^*; \theta) \right\}
\]

\[
\leq E \left\{ R_n(\hat{d}; \theta) - \hat{R}_1(\hat{d}) + \hat{R}_1(d^*) - R_n(d^*; \theta) \right\}
\]

\[
\leq 2E \sup_{d \in D} \left| R_n(\hat{d}; \theta) - \hat{R}_1(\hat{d}) \right|
\]

\[
= 2E \sup_{d \in D} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ \theta_i - d(X_i) \right\}^2 - \frac{1}{n} \sum_{i=1}^{n} \left\{ X_i - d(X_i) \right\}^2 - 2\sigma^2 \frac{1}{n} \sum_{i=1}^{n} d'(X_i) + \sigma^2 \right|
\]

\[
= 2E \sup_{d \in D} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ -(X_i - \theta_i)^2 - 2\theta_i(X_i - \theta_i) + 2(X_i - \theta_i)d(X_i) - 2\sigma^2 d'(X_i) + \sigma^2 \right\} \right|
\]

\[
= 2E \sup_{d \in D} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ \sigma^2 - (X_i - \theta_i)^2 - 2\theta_i(X_i - \theta_i) + 2(X_i - \theta_i)d(X_i) \right\} \right|
\]

\[
- 2\sigma^2 E_x d'(X_i) + 2\sigma^2 E_x d'(X_i) - 2\sigma^2 d'(X_i) \right|
\]

\[
= 2E \sup_{d \in D} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ \sigma^2 - (X_i - \theta_i)^2 - 2\theta_i(X_i - \theta_i) + 2(X_i - \theta_i)d(X_i) \right\} \right|
\]

\[
- 2E_x \left\{ (X_i - \theta_i)d(X_i) \right\} + 2\sigma^2 E_x d'(X_i) - 2\sigma^2 d'(X_i) \right|
\]

\[
\leq 2E \left| \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i)^2 - \sigma^2 \right| + 4E \left| \frac{1}{n} \sum_{i=1}^{n} (X_i - \theta_i)\theta_i \right|
\]

\[
+ 4E \sup_{d \in D_n} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ (X_i - \theta_i)d(X_i) - E_x (X_i - \theta_i)d(X_i) \right\} \right|
\]

\[
+ 4E \sup_{d \in D_n} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ d'(X_i) - E_x d'(X_i) \right\} \right|
\]

\[
\leq \frac{2\sqrt{2}\sigma^2}{\sqrt{n}} + \frac{2\sigma C_n}{\sqrt{n}} + O \left[ n^{-1/2} \left\{ \log n + C_n (\log n)^{1/2} \right\} \right] + o \left[ n^{-1/2} \left\{ C_n + \sigma (\log n)^{1/2} \right\}^2 \right],
\]

where the * equality is an application of Stein’s lemma [47].

Finally, we recall that \( b_n = \sigma(K \log n)^{1/2} \) is hidden in the numerator of the final two big-O terms above as a multiplicative factor. This suggests that we take \( K = 3 \) so that both the estimation error and approximation error go to zero at the same rate, up to log-terms. Thus

\[
R(\hat{d}; \theta) - R(d^*; \theta) = O \left\{ n^{-1/2} \left( C_n + \log^{1/2} n \right)^2 \right\}.
\]

\[ \square \]

7.7 Proof of Proposition 6

**Proposition.** Let \( Z \sim N(\mu, \sigma^2) \). Let \( g : \mathbb{R} \to \mathbb{R} \) have finite total variation and let \( \mathcal{J}(g) = \{ t_1, t_2, \ldots \} \) be the countable set of locations where \( g \) has a discontinuity. Let \( g' \) be the derivative of \( g \) almost everywhere
and assume that $E|g'(Z)| < \infty$. Then

$$\frac{1}{\sigma^2}E[(Z - \mu)g(Z - \mu)] = E[g'(Z - \mu)] + \sum_{t_k \in J(g)} \phi_\sigma(t_k - \mu) \left( \lim_{x \uparrow t_k} g(x) - \lim_{x \downarrow t_k} g(x) \right).$$

Proof. Let $Z \sim N(0, 1)$ let $\phi$ denote the pdf of $Z$. Fix $f : \mathbb{R} \to \mathbb{R}$ such that $f$ has bounded variation, $TV(f) < \infty$. Because $f$ has bound variation, it has at most a countable number of discontinuities (this follows from $f$ being the difference of two bounded, monotone non-decreasing function), which must be either jump-type or removable-type discontinuities. Let $J(f) = \{t_1, t_2, \ldots \}$ denote the set locations where $f$ has a discontinuity. Assume the following notational shorthand:

$$\lim_{t \uparrow x} f(t) = f(x-) \quad \text{and} \quad \lim_{t \downarrow x} f(t) = f(x+).$$

Observe that

$$E\{f'(Z)\} = \int_{-\infty}^{\infty} f'(z) \phi(z) dz$$

$$= \int_0^\infty f'(z) \phi(z) dz - \int_{-\infty}^0 f'(z) (-\phi(z)) dz$$

$$(i) = \int_0^\infty f'(z) \left( \int_x^\infty t \phi(t) dt \right) dz - \int_{-\infty}^0 f'(z) \left( \int_{-\infty}^z t \phi(t) dt \right) dz$$

$$(ii) = \int_0^\infty t \phi(t) \left( \int_0^t f'(z) dz \right) dt - \int_{-\infty}^0 t \phi(t) \left( \int_0^t f'(z) dz \right) dt,$$

where $\phi(t)$ is the density function of a $N(0, 1)$ random variable, (i) comes from $-t \phi(t) = \phi'(t)$, and (ii) is Fubini’s Theorem. Notice that by the fundamental theorem of Lebesgue integral calculus we have:

$$f(t) + f(0) = \int_0^t f'(x) dx + \sum_{t_i \in J(f)} \{f(t_i) + f(t_i) - f(t_i) - f(t_i)\} 1(0 \leq t_i \leq t).$$

Now we can rearrange the first term in the above decomposition of $E\{f'(Z)\}$:

$$\int_0^\infty t \phi(t) \left( \int_0^t f'(z) dz \right) dt = \int_0^\infty t \phi(t) \left[ f(t) + f(0) - \sum_{t_i \in J(f)} \{f(t_i) + f(t_i) - f(t_i)\} 1(0 \leq t_i \leq t) \right] dt$$

$$= \int_0^\infty t \phi(t) \left\{ f(t) + f(0) \right\} dt$$

$$- \int_0^\infty t \phi(t) \left[ \sum_{t_i \in J(f)} \{f(t_i) + f(t_i) - f(t_i)\} 1(0 \leq t_i \leq t) \right] dt$$

$$= \int_0^\infty t \phi(t) \left\{ f(t) + f(0) \right\} dt$$

$$- \sum_{t_i \in J(f)} \{f(t_i) + f(t_i) - f(t_i)\} \int_0^\infty t \phi(t) 1(0 \leq t_i \leq t) dt$$

$$= \int_0^\infty t \phi(t) \left\{ f(t) + f(0) \right\} dt - \sum_{t_i \in J(f) : t_i > 0} \{f(t_i) + f(t_i) - f(t_i)\} \int_0^\infty t \phi(t) dt$$

$$= \int_0^\infty t \phi(t) \left\{ f(t) + f(0) \right\} dt - \sum_{t_i \in J(f) : t_i > 0} \{f(t_i) + f(t_i) - f(t_i)\} E\{Z \cdot 1(Z \geq t_i)\},$$

where (i) is Fubini’s theorem, noting that $J(f)$ may be countably infinite. The second term follows analogously. Notice that $E\{Z \cdot 1(Z \leq a)\} = -\phi(a)$ and $E\{Z \cdot 1(Z \geq a)\} = \phi(a)$ for all $a \geq 0$. So, putting these
results together we get:

\[
E\{f'(Z)\} = \left[ \int_0^\infty t\phi(t) \sum_{t_i \in J(f): t_i > 0} \{f(t_i)_+ - f(t_i)_-\} E\{Z \cdot 1(Z \geq t_i)\} \right. \\
\left. - \int_{-\infty}^0 t\phi(t) \sum_{t_i \in J(f): t_i < 0} \{f(t_i)_+ - f(t_i)_-\} E\{Z \cdot 1(Z \leq t_i)\} \right]
\]

\[
= E\{Zf(Z)\} - \sum_{t_i \in J(f): t_i > 0} \{f(t_i)_+ - f(t_i)_-\} \phi(t_i) \\
\]

\[
= E\{Zf(Z)\} - \sum_{t_i \in J(f): t_i < 0} \{f(t_i)_+ - f(t_i)_-\} \phi(t_i) \\
\]

\[
= E\{Zf(Z)\} - \sum_{t_i \in J(f)} \{f(t_i)_+ - f(t_i)_-\} \phi(t_i). \\
\]

The last equality comes from the fact that if \(0 \notin J(f)\), then \(f(0)_+ - f(0)_- = 0\). We note that by our use of the fundamental theorem of Lebesgue integral calculus, removable-type discontinuities do not affect the value of the expectation because \(f(t_i)_+ - f(t_i)_- = 0\) when \(f\) has a removable-type discontinuity at \(t_i\). We chose the notation \(J(f)\) to emphasize the importance of only jump-type discontinuities based on this fact.

Finally our result follows by a change of variables. Let \(\mu, \sigma \in \mathbb{R}\) such that \(\sigma > 0\). Define \(Z = (X - \mu)/\sigma\) and \(f(z) = g(\sigma z + \mu)\). Now,

\[
\sigma^{-2}E\{(X - \mu)h(X)\} = \sigma^{-1}E\{Zf(Z)\} \\
= \sigma^{-1} \left[ E\{f'(Z)\} + \sum_{t_i \in J(f)} \{f(t_i)_+ - f(t_i)_-\} \phi(t_i) \right] \\
= \sigma^{-1} \left[ E\{\sigma g'(X)\} + \sum_{u_i \in J(g)} \{g(u_i)_+ - g(u_i)_-\} \phi_\sigma(u_i - \mu) \right] \\
= E\{g'(X)\} + \sum_{u_i \in J(g)} \{g(u_i)_+ - g(u_i)_-\} \phi_\sigma(u_i - \mu),
\]

where \(\phi_\sigma(t)\) is the density function of a \(N(0, \sigma^2)\) random variable.

\[\square\]

### 7.8 Proof of Theorem \(\text{[7]}\)

**Theorem.** Let \(h > 0\). For every \(g \in D_{0,n}\) \([13]\) that is right continuous at \(X_1, \ldots, X_n\), there exists a piecewise constant function, \(\tilde{g} \in D_{0,n}\), that has at most \(n - 1\) knots and satisfies \(\tilde{g}(X_i) = g(X_i)\) from the right and \(\tilde{R}_0(\tilde{g}; h) \leq R_0(g; h)\). The knots of \(\tilde{g}(x)\) lie at the minimum of \(\hat{f}_h(t)\) between each consecutive order statistics of \(X_1, \ldots, X_n\).

**Proof.** Let \(x_1 < \cdots < x_n\) be the order statistics of \(X_1, \ldots, X_n\) and let \(g \in D_{0,n}\) be right continuous at each \(x_i\). First notice that by the extreme value theorem, because \(\hat{f}_h(t)\) is continuous, there is a minimum that it obtains at least once on any closed interval \([a, b] \subset \mathbb{R}\), so

\[
\int_a^b \hat{f}_h(x) g'(x) dx \geq \int_a^b \left\{ \min_{x \in [a,b]} \hat{f}_h(x) \right\} g'(x) dx \\
= \left\{ \min_{x \in [a,b]} \hat{f}_h(x) \right\} \int_a^b g'(x) dx
\]
Now, let $\hat{g} \in \mathcal{D}_{0,n}$ be a degree-zero (piecewise constant) spline such that $\hat{g}(x_i) = g(x_i)$ for each $i = 1, \ldots, n$ from the right. This $\hat{g} \in \mathcal{D}_{0,n}$ exists because its piecewise constant structure ensures that $TV(\hat{g}) \leq TV(g)$ and if $g$ is bounded or monotone, $\hat{g}$ is has the same bounds and is monotone. Let $t_i = \arg \min_{x \in [x_i, x_{i+1}]} \hat{f}_h(x)$ for $i = 1, \ldots, n - 1$ be the $n - 1$ knots for $\hat{g}$. Notice that because $x_i$ are distinct by assumption (and $X_i$ are distinct almost surely), the definition of $\hat{f}_h(t_i)$ gives us that each of the $t_i$ must be distinct and lie in the open interval $(x_i, x_{i+1})$. Further, notice that $\hat{g}$ has at most $n - 1$ jump discontinuities and is constant on the resulting $n$ open intervals: $(-\infty, t_1), (t_1, t_2), \ldots, (t_n, \infty)$.

From the fundamental theorem of Lebesgue integral calculus we have:

$$g(b) - g(a) = \int_a^b g'(x)dx + \sum_{t_k \in J \cap [a,b]} \{g(t_k) - g(t_k)^-\}.$$

Combining these first two statements and using the definition of $t_i$, we get that:

$$\int_{x_i}^{x_{i+1}} \hat{f}_h(x)g'(x)dx + \sum_{t_k \in J \cap [x_i, x_{i+1}]} \hat{f}_h(t_k)\{g(t_k) - g(t_k)^-\}$$

$$\geq \hat{f}_h(t_i) \int_{x_i}^{x_{i+1}} g'(x)dx + \hat{f}_h(t_i) \sum_{t_k \in J \cap [x_i, x_{i+1}]} \{g(t_k) - g(t_k)^-\}$$

$$= \hat{f}_h(t_i) \left[ \int_{x_i}^{x_{i+1}} g'(x)dx + \sum_{t_k \in J \cap [x_i, x_{i+1}]} \{g(t_k) - g(t_k)^-\} \right]$$

$$= \hat{f}_h(t_i)\{g(x_{i+1}) - g(x_i)^-\}.$$

Also notice that because $g$ is monotone non-decreasing (one approach to extending this proof to functions with bound variation is to restrict the domain to $[x_i, x_n]$, to avoid potentially difficult asymptotic behavior),

$$\int_{-\infty}^{\infty} \hat{f}_h(x)g'(x)dx = \int_{-\infty}^{x_1} \hat{f}_h(x)g'(x)dx + \int_{x_1}^{x_n} \hat{f}_h(x)g'(x)dx + \int_{x_n}^{\infty} \hat{f}_h(x)g'(x)dx$$

$$\geq 0 + \int_{x_1}^{x_n} \hat{f}_h(x)g'(x)dx + 0$$

$$= \sum_{i=1}^{n-1} \int_{x_i}^{x_{i+1}} \hat{f}_h(x)g'(x)dx,$$

and

$$\sum_{t_k \in J \cap (-\infty, x_1)} \hat{f}_h(t_k)\{g(t_k)^+ - g(t_k)^-\} + \sum_{t_k \in J \cap [x_1, x_n)} \hat{f}_h(t_k)\{g(t_k) - g(t_k)^-\} + \sum_{t_k \in J \cap [x_n, \infty)} \hat{f}_h(t_k)\{g(t_k)^+ - g(t_k)^-\}$$

$$\geq 0 + \sum_{t_k \in J \cap [x_1, x_n)} \hat{f}_h(t_k)\{g(t_k) - g(t_k)^-\} + 0$$

$$= \sum_{i=1}^{n-1} \sum_{t_k \in J \cap [x_i, x_{i+1})} \hat{f}_h(t_k)\{g(t_k)^+ - g(t_k)^-\}.$$

Finally, because $\hat{g}(x_i) = g(x_i)$ from the right (and $g$ is right continuous) for each $i = 1, \ldots, n$ and $\hat{g}$ has
its jump points at $t_i$,

$$
\hat{R}_0(g; h) = \frac{1}{n} \sum_{i=1}^{n} \langle x_i - g(x_i) \rangle^2 + 2\sigma^2 \int_{-\infty}^{\infty} \hat{f}_h(x)g'(x)dx + 2\sigma^2 \sum_{t_k \in \mathcal{J}(g)} \hat{f}_h(t_k)\{g(t_k) + g(t_k)\} - \sigma^2
$$

$$
\geq \frac{1}{n} \sum_{i=1}^{n} \langle x_i - g(x_i) \rangle^2
$$

$$
+ 2\sigma^2 \sum_{i=1}^{n-1} \left[ \int_{x_i}^{x_{i+1}} \hat{f}_h(x)g'(x)dx + \sum_{t_k \in \mathcal{J}(g)[x_i, x_{i+1}]} \hat{f}_h(t_k)\{g(t_k) + g(t_k)\} \right] - \sigma^2
$$

$$
\geq \frac{1}{n} \sum_{i=1}^{n} \langle x_i - g(x_i) \rangle^2 + 2\sigma^2 \sum_{i=1}^{n-1} \hat{f}_h(t_i)\{g(x_{i+1}) - g(x_i)\} - \sigma^2
$$

$$
= \frac{1}{n} \sum_{i=1}^{n} \langle x_i - \tilde{g}(x_i) \rangle^2 + 2\sigma^2 \sum_{i=1}^{n-1} \hat{f}_h(t_i)\{\tilde{g}(x_{i+1}) - \tilde{g}(x_i)\} - \sigma^2
$$

$$
\overset{(i)}{=} \frac{1}{n} \sum_{i=1}^{n} \langle x_i - \tilde{g}(x_i) \rangle^2 + 2\sigma^2 \sum_{i=1}^{n-1} \hat{f}_h(t_i)\{\tilde{g}(x_{i+1}) - \tilde{g}(x_i)\} - \sigma^2
$$

$$
\overset{(i)}{=} \hat{R}_0(\tilde{g}; h).
$$

We note that $\tilde{g}$ is constant almost everywhere and only has discontinuities at $t_i \in (x_i, x_{i+1})$. These facts imply: (i) $g(x_{i+1}) - g(x_i) = g(x_{i+1}) + g(x_i)$ for each $i = 1, \ldots, n - 1$, and (ii) the integral term in $\hat{R}_0(\tilde{g}; h)$ is zero.

7.9 Proof of Theorem

Theorem. Let $X_i \sim N(\theta_i, \sigma^2)$ be independent such that $\sigma^2$ is known and $\max_{i=1}^{n}|\theta_i| < C_n$. Further, let $b_n = (8/3)\sigma^2 \log(n)1/2$ and $h_n > 0$ such that $h_n \ll n^{-1/6}$. Define $\hat{d}_{h_n}(x)$ as in (15) and let $d^*(x)$ be the optimal separable estimator [4], then

$$
R(\hat{d}_{h_n}; \theta) - R(d^*; \theta) = O \left( n^{-1/3} \left( C_n + \log^{1/2} n \right)^2 \right).
$$

Proof: Most of proof follows identically to the proof of Theorem [5] except additional care needs to be paid to the estimation error of the penalty and the approximation error’s probability bound has a 4 rather than a 6 because the function class no longer has its total variation constraint.

Define $f_v(x) = n^{-1} \sum_{i=1}^{n} \phi_v(x - \theta_i)$ for $v = (\sigma^2 + h_n^2)^{1/2}$, observe that $f_v(x) = E\hat{f}_{h_n}(x)$ and $f'_v(x) = E\hat{f}'_{h_n}(x)$. For brevity of notation, define $\beta_d(t_k) = d(t_k)_{+} - \beta_d(t_k)_{-}$ for any $d \in D_{n, \theta}$ and corresponding $\mathcal{J}(d)$. Rather than the penalty estimation term in the proof of Theorem [5]

$$
E \sup_{d \in D_{n, \theta}} \left| \frac{1}{n} \sum_{i=1}^{n} \{d'(X_i) - E_X d'(X_i)\} \right|
$$

our task is now to bound:

$$
E \sup_{d \in D_{n, \theta}} \left| \int_{-\infty}^{\infty} f_v(x)d'(x)dx + \sum_{t_k \in \mathcal{J}(d)} \beta_d(t_k)f_\theta(t_k) - \int_{-\infty}^{\infty} \hat{f}_{h_n}(x)d'(x)dx - \sum_{t_k \in \mathcal{J}(d)} \beta_d(t_k)\hat{f}_{h_n}(t_k) \right|
$$

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This term is challenging to analyze because both $D_{0,n}$ and $\hat{f}_{h_n}(x)$ are random. To address this challenge, we introduce $f_n(x)$ and use the triangle inequality to study a structural error term and a random error term:

$$E \sup_{d \in D_{0,n}} \left| \int_{-\infty}^{\infty} f_0(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_0(t_k) - \int_{-\infty}^{\infty} \hat{f}_h(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)\hat{f}_h(t_k) \right|$$

$$\leq E \sup_{d \in D_{0,n}} \left| \int_{-\infty}^{\infty} f_0(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_0(t_k) - \int_{-\infty}^{\infty} f_n(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)f_n(t_k) \right|$$

$$+ E \sup_{d \in D_{0,n}} \left| \int_{-\infty}^{\infty} f_n(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_n(t_k) - \int_{-\infty}^{\infty} \hat{f}_h_n(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)\hat{f}_h_n(t_k) \right| .$$

Starting with the structural term, we apply Proposition 6 utilizing the fact that $f_n(t) = E\hat{f}_{h_n}(x)$ and that $v \geq \sigma > 0$. Define $Y_i = X_i + Z_i$ where $Z_i \sim N(0,h_n^2)$ is independent from all other random variables. Now we can bound the structural error utilizing the fact that the only randomness in this term is in $D_{0,n}$:

$$E \sup_{d \in D_{0,n}} \left| \int_{-\infty}^{\infty} f_0(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_0(t_k) - \int_{-\infty}^{\infty} f_n(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)f_n(t_k) \right|$$

$$= E \sup_{d \in D_{0,n}} \left| \frac{1}{n} \sum_{i=1}^{n} E_{X_i} \left\{ \frac{X_i - \theta_i}{\sigma^2} d(X_i) \right\} - \frac{1}{n} \sum_{i=1}^{n} E_{Y_i} \left\{ \frac{Y_i - \theta_i}{v^2} d(Y_i) \right\} \right|$$

$$= E \sup_{d \in D_{0,n}} \left| \frac{1}{n} \sum_{i=1}^{n} \int_{-\infty}^{\infty} \frac{x - \theta_i}{\sigma^2} \frac{1}{\sigma} \phi \left( \frac{x - \theta_i}{\sigma} \right) d(x)dx - \frac{1}{n} \int_{-\infty}^{\infty} \frac{x - \theta_i}{v^2} \frac{1}{v} \phi \left( \frac{x - \theta_i}{v} \right) d(x)dx \right|$$

$$\leq E \sup_{d \in D_{0,n}} \left| \frac{1}{n} \sum_{i=1}^{n} \int_{-\infty}^{\infty} \frac{y}{\sigma^2} \phi \left( \frac{y}{\sigma} \right) - \frac{y}{v^2} \phi \left( \frac{y}{v} \right) d(y + \theta_i)dy \right|$$

$$\leq E \left\{ \sup_{d \in D_{0,n}} \sup_{x \in \mathbb{R}} |d(x)| \right\} \cdot \int_{-\infty}^{\infty} \left| \frac{y}{\sigma^2} \phi \left( \frac{y}{\sigma} \right) - \frac{y}{v^2} \phi \left( \frac{y}{v} \right) \right| dy$$

$$= \frac{2}{\sqrt{2\pi}} \left( \frac{1}{\sigma} - \frac{1}{v} \right) \cdot E \left\{ \sup_{d \in D_{0,n}} \sup_{x \in \mathbb{R}} |d(x)| \right\}$$

$$\leq \frac{2}{\sqrt{2\pi}} \left( \frac{1}{\sigma} - \frac{1}{v} \right) \cdot E \left\{ \max_{i=1}^{n} |X_i| + b_n \right\}$$

$$\leq \frac{2}{\sqrt{2\pi}} \left( \frac{1}{\sigma} - \frac{1}{v} \right) \cdot \left\{ (2\sigma^2 \log(2n))^{1/2} + C_n + b_n \right\}$$

$$\leq \frac{2}{\sqrt{2\pi}} \left( \frac{1}{\sigma} - \frac{1}{v} \right) \cdot \left\{ (2\sigma^2 \log(2n))^{1/2} + C_n + b_n \right\}$$

$$= \frac{2}{(2\pi)^{1/2}} \left( \frac{\sigma^{-1} - (\sigma^2 + h_n^2)^{-1/2}}{\sigma^{-1} - (\sigma^2 + h_n^2)^{-1/2}} \right).$$

The aggressive use of triangle inequality in the first inequality may seem overly aggressive at first, but we note that if $\theta_1 = \cdots = \theta_n = 0$, then the bound is actually an equality. The following step where we sup-out the $d(x)$ may be loose. The last inequality is an application of a Gaussian maximal inequality. We observe that as $h_n \downarrow 0$, the structural error term converges to zero.
Next we bound the random error term. To do this we will again use symmeterization and a chaining bound utilizing the fact that $f_n(t) = E\hat{f}_n(t)$; however, we will first need to define and study the new function class:

$$G_{n,h} = \left\{ g(y) = \int_{-\infty}^{\infty} \phi_h(x-y)d'(x)dx + \sum_{t_k \in J(d)} \phi_h(t_k-y)\beta_d(t_k) : d \in D_{0,n} \right\}$$

for some $h > 0$. In particular, we will demonstrate that $g \in G_{n,h}$ is bound and has bound total variation. Fixed $h > 0$ and let $\tau_n$ be such that $TV(d) \leq \tau_n < \infty$ for every $d \in D_{0,n}$ (for monotone functions this is just the range). We begin by showing that $G_{n,h}$ is uniformly bounded. Observe that by the triangle inequality, we can bound the range of every $g(y)$ as follows:

$$|g(y)| = \left| \int_{-\infty}^{\infty} \phi_h(x-y)d'(x)dx + \sum_{t_k \in J(d)} \phi_h(t_k-y)\beta_d(t_k) \right|$$

$$\leq \int_{-\infty}^{\infty} |\phi_h(x-y)|d'(x)|dx + \sum_{t_k \in J(d)} \phi_h(t_k-y)|\beta_d(t_k)|$$

$$\leq (2\pi h^2)^{-1/2}\int_{-\infty}^{\infty} |d'(x)||dx + (2\pi h^2)^{-1/2}\sum_{t_k \in J(d)} |\beta_d(t_k)|$$

$$= (2\pi h^2)^{-1/2} \cdot TV(d)$$

Next we bound the total variation of $g(y)$ by applying the triangle inequality and Fubini’s theorem:

$$TV(g) = \int_{-\infty}^{\infty} |g'(y)| \, dy$$

$$= \int_{-\infty}^{\infty} \left| \frac{\partial}{\partial y} \int_{-\infty}^{\infty} \phi_h(x-y)d'(x)dx + \sum_{t_k \in J(d)} \frac{\partial}{\partial y} \phi_h(t_k-y)\beta_d(t_k) \right| \, dy$$

$$= \int_{-\infty}^{\infty} \left| \int_{-\infty}^{\infty} \frac{x-y}{h^2} \phi_h(x-y) \, dx + \sum_{t_k \in J(d)} \frac{t_k-y}{h^2} \phi_h(t_k-y)\beta_d(t_k) \right| \, dy$$

$$\leq \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{|x-y|}{h^2} \phi_h(x-y) \, dx \, dy + \sum_{t_k \in J(d)} \left| \frac{t_k-y}{h^2} \phi_h(t_k-y)\beta_d(t_k) \right| \, dy$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{|x-y|}{h^2} \phi_h(x-y) \, dx \, dy + \sum_{t_k \in J(d)} \int_{-\infty}^{\infty} \frac{|t_k-y|}{h^2} \phi_h(t_k-y)\beta_d(t_k) \, dy$$

$$= \int_{-\infty}^{\infty} 2(2\pi h^2)^{-1/2}|d'(x)||dx + \sum_{t_k \in J(d)} 2(2\pi h^2)^{-1/2}|\beta_d(t_k)|$$

$$= 2(2\pi h^2)^{-1/2} \cdot TV(d)$$

$$\leq 2\tau_n(2\pi h^2)^{-1/2}.$$

Thus $G_{n,h}$ inherits the boundedness and bounded total variation from $D_{0,n}$ for any $h > 0$. Moreover both the range and total variation of functions in $G_{n,h}$ are bound by $2\tau_n(2\pi h^2)^{-1/2}$, which will make our chaining bounds simple.

Proceeding by a symmeterization argument, let $X_i^\epsilon$ be independent copies of $X_i$ and let $\epsilon_i$ be independent Rademacher random variables. Then,
Before proceeding with the symmeterization argument, observe that by Fubini’s theorem and our definition of \( \mathcal{G}_{n,h} \), for every \( d \in \mathcal{D}_0 \) and \( h_n > 0 \) there exists a \( g \in \mathcal{G}_{n,h} \) such that:

\[
\int_{-\infty}^{\infty} f_v(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_v(t_k)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n} \sum_{i=1}^{\infty} \phi_h(x - \theta_i)d'(x)dx + \frac{1}{n} \sum_{i=1}^{n} \sum_{t_k \in J(d)} \beta_d(t_k)\phi_v(x - \theta_i)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n} \sum_{i=1}^{\infty} E_{X_i} \phi_h(x - X_i)d'(x)dx + \frac{1}{n} \sum_{i=1}^{n} \sum_{t_k \in J(d)} \beta_d(t_k)E_{X_i} \phi_h(x - X_i)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} E_{X_i} \left\{ \int_{-\infty}^{\infty} \phi_h(x - X_i)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)\phi_h(x - X_i) \right\}
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} E_{X_i}g(X_i)
\]

and

\[
\int_{-\infty}^{\infty} \hat{f}_{h_n}(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)\hat{f}_{h_n}(t_k)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n} \sum_{i=1}^{\infty} \phi_h(x - \theta_i)d'(x)dx + \frac{1}{n} \sum_{i=1}^{n} \sum_{t_k \in J(d)} \beta_d(t_k)\phi_h(x - \theta_i)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \sum_{i=1}^{\infty} E_{X_i} \phi_h(x - X_i)d'(x)dx + \frac{1}{n} \sum_{i=1}^{n} \sum_{t_k \in J(d)} \beta_d(t_k)\phi_h(x - X_i)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} g(X_i)
\]

Putting these together, we can proceed with our symmeterization argument:

\[
E_X \sup_{d \in D_n} \left| \int_{-\infty}^{\infty} f_v(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_v(t_k) - \int_{-\infty}^{\infty} \hat{f}_{h_n}(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)\hat{f}_{h_n}(t_k) \right|
\]

\[
= E_X \sup_{g \in \mathcal{G}_{n,h}} \left| \frac{1}{n} \sum_{i=1}^{n} E_{X_i}g(X_i) - \frac{1}{n} \sum_{i=1}^{n} g(X_i) \right|
\]

\[
= E_X \sup_{g \in \mathcal{G}_{n,h}} \left| \frac{1}{n} \sum_{i=1}^{n} E_{X_i}g(X_i) - \frac{1}{n} \sum_{i=1}^{n} g(X_i) \right|
\]

\[
= E_X \sup_{g \in \mathcal{G}_{n,h}} \left| \frac{1}{n} \sum_{i=1}^{n} E_{X_i}g(X_i) - \frac{1}{n} \sum_{i=1}^{n} g(X_i) \right|
\]

\[
= E_X \sup_{g \in \mathcal{G}_{n,h}} \left| \frac{1}{n} \sum_{i=1}^{n} \{g(X_i) - g(X_i)\} \right|
\]

\[
\leq E_{X,X'} \sup_{g \in \mathcal{G}_{n,h}} \left| \frac{1}{n} \sum_{i=1}^{n} \{g(X_i) - g(X_i)\} \right|
\]

\[
= E_{X,X'} \sup_{g \in \mathcal{G}_{n,h}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i g(X_i) \right|
\]

\[
\leq 2E_{X} \sup_{g \in \mathcal{G}_{n,h}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i g(X_i) \right|
\]

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Now we will use a chaining bound to finish our bound on the random term. Define \( D_n = 2\tau_n(2\pi h_n^2)^{-1/2} \), where because \( D_{0,n} \) is uniformly bound and monotone non-decreasing, \( \tau_n = \max_{n=1}^{n} X_i - \min_{n=1}^{n} X_i + 2b_n \). Then, using our properties of \( G_{n,h,n} \), Lemma 11, metric entropy results \([54]\), and Gaussian maximal inequalities \([8]\) we have:

\[
E_X \sup_{d \in D_n} \left| \int_{-\infty}^{\infty} f_d(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_d(t_k) - \int_{-\infty}^{\infty} \hat{f}_h(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)\hat{f}_h(t_k) \right| 
\leq 2E_X \sup_{g \in \mathcal{G}_n} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i g(X_i) \right| 
\leq 2E_X \left[ Cn^{-1/2} \int_{0}^{D_n} \{ \log N(G_{n,h,n}; L_n; t) \}^{1/2} dt \right] 
\leq 2E_X \left\{ Cn^{-1/2} \int_{0}^{D_n} (A_3 D_n/t) dt \right\} 
= \frac{4C\sqrt{\pi}}{\sqrt{n}} E_X \{ D_n \} 
= 8CA_3^{1/2}(2\pi h_n^2)^{-1/2}E_X \{ \tau_n \} 
= C_3(2\pi h_n^2)^{-1/2}E_X \{ \tau_n \} 
= C_3(2\pi h_n^2)^{-1/2}E_X \{ X_{(n)} - X_{(1)} + 2b_n \} 
\leq C_3(2\pi h_n^2)^{-1/2}E_X \left\{ \max_{i=1}^{n} |X_i - \theta_i| + C_n + b_n \right\} 
\leq C_3(2\pi h_n^2)^{-1/2} \left\{ (2\sigma^2 \log(2n))^{1/2} + C_n + b_n \right\} ,
\]

where \( A_3 > 0 \) and \( C_3 = 8CA_3^{1/2} \) are constants. We observe that as \( h_n \downarrow 0 \), the random error term grows. This suggests that we need to optimize \( h_n \) to balance both the structural error and the random error.

Putting our results together we bound the estimation of the penalty term as:

\[
E \sup_{d \in D_{0,n}} \left| \int_{-\infty}^{\infty} f_d(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_d(t_k) - \int_{-\infty}^{\infty} \hat{f}_h(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)\hat{f}_h(t_k) \right| 
\leq 2 \left\{ (2\sigma^2 \log(2n))^{1/2} + C_n + b_n \right\} \{ \sigma^{-1} - (\sigma^2 + h_n^2)^{-1/2} \} 
+ C_3(2\pi h_n^2)^{-1/2} \left\{ (2\sigma^2 \log(2n))^{1/2} + C_n + b_n \right\} 
= C_3 \left\{ (2\sigma^2 \log(2n))^{1/2} + C_n + b_n \right\} \cdot \left\{ (2/C_3) \left\{ \sigma^{-1} - (\sigma^2 + h_n^2)^{-1/2} \right\} + (nh_n^2)^{-1/2} \right\} 
\]

This bound suggests that large \( n \), the optimal \( h_n \) satisfies \( h_n \sim \sigma n^{-1/6} \). Thus we get our bound on the estimation error of the penalty term:

\[
E \sup_{d \in D_{0,n}} \left| \int_{-\infty}^{\infty} f_d(x)d'(x)dx + \sum_{t_k \in J(d)} \beta_d(t_k)f_d(t_k) - \int_{-\infty}^{\infty} \hat{f}_h(x)d'(x)dx - \sum_{t_k \in J(d)} \beta_d(t_k)\hat{f}_h(t_k) \right| 
= \left\{ (2\sigma^2 \log(2n))^{1/2} + C_n + b_n \right\} \cdot O \left( n^{-1/3} \right) 
= O \left\{ n^{-1/3} \left( C_n + \log^{1/2}(n) \right) \right\} ,
\]

when \( b_n = \{ \sigma^2 K \log(n) \}^{1/2} \).
This rate bound dominates the convergence of the estimation error. With a slower rate of convergence in the estimation error, we choose a smaller value for $K$ to balance the convergence rates between the estimation error and approximation error. Letting $K = 8/3$, we get the following bound on approximation error:

$$O\left\{n^{-1/3} \left(C_n + \log^{1/2} n \right)^2 \right\}.$$ 

Putting these bounds together in the same manner as the proof of Theorem 8 completes the proof.

7.10 Proof of Corollary 8.1

**Corollary.** Let $X_i \sim N(\theta_i, \sigma^2)$ be independent such that $\sigma^2$ is known and $\max_{i=1}^n |\theta_i| < C_n$. Further, let $b_n = \left\{(8/3)\sigma^2 \log(n)\right\}^{1/2}$, $\lambda_n = \max_{i=1}^n X_i - \min_{i=1}^n X_i + 2b_n$, and $h_n > 0$ such that $h_n \asymp \sigma n^{-1/6}$. Define the new function class:

$$C_{0,n} = \left\{d : \mathbb{R} \to \left[\min_i X_i - b_n, \max_i X_i + b_n\right] \mid TV(d) \leq \lambda_n \right\},$$

and the corresponding estimator $\bar{d}_{h_n} = \arg\min_{d \in C_{1,n}} \hat{R}_0(d; h_n)$. Let $d^*(x)$ be the optimal separable estimator (1), then

$$R(\bar{d}_{h_n}; \theta) - R(d^*; \theta) = O\left\{n^{-1/3} \left(C_n + \log^{1/2} n \right)^2 \right\}.$$ 

**Proof.** This proof follows almost immediately from the proof of Theorem 8. We notice that the addition of a total variation constraint increases the constant in the probability term bound in the approximation error from 4 to 6. Further, since the analysis of $G_{n,h}$ is already in terms of total variation, it applies to the function class $C_{0,n}$ without modification. \qed