High-dimensional Index Volatility Models via Stein’s Identity

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Abstract

We study estimation of the parametric components of single and multiple index volatility models. Using the first- and second-order Stein’s identity, we develop methods that are applicable for estimation of the variance index in a high-dimensional setting requiring finite moment condition, which allows for heavy-tailed data. Our approach complements the existing literature in a low-dimensional setting, while relaxing the conditions on estimation, and provides a novel approach in a high-dimensional setting. We prove that the statistical rate of convergence of our variance index estimators consists of a parametric rate and a nonparametric rate, where the latter appears from the estimation of the mean link function. However, under standard assumptions, the parametric rate dominates the rate of convergence and our results match the minimax optimal rate for the mean index estimation. Simulation results illustrate finite sample properties of our methodology and back our theoretical conclusions.

1 Introduction

We consider the following index volatility model:

\[ y \mid x = f(\langle \beta^*, x \rangle) + g(G^T x) \epsilon \]

where \( y \) is the response variable, \( x \in \mathbb{R}^d \) is the vector of predictors, and \( \epsilon \) is a random error independent of \( x \) with \( \mathbb{E}[\epsilon] = 0 \) and \( \mathbb{E}[\epsilon^2] = 1 \). In the model above, the conditional mean and variance of the response depend on the multivariate predictors only through linear projections. The unknown parts of this semi-parametric model are signals \( \beta^* \in \mathbb{R}^d \) and \( G^* = (\gamma_1^*, \ldots, \gamma_v^*) \in \mathbb{R}^{d \times v} \), which are parametric components satisfying \( \beta^T \beta^* = 1 \) and \( G^T G^* = I_v \) for identifiability, and unknown link functions \( f : \mathbb{R} \to \mathbb{R} \) and \( g : \mathbb{R}^v \to \mathbb{R} \), which are nonparametric components. Li (1991) termed the linear space spanned by the direction of the projections as effective dimension reduction (e.d.r.). In this paper, we focus our attention to the estimation of \( G^* \).

In order to emphasize the main contribution of the work, we assume that the conditional mean of \( y \) given \( x \) follows a single index model. We note, however, that this assumption is not crucial and we will be able to estimate \( G^* \) as long as the mean function can be estimated sufficiently quickly, as we illustrate later. Estimators of \( f(\cdot) \) and \( g(\cdot) \) only depend on the projection of predictors \( x \) onto the e.d.r. direction. In particular, one can apply local polynomial regression or a spline-based method on \( \{y_i, \hat{\beta}^T x_i, \hat{G}^T x_i\}_{i=1}^n \) to estimate \( f(\cdot) \) and \( g(\cdot) \) once \( \hat{\beta} \) and \( \hat{G} \) are computed. Furthermore, the estimation of the nonparametric components does not depend on the ambient dimensionality \( d \).
of the problem. Thus our focus will be on estimating parametric components in a high-dimensional setting, allowing for heavy-tails of the covariates $x$, without using knowledge of $f$ and $g$.

Model in (1) has been widely studied in the literature as it allows for flexible modeling of data without making rigid assumptions that parametric models make, while at the same time allowing for tractable estimation without suffering from the curse of dimensionality that affects fully nonparametric methods (Robins and Ritov, 1997; Bach, 2017). When the variance function is constant and does not depend on the predictors $x$, the model (1) becomes the homoscedastic single index model (SIM), which plays a prominent role in econometrics and applied quantitative sciences (see, for example, Sharpe (1963); Collins and Barry (1986); Stock and Watson (1988)). Due to its wide-ranged applicability, a number of estimation procedures were proposed and studied (see Ichimura (1993); Härdle et al. (1993); Horowitz and Härdle (1996); Xia et al. (2002b); Delecroix et al. (2006) and references therein). Li (1991) developed the sliced inverse regression (SIR), which is one of the first widespread methods for estimating the e.d.r. direction. Subsequently, a number of more advanced methods were proposed for estimating single and multiple index models. Hristache et al. (2001) estimated the e.d.r. direction by iteratively estimating $\beta^*$ and $f'$. Gaïffas and Lecué (2007) used an aggregation algorithm with local polynomial estimator to estimate $f$ at the minimax rate, while Lepski and Serdyukova (2014) developed a procedure that adapts to the smoothness of $f$. In a setting where the dimension of the predictors, $d$, increases with the sample size, $n$, Zhu and Zhu (2009) developed a penalized inverse regression method with a nonconcave SCAD penalty and their estimator $\hat{\beta}$ is asymptotically normal as long as $d = O(n^{1/3})$. Finally, a number of papers have studied other index structures. For example, Carroll et al. (1997), Müller (2001), and Wang et al. (2010) studied partial-linear index model; Ait-Saïdi et al. (2008) and Lian (2011) studied functional index model; and Wong et al. (2008), Xue and Wang (2012), and Ma and Song (2015) studied varying-coefficient index model.

The above mentioned literature, while able to attain either $\sqrt{n}$-consistency or asymptotic normality for estimating parametric components, have two limitations. First, most of them require the predictors $x$ to have Gaussian or elliptically symmetric distribution. Second, they focus on estimation in a low dimensional setting where the sample size $n$ far exceeds the dimension of predictors, $d$. More recent literature, that is closer to the approach we take in this paper, addressed the two limitations by incorporating Stein’s identity into estimation of index models. Babichev and Bach (2018) developed a sliced inverse regression method based on Stein’s identity that allows for estimation under weak conditions on the distribution of $x$, albeit in a low dimensional setting. Plan and Vershynin (2016) studied estimation of single index models in a high-dimensional setting with Gaussian design and showed that the generalized Lasso gives rate optimal estimation for the parametric part of the model. Yang et al. (2017a) extended the above work to heavy-tail designs, while maintaining the optimal statistical rate using the first-order Stein’s identity, and further, Yang et al. (2017b) developed methodology for estimation of multiple index models. Na et al. (2018) illustrated how to estimate varying-coefficient index models. Furthermore, Stein’s method has also been applied into risk estimation in Gaussian sequence model and normal approximation in recent work (Chen et al., 2011; Bellec and Zhang, 2018).

Allowing for conditional heteroscedasticity extends the applicability of the model even further. In financial time series, the function $g(\cdot)$ is usually interpreted as diffusion or volatility, with a long history in stochastic process, dating back to Doob (1953). Development of the heteroscedastic model is attributed to Engle et al. (1987). Estimating the function $g(\cdot)$ does not only help in the estimation of the mean, but is interesting in its own right (see Box and Hill (1974); Bickel (1978); Box and
Meyer (1986) and references therein). Härdle et al. (1993) first considered model (1) with \( v = 1 \) and termed it single index volatility model, which was subsequently studied in Xia et al. (2002a). Zhang (2018) extended the quasi-likelihood estimator of Xia (2006) to low-dimensional single index volatility model. Chiou and Müller (2004) proposed a semiparametric quasi-likelihood approach to estimating multiple index models with purely nonparametric variance function. Klein and Vella (2009) studied a special case of a single index volatility model and built a likelihood-based estimator for unknown variance function using local smoothing. Van Keilegom and Wang (2010) studied general semiparametric location-dispersion model with applications to index volatility models. Fang et al. (2015) proposed a two-step procedure for fitting a heteroscedastic additive partial-linear model, while Lian et al. (2015) extended the method of Wang et al. (2010) for fitting a model where both mean function and variance function are in partial-linear single index form.

In this paper, we consider a generalization of the single index volatility model with \( v > 1 \), which we call multiple index volatility model. Compared to the existing literature on index volatility modeling, we focus our attention on estimation in a high-dimensional setting, which is possible under an assumption that \( \mathbf{G}^* \) is sparse. We focus on the random design setting with weak assumptions on the predictors, that allow for heavy-tailed designs, and develop an estimator that can estimate parametric components without knowing the link function, as is needed in applications (Boufounos and Baraniuk, 2008; Yi et al., 2015). In particular, we avoid iterative estimation of \( \mathbf{G}^* \) and \( g(\cdot) \) that is common in the literature on index volatility modeling and requires some knowledge of \( g(\cdot) \). While our estimator of \( \mathbf{G}^* \) can skip the estimation of \( g(\cdot) \), it does rely on having a good estimator of the conditional mean. Some necessary results concerning the mean estimation are discussed in Section 2, while detailed theoretical analysis is given in Appendix A. The effect of the mean estimation will be evident from the obtained statistical convergence results, which can be decomposed into two parts: (i) nonparametric rate, originating from estimation of \( f \), and (ii) parametric rate at which we can estimate \( \mathbf{G}^* \) under the knowledge of \( f(\cdot) \). In a high-dimensional setting, it is often the latter, parametric part, that dominates the converge rate, as long as \( f(\cdot) \) is sufficiently smooth.

The main contributions of the paper can be summarized as follows. We develop a flexible method for estimating \( \mathbf{G}^* \) in model (1) based on Stein’s identity that is suitable for single and multiple index volatility models. Our analysis does not require sub-Gaussian design or the knowledge of the link function \( g(\cdot) \). We establish the first result on high-dimensional heavy-tailed index volatility models. As a byproduct, the result on low-dimensional setting is also provided. While developing our methodology, we illustrate how the Stein’s identity can be used for the problem of variance estimation, which is of independent interest. Finally, we illustrate finite sample properties through a series of experiments, including scenarios for which there were no suitable estimators before.

### 1.1 Notation

Here we summarize the notation that is used throughout the paper. We use bold symbols to denote column vectors. For any two vectors \( \mathbf{a} \) and \( \mathbf{b} \), we use \( (\mathbf{a}; \mathbf{b}) \) to denote a column vector obtained by stacking them together. We use \( e \) to denote the canonical basis of \( \mathbb{R}^r \) for some \( r \) that will depend on the context. Given an integer \( k \), we use \( \{k\} \) to denote the set \( \{1, 2, \ldots, k\} \). For any two scalar \( a \) and \( b \), we let \( a \wedge b = \min\{a, b\} \) and \( a \vee b = \max\{a, b\} \). For positive \( a, b \), we write \( a \lesssim b \) (\( a \gtrsim b \)), if there exists a constant \( c \) such that \( a/b \leq c \) (\( b/a \leq c \)). We denote \( a \asymp b \), if \( a \lesssim b \) and \( a \gtrsim b \). For a vector \( \mathbf{\beta} \in \mathbb{R}^d \), we define \( \|\mathbf{\beta}\|_0 = |\text{supp}(\mathbf{\beta})| \). We say \( \mathbf{\beta} \) is \( s \)-sparse if \( \|\mathbf{\beta}\|_0 \leq s \). The norm \( \| \cdot \|_p \) represents either the \( l_p \) norm of a vector or the induced \( p \)-norm for a matrix (for \( p = 2 \) the norm is used without a subscript). For a matrix \( \mathbf{A} \in \mathbb{R}^{m \times n} \), we let \( \|\mathbf{A}\|_* \) denote the nuclear norm, \( \|\mathbf{A}\|_F \).
denote the Frobenius norm, and \( \|A\|_{p,q} = \left( \sum_{i=1}^{n} \sum_{j=1}^{m} |A_{ij}|^{p} \right)^{1/q} \). We use \( I_r \) to denote \( r \times r \) identity matrix. For a random variable \( v \), we define \( \mathbb{E}_v[\cdot] = \mathbb{E}[\cdot \mid v] \), which is expectation conditional on \( v \). Also, a sequence of variable \( v_n \) is written as \( v_n = O_P(a_n) \) if \( v_n/a_n \) is stochastically bounded. We use \( C^r(\mathbb{R}) \) to denote all \( r \) times continuously differentiable functions and \( \mathbb{Q}^{d \times d} \) to denote all \( d \times d \) orthogonal matrices.

## 2 Preliminary

In this section, we present the first- and second-order Stein’s identities that will be used as fundamental tools in our estimation. Furthermore, we introduce the finite moment condition and some basic results on the mean estimation, under which we develop detailed estimation procedures in Sections 3 and 4.

### 2.1 Stein’s Identity

Stein (1981) described the first-order Stein’s identity for a Gaussian random variable, which was further extended to general random variables in Stein et al. (2004). To present the first-order Stein’s identity, we need the following definition.

**Definition 2.1** (First-order regularity condition). Suppose \( X \) is a \( \mathbb{R}^d \) random vector with a differentiable density \( p_X : \mathbb{R}^d \to \mathbb{R} \), whose support is denoted as \( \mathcal{X} \subseteq \mathbb{R}^d \). Further, we suppose \( p_X(x) \) is strictly positive in the interior of \( \mathcal{X} \) with \( |p_X(x)| \to 0 \) as \( x \) goes to the boundary. Let \( S_X : \mathcal{X} \to \mathbb{R}^d \) be the first-order score function defined as \( S_X(x) = -\nabla_x \log p_X(x) \). A differentiable function \( f : \mathcal{X} \to \mathbb{R} \) together with \( X \) satisfies the first-order regularity condition if both \( \mathbb{E}[|f(X) \cdot S_X(X)|] \) and \( \mathbb{E}[|\nabla_x f(X)|] \) exist.

With this definition, we have the following theorem.

**Theorem 2.2** (First-order Stein’s identity, Stein et al. (2004)). If function \( f \) together with random vector \( X \) satisfies the first-order regularity condition, then we have

\[
\mathbb{E}[f(X) \cdot S_X(X)] = \mathbb{E}[\nabla_x f(X)].
\]

In order to generalize to the second-order identity, we define the second-order regularity condition.

**Definition 2.3** (Second-order regularity condition). Suppose the same conditions as in Definition 2.1 hold. Let \( H_X : \mathcal{X} \to \mathbb{R}^{d \times d} \) be the second-order score function defined as \( H_X(x) = \nabla^2_x p_X(x)/p_X(x) \). A twice differentiable function \( f : \mathcal{X} \to \mathbb{R} \) together with \( X \) satisfies the second-order regularity condition if both \( \mathbb{E}[|f(X) \cdot H_X(X)|] \) and \( \mathbb{E}[|\nabla_x^2 f(X)|] \) exist.

**Theorem 2.4** (Second-order Stein’s identity, Janzamin et al. (2014)). If function \( f \) together with random vector \( X \) satisfies the second-order regularity condition, then we have

\[
\mathbb{E}[f(X) \cdot H_X(X)] = \mathbb{E}[\nabla_x^2 f(X)].
\]

In what follows, we will omit the subscript in \( \nabla_x f \) and \( S_X, H_X \) and write \( \nabla f, S, H \) whenever it is clear from the context. It is easy to see that when \( X \sim \mathcal{N}(0, I_d) \), then \( S(X) = X, H(X) = XX^T - I_d \). Furthermore, by above two theorems, we get

\[
\mathbb{E}[f(X) \cdot X] = \mathbb{E}[\nabla f(X)] \quad \text{and} \quad \mathbb{E}[f(X) \cdot (XX^T - I_d)] = \mathbb{E}[\nabla^2 f(X)].
\]
if \( f \) satisfies both regularity conditions. The regularity conditions are fairly mild and are required in the literature on Stein-based estimators. See, for example, Babichev and Bach (2018); Yang et al. (2017a); Na et al. (2018) and references therein. In addition to the regularity conditions above, we will need a moment assumption for the model (1).

**Assumption 2.5** (Finite moment assumption). We say finite \( p \)-th moment assumption holds for the model (1), if \( \mathbb{E}[|\epsilon|^p] < \infty \) and there exists \( M_p > 0 \) such that

\[
\mathbb{E}[|f(\beta^T x)|^p] + \mathbb{E}[|g(G^T x)|^p] \leq M_p, \quad \forall j, k \in [d].
\]

Furthermore, we have

\[
\mathbb{E}[|y|^p] \leq \mathbb{E}[|f(\langle x, \beta^* \rangle)|^p] + \mathbb{E}[|g(G^T x)|^p] \cdot \mathbb{E}[|\epsilon|^p] \leq M_p.
\]

In the above assumption, we assume that \( \mathbb{E}[|\epsilon|^p] \) is a constant and do not keep the track of it. On the other hand, we explicitly keep track of the quantity \( M_p \). Although the above assumption does not explicitly put restrictions on the tails of \( x \), it does allow for certain types of heavy-tailed designs, including the gamma and \( t \)-distribution. Furthermore, when the predictor \( x \) has i.i.d entries, \( \mathbb{E}[|H(x)_{jk}|^p] \) is bounded as long as the \( p \)-th moment of \( S(x)_j \) and its derivative are bounded.

### 2.2 Mean Estimation

Our estimator for \( G^* \) in the model (1) relies on a good estimator of the conditional mean. Since the variance estimation procedure does not depend on the specific form of the conditional mean function, in order to simplify the presentation, let’s consider the following model first,

\[
y \mid x = f(x) + g(G^T x)\epsilon,
\]

where \( x \in \mathbb{R}^d \) is the predictor vector, \( \epsilon \) is noise with \( \mathbb{E}[\epsilon | x] = 0 \), and \( f(\cdot) \) is an unknown function that is not necessarily of the index form. While this model is not suitable in a high-dimensional setting, it helps us illustrate the main requirements on the conditional mean estimator. Detailed estimation procedure, assumptions, and convergence results for the index model (1) are provided in Appendix A.

Under the model (2) with \( x \) belonging to a compact set, a number of standard nonparametric methods can be used to estimate \( f(\cdot) \), such as local polynomial regression. Suppose we use \( n \) independent samples, say \( D = \{y_i, x_i\}_{i=1}^n \) to estimate \( \hat{f} \), under suitable regularity conditions (see, for example, the Condition 1 in Fan (1993) for one-dimensional case), the pointwise mean squared error can be upper-bounded as

\[
\mathbb{E}[|\hat{f}(x) - f(x)|^2 \mid x = x_0] \leq e_f(x_0, n, d)
\]

for some error function \( e_f(x_0, n, d) \) depending on the evaluation point \( x_0 \), dimension \( d \) and sample size \( n \). In particular, when \( f \in \Sigma(k, L) \) where \( \Sigma(k, L) \) denotes the Hölder class (see Definition 1.2 in Tsybakov (2009)), the integrated mean squared error satisfies

\[
\mathbb{E}[|\hat{f}(x) - f(x)|^2] \leq \mathbb{E}[e_f(x, n, d)] \leq \Upsilon \cdot n^{-\frac{2k}{2k+d}},
\]

for some constant \( \Upsilon \), which is also the minimax rate (Györfi et al., 2002).
Different from the above discussed mean estimation, in order to have precise variance information for a given \( \hat{f} \), we require a slightly stronger result on \( \hat{f} \). Suppose \( W(x) \) is an entry of either first- or second-order score variable. We require that the weighted mean squared error, for the given \( \hat{f} \), is well controlled. In particular,

\[
\mathbb{E}[|\hat{f}(x) - f(x)|^2 \cdot W(x) \mid D] \leq \sqrt{\mathbb{E}[|\hat{f}(x) - f(x)|^4 \mid D] \cdot \sqrt{\mathbb{E}[W(x)^2]}}
\]

where the second inequality is due to the Markov’s inequality and holds with probability \( 1 - \delta \). To have the weighted mean squared error bounded, we require the mean estimator to satisfy

\[
\bar{e}_f(n, d) = \sqrt{\mathbb{E}[e_f(x, n, d)]} < \infty
\]

where

\[
e_f(x_0, n, d) := \mathbb{E}[|\hat{f}(x) - f(x)|^4 \mid x = x_0].
\]

Compared to the bounded second moment in (3), here we require the fourth moment to be bounded in (7), due to the application of the Cauchy-Schwarz in (5). When the covariate vector \( x \) is supported on a compact set and its density is bounded away from zero, one can simply show that \( e_f(x, n, d) \) is uniformly upper bounded and, in fact, converges to zero at the rate of \( n^{-2k_2k_2} \), and as a result has all the moments bounded.

In order to emphasize the main contribution, which is the variance estimation, we use the local linear estimator proposed in Fan (1993) and derive an explicit formula for \( \bar{e}_f(n, d) \) under the model (1) in Appendix A. We prove that (6) holds under a tail condition on \( \bar{e}_f(x, n, d) \), which is satisfied for any compact designs, as well as for any link functions \( f \) with appropriate decay properties. We note that an alternative proof technique is possible using uniform convergence result of \( \hat{f} \), see Hansen (2008), which, however, would require different regularity conditions.

Under the condition (6), the following theorem provides a result on the mean estimation that will allow us to estimate \( G^* \) in model (2).

**Theorem 2.6.** Suppose there is an estimator \( \hat{f} \) of the conditional mean under the model (2) which is calculated from \( n \) samples \( D = \{y_i, x_i\}_{i=1}^n \) and satisfies condition (6). Let \( W(x) \) be either \( S(x) \) or \( H(x) \) and assume that each entry of \( W(x) \) has a finite 2nd moment bounded by \( M_2 \). Then for any \( 0 < \delta < 1 \), we have

\[
P\left( \mathbb{E}[|\hat{f}(x) - f(x)|^2 \cdot W(x) \mid D] \geq \sqrt{M_2 \cdot \bar{e}_f(n, d)} \right) \leq \delta.
\]

The following result is an immediate corollary for the index model (1).

**Corollary 2.7.** Suppose \( \hat{\beta} \) and \( \hat{f} \) are estimators of \( \beta^* \) and \( f \) under the model (1), calculated from two independent sample sets \( D_1 \) and \( D_2 \) with size \( n \) for each. We define the mean quartic error as

\[
\bar{e}_f(\hat{\beta}^T x, n, 1) := \mathbb{E}[|\hat{f}(\langle \hat{\beta}, x \rangle) - f(\langle \beta^*, x \rangle)|^4 \mid x, D_1]
\]
We start our analysis by focusing on single index volatility models, which are a sub-class of models where probability is taken over randomness in \( \mu \) which satisfy the error rate in (11). Furthermore, to simplify the presentation of the paper, we assume that estimation of \( G \) can be estimated using the approach proposed in Yang et al. (2017a), while \( \hat{f} \) can be estimated by local linear regression (Fan, 1993). However, note that a number of alternative procedures, such as smoothing splines (de Boor, 2001; Green and Silverman, 1993), wavelets (Johnstone, 2011; Mallat, 2009) could be used, since under standard assumptions the quantity in (9) can be uniformly bounded over evaluation points. We show that the condition (10) follows from an explicit formula for \( \bar{e}_f(n, 1) \). In particular, we show that \( \hat{\gamma} \) satisfies the condition in (11). In Appendix A we will provide a simple estimator that satisfies the condition (11). In particular, we focus on the following model

\[ y | x = f(\langle x, \beta^* \rangle) + g(\langle x, \gamma^* \rangle) \epsilon, \]

and develop a procedure for estimating \( \gamma^* \). As discussed in Section 2, we assume existence of estimators \( \hat{\beta} \) and \( \hat{f} \) that satisfy the condition (11). We present our estimators based on the first- and second-order Stein’s identities in the following two subsections.

### 3 Single Index Volatility Model

We start our analysis by focusing on single index volatility models, which are a sub-class of models in (1) with \( v = 1 \). In particular, we focus on the following model

\[ y | x = f(\langle x, \beta^* \rangle) + g(\langle x, \gamma^* \rangle) \epsilon, \]

and assume \( e_f(\hat{\beta}, n, 1) := E[\bar{e}_f(\hat{\beta}^T x, n, 1) | D_1] < \infty, \)

\[ P(\sqrt{e_f(\hat{\beta}, n, 1) \geq \bar{e}_f(n, 1)} \leq \delta, \forall 0 < \delta < 1, \]

for some rate \( \bar{e}_f(n, 1) \). Let \( W(x) \) be either \( S(x) \) or \( H(x) \) and assume that each entry of \( W(x) \) has a finite 2nd moment bounded by \( M_2 \). Then we have

\[ P(\|E[\hat{f}(\hat{\beta}, x)] - f(\langle \beta^* \rangle, x)\|_2 \cdot W(x) | D_1, D_2 \geq \frac{\sqrt{M_2 \cdot \bar{e}_f(n, 1)}}{\delta}) \leq 2\delta, \]

where probability is taken over randomness in \( D_1 \) and \( D_2 \).

Estimation procedures we develop in Section 3 and 4 for \( G^* \) assume that the mean estimation satisfies the condition in (11). In Appendix A we will provide a simple estimator that satisfies the condition (11). In particular, we show that \( \hat{\beta} \) can be estimated using the approach proposed in Yang et al. (2017a), while \( \hat{f} \) can be estimated by local linear regression (Fan, 1993). However, note that a number of alternative procedures, such as smoothing splines (de Boor, 2001; Green and Silverman, 1993), wavelets (Johnstone, 2011; Mallat, 2009) could be used, since under standard assumptions the quantity in (9) can be uniformly bounded over evaluation points. We show that the condition (10) follows from an explicit formula for \( \bar{e}_f(\hat{\beta}^T x, n, 1) \). In particular, when \( f \in \Sigma(2, L) \), Theorem A.3 shows that \( \bar{e}_f(n, 1) \approx n^{-4/5} \). Our analysis recovers the existing results on estimating \( f \) under model (1) when \( x \) is in a compact set, however, a more careful analysis is needed when \( x \) is heavy-tailed.

In the following two sections, we assume existence of the estimators of \( \hat{\beta} \) and \( \hat{f} \) under model (1), which satisfy the error rate in (11). Furthermore, to simplify the presentation of the paper, we assume that estimation of \( G^* \) is done on an independent sample set with size \( n \), which ensures the independence of \( \hat{G} \) from \( \hat{\beta} \) and \( \hat{f} \). This can be achieved through data splitting and will not affect the statistical rate of convergence, but only the constants.

### 3.1 First-order estimation

Suppose the function \( g^2(\langle x, \gamma^* \rangle) \) together with \( x \) satisfies the first-order regularity condition. Then

\[ E[(y - f(\langle x, \beta^* \rangle))^2 S(x)] = E[c^2 g^2(\langle x, \gamma^* \rangle)S(x)] = 2\mu_1 \gamma^* = \gamma, \]

where \( \mu_1 = E[g(\langle x, \gamma^* \rangle)g'(\langle x, \gamma^* \rangle)] \). Note that whenever \( \mu_1 \neq 0 \), the line spanned by \( \gamma^* \) is identifiable from \( \gamma \). In particular, one can estimate \( \pm \gamma^* \) by normalizing the estimator of \( \gamma \). If we
further assume that $\mu_1 > 0$, one can fully identify $\gamma^*$ from $\gamma$ (Xia, 2006; Wang et al., 2010). We take a different approach and, in order to avoid issues with normalization, use the following distance 

$$\text{dist}(\hat{\gamma}, \gamma^*) = 1 - \frac{\langle \hat{\gamma}, \gamma^* \rangle}{\|\gamma\|_2},$$

(14) as a surrogate for $\|\hat{\gamma} - \gamma\|_2^2$, to quantify the convergence rate for the first-order estimator. We will estimate $\hat{\gamma}$ by replacing the left hand side in (13) by its truncated empirical counterpart.

**Definition 3.1** (Truncation function). For a scalar $v \in \mathbb{R}$, the truncation function is defined as $\Psi_\tau(v) = v \cdot 1_{|v| \leq \tau}$. For a vector or matrix $v$, the truncation function $\Psi_\tau(v)$ is applied elementwise.

In a low-dimensional setting, we estimate $\hat{\gamma}$ as 

$$\hat{\gamma}_1 = \frac{1}{n} \sum_{i=1}^{n} \left( \Psi_\tau(y_i) - \Psi_\tau(\hat{f}(x_i^T \hat{\beta})) \right)^2 \cdot \Psi_\tau(S(x_i)).$$

(15) The following theorem gives us its statistical convergence rate.

**Theorem 3.2** (Low-dimensional first-order estimator). Suppose the function $g^2(\langle x, \gamma^* \rangle)$ together with $x$ satisfies the first-order regularity condition. Furthermore, suppose Assumption 2.5 with $p \geq 6$ and Assumption A.2 (a,b) hold and $\mu_1 \neq 0$. Then for any $0 < \delta < 1$, there exist constants $N_\delta$ (depending on $\delta$) and $\Upsilon$ such that the estimator (15) with $\tau = \Upsilon \left( \frac{nM_6 \log(12d/\delta)}{d} \right) \frac{1}{\delta}$ satisfies

$$P \left( \|\hat{\gamma}_1 - \gamma\|_2 \leq \Upsilon \left( \sqrt{\frac{M_6 d \log(12d/\delta)}{n}} + \sqrt{\frac{M_6 d \cdot \bar{e}_{f,\delta}(n,1)}{\delta}} \right) \right) \geq 1 - \delta,$$

for all $n \geq N_\delta$. In addition, if the conditions of Theorem A.1 and A.3 are satisfied, then we have 

$$\text{dist}(\hat{\gamma}_1, \gamma^*) = O_P \left( \frac{d \log d}{\mu_1^2 n} \right).$$

Assumption A.2 (a,b) guarantees the 6th moment of $|\hat{f}(x^T \hat{\beta})|$ is finite for a given $\hat{f}$ and $\hat{\beta}$, that is, $\mathbb{E}_{\beta,f}[|\hat{f}(x^T \hat{\beta})|^6] \leq M_6$ with high probability. The convergence rate consists of two parts: parametric rate and nonparametric rate. When $f \in \Sigma(2, L)$, Theorem A.3 shows that $\bar{e}_{f,\delta}(n,1) \approx n^{-4/5}$ and therefore the parametric rate is the dominant term above. Similarly, when a one-dimensional function $f \in \Sigma(k, L)$, we have that $\bar{e}_{f,\delta}(n,1) \approx n^{-2k/(k+1)}$, and the dominant term will always be the parametric rate.

In a high-dimensional setting, estimation of $\gamma^*$ is possible under additional structural assumptions on the unknown vector. It is common to assume that $\gamma^*$ is sparse and satisfies $\|\gamma^*\|_0 \leq s$. Under this assumption, we propose the following $\ell_1$ penalized estimator

$$\hat{\gamma}_2 = \arg \min_{\gamma} \frac{1}{2} \|\gamma\|^2 - \langle \gamma, \hat{\gamma}_1 \rangle + \lambda \|\gamma\|_1.$$ 

(16) It is well known that $\hat{\gamma}_2$ can be obtained by soft-thresholding $\hat{\gamma}_1$ as $\hat{\gamma}_2 = \phi_\lambda(\hat{\gamma}_1)$ where the soft-thresholding function, $\phi(v) = (1 - \lambda/|v|)_+ \cdot v$, is applied elementwise. We have the following convergence result.

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**Theorem 3.3** (High-dimensional first-order estimator). Suppose the conditions of Theorem 3.2 are satisfied and further suppose $\|\gamma^*\|_0 \leq s$. Then, for the same constants $\Upsilon$ and $N_\delta$, the estimator (16) with $\tilde{\gamma}_1$ as in Theorem 3.2 and

$$\lambda \geq 2\Upsilon \left( \sqrt{\frac{M_6 \log(12d/\delta)}{n}} + \frac{\sqrt{M_6 \cdot \tilde{e}_{f,\delta}(n, 1)}}{\delta} \right)$$

satisfies

$$P\left( \|\tilde{\gamma}_2 - \gamma\|_2 \leq 3\sqrt{s}\lambda \quad \text{and} \quad \|\tilde{\gamma}_2 - \gamma\|_1 \leq 12s\lambda \right) \geq 1 - \delta,$$

for all $n \geq N_\delta$. In addition, if the conditions of Theorem A.1 and A.3 are satisfied, we have

$$\text{dist}(\tilde{\gamma}_2, \gamma^*) = O_P\left( \frac{s \log d}{\mu_1 n} \right).$$

The above two theorems show that $\gamma^*$ can be estimated at a parametric rate in a low-dimensional setting and at the rate $\sqrt{s \log d/\delta n}$ in a high-dimensional setting. These rates are minimax optimal when estimating mean signal $\beta^*$ in homoscedastic index model (Lin et al., 2017). The results only hold asymptotically due to the estimation of the link function $f$.

### 3.2 Second-order estimation

In this section, we develop the second-order estimation procedure for $\gamma^*$. Though the first-order estimator is easy to compute and has good statistical convergence rate, it has been observed in the literature that second-order estimators are more robust and the regularity condition allows for estimation under a wider class of functions (Babichev and Bach, 2018).

Suppose the function $g^2(\langle x, \gamma^* \rangle)$ together with $x$ satisfies the second-order regularity condition. Under the model (12), we have

$$U^* := \mathbb{E}[y - f(\langle x, \beta^* \rangle)]^2H(x) = \mathbb{E}[\kappa^2 g^2(\langle x, \gamma^* \rangle)H(x)] = 2\mu_2 \gamma^* \gamma^T,$$

where $\mu_2 = \mathbb{E}[g'(x^T \gamma^*)]^2 + \mathbb{E}[g(x^T \gamma^*)g''(x^T \gamma^*)]$. Suppose $\mu_2 \neq 0$, one strategy for estimating $\pm \gamma^*$ is based on estimating the matrix $U^*$ and extracting its leading eigenvector. In a low-dimensional setting, this strategy leads to our second-order estimator, which is defined as

$$\tilde{\gamma}_3 \in \arg \max_{\|\gamma\|_2 \leq 1} \|\gamma^T \left( \frac{1}{n} \sum_{i=1}^n (\Psi_\tau(y_i) - \Psi_\tau(f(x^T \tilde{\beta})))^2 \cdot \Psi_\tau(H(x_i)) \right) \|.$$

The following theorem establishes its rate of convergence.

**Theorem 3.4** (Low-dimensional second-order estimator). Suppose the function $g^2(\langle x, \gamma^* \rangle)$ together with $x$ satisfies the second-order regularity condition. Furthermore, suppose Assumption 2.5 with $p \geq 6$ and Assumption A.2 (a,b) hold and $\mu_2 \neq 0$. Then for any $0 < \delta < 1$, there exist constants $N_\delta$ (depending on $\delta$) and $\Upsilon$ such that the estimator (18) with $\tau = \Upsilon \left( \frac{nM_6}{\log(12d/\delta)} \right)^{1/2}$ satisfies

$$P\left( \min_{i=1}^{\pm 1} \|\tilde{\gamma}_3 - \gamma^*\|_2 \leq \frac{\Upsilon}{\mu_2} \left( \frac{d \sqrt{M_6 \log(12d^2/\delta)}}{n} + \frac{d \sqrt{M_6 \cdot \tilde{e}_{f,\delta}(n, 1)}}{\delta} \right) \right) \geq 1 - \delta,$$
for all \( n \geq N_\delta \). In addition, if the conditions of Theorem A.1 and A.3 are satisfied, then we have

\[
\min_{i=\pm 1} \| \hat{\gamma}_i - \gamma^* \|_2 = O_P\left( \frac{d}{\mu_2} \sqrt{\frac{\log d}{n}} \right).
\]

Based on \( \hat{U} \) defined in (18), we propose to estimate \( \gamma^* \) with the second-order Stein’s identity in a high-dimensional setting. Our estimator is built on the optimization algorithm that was proposed as a convex relaxation for sparse PCA problem (Vu et al., 2013). Given a symmetric matrix \( A \), tuning parameter \( \lambda \), and an integer \( r \), we denote \( T_\lambda(A, r) \) to be the optimal solution of the following optimization program

\[
T_\lambda(A, r) = \arg \max_V \langle V, A \rangle - \lambda \| V \|_{1,1},
\]

s.t. \( 0 \leq V \leq I_d, \ Trace(V) = r. \tag{19}
\]

The constraint set in (19) is called the Fantope of order \( r \), which is the convex hull of rank-\( r \) projection matrices (Vu et al., 2013). The tuning parameter \( r \) controls the number of eigenvectors we aim to estimate, while \( \lambda \) controls the overall sparsity of eigenvectors. Let \( \hat{V} = T_\lambda(\hat{U}, 1) \) where \( \hat{U} \) is defined in (18). Our high-dimensional second-order estimator of \( \gamma^* \) is defined as

\[
\hat{\gamma}_4 = \arg \max_{|\gamma|_2 \leq 1} | \gamma^T \hat{V} \gamma |. \tag{20}
\]

**Theorem 3.5** (High-dimensional second-order estimator). Suppose the conditions of Theorem 3.4 are satisfied and further suppose \( \| \gamma^* \|_0 \leq s \). Then, there exist constants \( Y \) and \( N_\delta \) such that the estimator (20) with \( \hat{U} \) as in Theorem 3.4 and

\[
\lambda \geq Y(\sqrt{\frac{M_6 \log(12d^2/\delta)}{n}} + \sqrt{M_6 \cdot e_{f,\delta}(n, 1) \delta})
\]

satisfies

\[
P\left( \min_{i=\pm 1} \| i \hat{\gamma}_4 - \gamma^* \|_2 \leq \frac{4\sqrt{2} s \lambda}{\mu_2} \right) \geq 1 - \delta,
\]

for all \( n \geq N_\delta \). In addition, if the conditions of Theorem A.1 and A.3 are satisfied, we have

\[
\min_{i=\pm 1} \| i \hat{\gamma}_4 - \gamma^* \|_2 = O_P\left( \frac{s}{\mu_2} \sqrt{\frac{\log d}{n}} \right).
\]

From the above two theorems, we see that the second-order estimator is \( \sqrt{n} \)-consistent in a low dimensional setting, while the rate of convergence in a high-dimensional setting is \( s\sqrt{\log d/n} \). Compared to the first-order estimators, the high-dimensional rate has an extra \( \sqrt{s} \) factor, which comes from the convex relaxation programming we are based on. The rate matches the one in Vu et al. (2013), even though the estimation is done on truncated data due to heavy-tailedness. We note, however, that the identifiability condition for the second-order method requiring \( \mu_2 \neq 0 \) is milder than \( \mu_1 \neq 0 \). For example, if \( x^T \beta^* \) has a symmetric distribution and \( g(x) = x^k \) for some \( k \), then \( \mu_1 = 0 \), while \( \mu_2 \neq 0 \). Therefore, each estimator has its own advantages.

So far, we have investigated first- and second-order estimators under model (12) and derived asymptotic results on their convergence in different settings. In the following, we will discuss an estimation procedure that can obtain a finite sample result in a setting where the mean and variance index are approximately orthogonal.
3.3 Estimation under orthogonality

In the previous two subsections, we discussed estimators of $\gamma^*$ that require estimation of $\beta^*$ and $f$. It is interesting to point out that estimation of $\gamma^*$ is possible without estimating $f$ in a certain setting. To illustrate this, we consider the model (12) in a high-dimensional setting. First, we note that if $\beta^*$ and $\gamma^*$ are suitably orthogonal, then our estimation procedure can take advantage of this property. Second, we note that two sparse vectors in high-dimensions are orthogonal to each other with high probability.

We illustrate the second point from a Bayesian point of view. Suppose that $\beta^*$ and $\gamma^*$ are drawn from a prior that puts a lot of mass on $s$-sparse vectors. For example, consider the following mixture distribution from which each entry of $\beta^*$ and $\gamma^*$ are drawn independently

$$
\beta_i^*, \gamma_i^* \sim (1-\pi) \cdot \delta_0 + \pi \cdot N(0,1), \quad \forall i \in [d]
$$

where $\delta_0$ is the Dirac function, putting all mass on 0, and $\pi = s/d$. Such a mixture distribution has been widely used in high-dimensional sparse parameter estimation (Johnstone and Silverman, 2004), variable selection (Mitchell and Beauchamp, 1988; Ishwaran and Rao, 2005), multi-task learning (Titsias and Lázaro-Gredilla, 2011), and Bayesian multiple testing (Scott and Berger, 2006). Under this prior, we have that $\beta^T \gamma^* = 0$ with high probability, since

$$
P(\beta^T \gamma^* = 0) \geq \prod_{i \in [d]} P(\beta_i^* \gamma_i^* = 0) = (1-\pi^2)^d \geq 1 - \frac{s^2}{d}.
$$

Next, we show that when $\beta^T \gamma^* = 0$, we can estimate $\gamma^*$ without estimating $f$.

We start with an estimator based on the first-order Stein’s identity. Suppose $f^2(\langle x, \beta^* \rangle)$ and $g^2(\langle x, \gamma^* \rangle)$ together with $x$ satisfy the first-order regularity condition, then

$$
\mathbb{E}[y^2 S(x)] = \mathbb{E}[f^2(\langle x, \beta^* \rangle) S(x)] + \mathbb{E}[g^2(\langle x, \gamma^* \rangle) S(x)] = 2\eta_1 \beta^* + \eta,
$$

(21)

where $\eta_1 = \mathbb{E}[f(x^T \beta^*) f'(x^T \beta^*)]$. We utilize (21) to obtain our estimator. First, we can use the procedure of Yang et al. (2017a) to estimate $\hat{\beta}$. Note that other estimators are also possible, as long as $\hat{\beta}$ satisfies the convergence rate in Theorem A.1. Next, given user specified thresholds $\tau$ and $\kappa$, we define $\hat{w} = \frac{1}{n} \sum_{i=1}^n \Psi_{\tau}(y_i)^2 \cdot \Psi_{\tau}(S(x_i))$ and its soft-thresholded version $\hat{w} = \phi_\lambda(\hat{w})$. Our estimator is given as

$$
\hat{\gamma}_5 = \phi_\lambda(\hat{w} - \langle \hat{\beta}, \hat{w} \rangle \cdot \hat{\beta}),
$$

(22)

where $\lambda$ is a user specified parameter that controls the sparsity of the estimator.

**Theorem 3.6** (First-order orthogonal estimation). Suppose $f^2(\langle x, \beta^* \rangle)$ and $g^2(\langle x, \gamma^* \rangle)$ together with $x$ satisfy the first-order regularity condition, $\|\beta^*\|_0 + \|\gamma^*\|_0 \leq s$, $\langle \beta^*, \gamma^* \rangle = 0$, and $\mu_1 \neq 0$ (defined in (13)). Furthermore, suppose Assumption 2.5 with $p \geq 6$ holds and $\hat{\beta}$ converges at the rate in Theorem A.1. Then for any $0 < \delta < 1$, we have a constant $C(\eta_1, \mu_1, \|\beta^*\|_1, \|\gamma^*\|_1)$ and the estimator (22) with $\tau = (\frac{M_\delta}{\log(2d/\delta)})^{\frac{1}{2}}, \kappa = 14 \sqrt{\frac{M_\delta \log(2d/\delta)}{n}}$, and $\lambda \geq C(\eta_1, \mu_1, \|\beta^*\|_1, \|\gamma^*\|_1) \kappa$ satisfies

$$
P\left( \|\hat{\gamma}_5 - \gamma\|_2 \leq 3\sqrt{s} \lambda \quad \text{and} \quad \|\hat{\gamma}_5 - \gamma\|_1 \leq 12s \lambda \right) \geq 1 - \delta.
$$
Unlike the results in the previous sections, the argument in Theorem 3.6 holds for finite sample size n. The choice of the tuning parameter λ depends on some quantities of β∗ and γ∗, which need to be tuned in practice. Even though our estimation is built on the identity (21), the above result still holds for η1 = 0.

The estimator based on the second-order Stein’s identity is obtained similarly. Suppose the functions f2((x, β∗)) and g2((x, γ∗)) together with x satisfy the second-order regularity condition. Then

$$E[y^2 H(x)] = E[f^2((x, β^*))H(x)] + E[g^2((x, γ^*))H(x)] = 2η_2β^*β^{**T} + 2μ_2γ^*γ^{**T},$$  \tag{23}

where η_2 = (E[(f'(xTβ*))^2] + E[f(xTβ*)f''(xTβ*)]) and μ_2 is defined same as (17). Let £U = \frac{1}{n} \sum_{i=1}^{n} \Psi_r(y_i)^2 \cdot \Psi_r(H(x_i)) be the truncated counterpart of the left hand side in (23), £U = £U − (£βT £ψ) · ββ^T, and £V = T_λ(£U, 1). Then our estimator can be computed as

$$\hat{γ}_6 ∈ \arg \max_{∥γ∥_2≤1} |γ^T £Vγ|. \tag{24}$$

**Theorem 3.7** (Second-order orthogonal estimation). Suppose f^2((x, β∗)) and g^2((x, γ∗)) together with x satisfy the second-order regularity condition, \(∥β^*∥_0 \vee ∥γ^*∥_0 ≤ s, <β^*, γ^*> = 0, \) and \(μ_2 \neq 0 \) (defined in (17)). Furthermore, suppose Assumption 2.5 with \(p ≥ 6 \) holds and β converges at the rate in Theorem A.1. Then for any \(0 < δ < 1 \), we have constant \(C'(η_2, μ_2, ∥β^*∥_1, ∥γ^*∥_1) \) and the estimator (24) with \(λ ≥ C'(η_2, μ_2, ∥β^*∥_1, ∥γ^*∥_1) \sqrt{\frac{M_0 log(6d/δ)}{n}} \) and \(τ = (\frac{nM_0}{log(6d/δ)})^{\frac{1}{2}} \) satisfies

$$P\left(\min_{i, j} ∥\hat{γ}_6 − γ^*∥_2 ≤ \frac{4V_s λ}{μ_2}\right) ≥ 1 − δ.$$

We conclude this section by noting that while the requirement \(β^T γ^* = 0 \) might seem restrictive, our proof technique can be trivially modified to allow for a relaxed assumption stating that \(∥β^T γ^*∥ ≤ \sqrt{log d/n} \) for the same estimator, which would be often satisfied in a high-dimensional setting. Compared to the results in the last two subsections, we can utilize the approximate orthogonality to obtain non-asymptotic results, rather than relying on estimation of f. Furthermore, we note that the orthogonality condition holds in applications of generalized linear mixed models, where predictors that contribute to the mean part will not be included in the variance part. Therefore, Theorem 3.6 and 3.7 are useful for orthogonal design generalized linear mixed models (Faraway, 2016; McCullagh, 2018).

### 4 Multiple Index Volatility Model

In this section, we study the model (1) with \(v > 1 \), which is a multiple index volatility model. We develop an estimator for \(G^* \) based on the second-order Stein’s identity. The first-order Stein’s identity is not directly applicable here, unless combined with sliced inverse regression. See Babichev and Bach (2018) for related issues in multiple index models.

Our starting point is the second-order identity, which states that

$$E[(y − f(x^T β^*))^2 H(x)] = E[y^2 (G^T x) H(x)] = 2G^* Λ G^{**T}, \tag{25}$$
where $\Lambda = \mathbb{E}[\nabla g(G^T x) \nabla^T g(G^T x) + g(G^T x) \nabla^2 g(G^T x)] \in \mathbb{R}^{v \times v}$. Let $\mu_3 = \lambda_{\text{min}}(\Lambda)$ be the minimum eigenvalue of $\Lambda$ and suppose $\mu_3 > 0$. Note that we could replace this identifiability condition by letting $\mu_3 = \lambda_{\text{max}}(\Lambda) < 0$. Our estimation procedure is similar to what we discussed in Section 3.2, however, we will extract top $v$ eigenvectors that will estimate $G^*$ up to an orthogonal transformation.

In a low-dimensional setting, starting from $\tilde{U}$, defined in (18), to estimate the left hand side of (25), we define $\tilde{G}_1$ as a solution to the following optimization program

$$\tilde{G}_1 \in \arg \max_{G \in \mathbb{R}^{d \times v}} \langle \tilde{U}, GG^T \rangle$$

s.t. $G^T G = I_v$. (26)

**Theorem 4.1** (Low-dimensional second-order estimator). Suppose conditions of Theorem 3.4 are satisfied and $\mu_3 > 0$. The estimator (26), with $\tilde{U}$ defined in (18) and $\tau = \Upsilon \left( \frac{nM_0}{\log(12d^2/\delta)} \right)^{\frac{1}{6}}$, satisfies

$$P \left( \frac{\inf_{Q \in \mathbb{R}^{v \times v}} \|\tilde{G}_1 - G^* Q\|_F}{\mu_3} \leq \frac{\Upsilon}{\mu_3} \left( d\sqrt{M_0 d \log(12d^2/\delta)} + d\sqrt{M_0 d \cdot \tilde{e}_{f,0}(n_1)} \right) \right) \geq 1 - \delta,$$

for $n$ large enough. Furthermore, if the conditions of Theorem A.1 and A.3 are satisfied, we have

$$\inf_{Q \in \mathbb{R}^{v \times v}} \|\tilde{G}_1 - G^* Q\|_F = O_P \left( \frac{d}{\mu_3} \sqrt{\frac{d \log d}{n}} \right).$$

In a high-dimensional setting, we let $\tilde{V} = \mathcal{T}_\lambda(\tilde{U}, v)$ be the first $v$ sparse eigenvectors of $\tilde{U}$ where $\mathcal{T}_\lambda(\cdot, \cdot)$ is defined in (19), then our high-dimensional estimator $\tilde{G}_2$ can be solved from (26) with $\tilde{U}$ replaced by $\tilde{V}$. Its statistical rate of convergence is given in next theorem.

**Theorem 4.2** (High-dimensional second-order estimator). Suppose conditions of Theorem 3.5 are satisfied (we replace $\|\gamma\|_0 \leq s$ by $\|G^*\|_{0, \text{max}} \leq s$) and $\mu_3 > 0$. Under the same setup of $\lambda$ as in Theorem 3.5, the estimator $\tilde{G}_2$ satisfies

$$P \left( \frac{\inf_{Q \in \mathbb{R}^{v \times v}} \|\tilde{G}_2 - G^* Q\|_F}{\mu_3} \leq \frac{4s \sqrt{v} \lambda}{\mu_3} \right) \geq 1 - \delta.$$

Furthermore, if the conditions of Theorem A.1 and A.3 are satisfied, we have

$$\inf_{Q \in \mathbb{R}^{v \times v}} \|\tilde{G}_2 - G^* Q\|_F = O_P \left( \frac{s}{\mu_3} \sqrt{\frac{v \log d}{n}} \right).$$

Analogously, in the orthogonal case, i.e. $\beta^T G^* = 0$, we redefine $\tilde{V}$ in (24) by setting $\tilde{V} = \mathcal{T}_\lambda(\tilde{U}, v)$ and apply (26) on $\tilde{V}$ to extract its first $v$ eigenvectors. The result is denoted as $\tilde{G}_3$, which is also our estimator of $G^*$ under orthogonal case. Its convergence rate is summarized next.

**Theorem 4.3** (Orthogonal estimation). Suppose conditions of Theorem 3.7 are satisfied with $\beta^T G^* = 0$, $\|G^*\|_{0, \text{max}} \leq s$, and $\mu_3 > 0$. Then, under the same setup of $\tau$ and $\lambda$ as in Theorem 3.7, the estimator $\tilde{G}_3$ satisfies

$$\inf_{Q \in \mathbb{R}^{v \times v}} \|\tilde{G}_3 - G^* Q\|_F \leq \frac{4\sqrt{v} \lambda}{\mu_3}$$

with probability at least $1 - \delta$. 

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The rate of convergence in the last two theorems is proportional to \( s \sqrt{\nu/\mu_3} \) as \( G^*G^*^T \) has at most \( s^2 \nu \) nonzero elements when \( \|G^*\|_{0,\text{max}} \leq s \). If, instead, the sparsity structure on \( G^* \) is assumed that \( G^* \) has at most \( s \) nonzero rows (Xu et al., 2010; Obozinski et al., 2011), then \( G^*G^*^T \) has at most \( s^2 \) nonzero elements and the rate would be proportional to \( s\lambda/\mu_3 \).

5 Numerical Experiment

We conduct extensive numerical experiments to validate the theoretical results presented in Section 3 and 4. We focus our attention to recovery of \( G^* \) and verify convergence rates in a high-dimensional setting assuming the knowledge of \( f \) and using Yang et al. (2017a) to estimate \( \beta^* \). Under this setup, all statements hold for finite sample. Also, only the step of estimating \( \beta^* \) contributes the error \( \tilde{e}_{f,\delta}(n,1) \), which is still in smaller order comparing to the error occurs in the step of estimating \( G^* \).

Specifically, we will empirically show that the estimation error is upper bounded by \( \sqrt{s \log d/n} \) for the first-order estimation and \( s \sqrt{\log d/n} \) for the second-order estimation. The estimation accuracy is measured using (14) for single index volatility models, and the sine distance, defined as

\[
\|\sin(\angle(\tilde{G},G^*))\|_F = \frac{1}{\sqrt{2}} \|\tilde{G}G^T - G^*G^*^T\|_F,
\]

for multiple index volatility model. Throughout the simulations, we set the mean link function to be \( f(x) = 2x + \cos(x) \) and consider three different distribution designs for \( x \): Gaussian, Student’s \( t \) distribution, and Gamma distribution. Table 1 summarizes the parameters for the distribution of \( x \), as well as the first- and second-order score functions. We let \( \epsilon \sim N(0,1) \). Simulation results are reported over 20 independent runs.

| Distribution  | Parameter               | First-order score   | Second-order score          |
|---------------|-------------------------|---------------------|----------------------------|
| Gaussian      | \( \mu = 0, \sigma = 1 \) | \( S(x) = x \)     | \( H(x) = x^2 - 1 \)      |
| Student’s \( t \) | degree of freedom 13  | \( S(x) = \frac{14x}{13+x^2} \) | \( H(x) = \frac{224x^2}{(13+x^2)^2} - \frac{14}{13+x^2} \) |
| Gamma         | \( k = 13, \theta = 2 \) | \( S(x) = \frac{1}{2} - \frac{12}{x} \) | \( H(x) = \frac{132}{x^2} - \frac{12}{x} + \frac{1}{4} \) |

Table 1: Distribution of covariate \( x \)

5.1 Single index experiment

We consider two estimators of \( \gamma^* \) here: \( \hat{\gamma}_2 \) in (16) and \( \hat{\gamma}_1 \) in (20). The optimization program in (19) is approximately solved using the ADMM-based algorithm proposed in Vu et al. (2013) with the Lagrange multiplier \( \rho = 1 \) (see equation (9) in Vu et al. (2013)). We consider three different variance link functions:

\[
g_1(x) = x^2 + x + \cos(x); \quad g_2(x) = x^2 + x + \exp(-x^2); \quad g_3(x) = x^2 + x + \frac{\exp(x)}{(1 + \exp(x))^2}.
\]

We set \( d = 100 \) and \( s = 10 \), and vary the sample size \( n \). For each \( i \in [n] \) and \( j \in [d] \), \( [x_i]_j \) is generated independently from the corresponding distributions. Unknown coefficients \( \beta^* \) and \( \gamma^* \) are generated as follows. We first randomly generate positions of non-zero indices from \([d]\). Then each non-zero entry is set equal to \( \pm 1/\sqrt{s} \) with probability \( 1/2 \). We set \( \tau = 10(n/\log d)^{\frac{1}{2}} \) and
Figure 1: Estimation error when estimating $\gamma^*$ in the single index volatility model (12). The lines indicate three different variance functions. Different columns correspond to different designs on $x$. The first row corresponds to the first-order estimator, while the bottom one to the second-order estimator.

From the plots we observe that our theory explains the relationship between the observed estimation error and the problem parameters. For example, when sample size is sufficiently large, from the first row of Figure 1, we observe that the estimation error linearly decreases with $\sqrt{s \log d/n}$ as suggested by Theorem 3.3. Furthermore, although there are small differences between different designs, we observe that for each design the error decreases linearly in the control parameters. Similar observation holds for the estimator $\hat{\gamma}_4$ which is based on the second-order Stein’s identity.
5.2 Multiple index experiment

We consider two estimators of $\mathbf{G}^*$ here: $\hat{\mathbf{G}}_2$ and $\hat{\mathbf{G}}_3$ described in Section 4. We set $d = 200$, $s = 10$, and $v = 3$. We let $\text{supp}(\gamma_j^*) = [(j - 1)s, js]$ and each entry in the support is set to $\pm 1/\sqrt{s}$ with equal probability. The variance link function is defined as $g(\mathbf{G}^* \mathbf{x}) = \sum_{j=1}^{v} g(\mathbf{x}^T \gamma_j^*)$ where $g \in \{g_1, g_2, g_3\}$ is the variance function used in the single index experiment. In this experiment, we let $\tau = 10(n/\log d)^{1/3}$, $\lambda = 0.01\sqrt{\log d/n}$. The results are shown in Figure 2 and again we observe that the error rate is correctly explained by our theory for sufficiently large sample size. In particular, we observe that the error rate decreases linearly with $s\sqrt{v\log d/n}$ as expected.
6 Discussion

We proposed new estimators for parametric components of index volatility models based on the first and second order Stein’s identities. Our approach lies in extracting the direction of variance by multiplying the score variables with residuals and using weighted mean squared minimization with truncation and regularization to accommodate for estimation in a high-dimensional and heavy-tailed setting. We rigorously proved statistical convergence rates of our estimators under both single and multiple index structures, which were then verified in finite samples through numerical experiments. In particular, our results were qualitatively the same under a range of designs, including heavy-tailed ones. The estimation rate is comprised of both the nonparametric and parametric rate, though the parametric rate is the dominant term and matches the corresponding rate in the mean estimation. We illustrated that when the mean index is orthogonal to the variance index, which would naturally be the case in many high-dimensional applications, we do not need to estimate the mean link function and can obtain finite sample results.

Our estimation procedures rely on estimation of the gradient of link function through Stein’s identities, which are aligned with the e.d.r. direction in index volatility models. Using this approach, we were able to naturally extend traditional fixed design setup to randomized design. The drawback of the approach based on Stein’s identity is that the prior knowledge of a distribution of covariates $\mathbf{x}$ is needed. In a low-dimensional setting, Babichev and Bach (2018) proposed an approach for estimating the first-order score function under the assumption that the score function can be represented as a finite linear combination of basis functions in a given dictionary. Extending their approach to a high-dimensional setting, as well as, to estimation of the second-order score functions seems challenging without strong assumptions on the underlying distribution of $\mathbf{x}$. We leave investigation of possible estimators for future work. Fortunately, in some applications, such as compressed sensing (Ai et al., 2014; Davenport et al., 2014) or phase retrieval (Candès et al., 2015a,b), the distribution of covariates is known.

In this work, we have focused on point estimation of the e.d.r. direction. Establishing tools that would allow for construction of confidence intervals and more generally uncertainty quantification is an important future direction. Another direction is improving the statistical rate obtained by the second-order estimation procedures, which arises from the finite moment condition on $H(\mathbf{x})$ that makes bounding of the restricted operator norm difficult. We note, however, that obtaining the error rate of $\sqrt{s \log d/n}$ under heavy-tailed design for sparse PCA is still an open problem. Finally, developing a robust version of the estimators based on absolute residuals, as used for robust variance estimation (Davidian and Carroll, 1987), would further enlarge potential for diverse applications of our methodology.
Supplemental Materials:
High-dimensional Index Volatility Models via Stein’s Identity

A Estimation of Index Mean Function

In this section, we present results on the mean estimation for the model (1). In particular, we develop an explicit formula for $\hat{c}_f(\hat{\beta}^T x, n, 1)$ and further derive a bound on its first moment, $\hat{e}_f(\hat{\beta}, n, 1)$, and error rate $\hat{e}_{f,\delta}(n, 1)$. Our estimation procedure is based on two steps. First, we use approach in Yang et al. (2017a) to estimate the mean index $\beta^\star$. Next, a local linear regression is applied to the pair $(y, \hat{\beta}^T x)$ to obtain the mean link function estimator $\hat{f}$. Finally, we use $\hat{f}(\langle \hat{\beta}, x \rangle)$ as an estimation of $f(\langle \beta^\star, x \rangle)$. To simplify the analysis, we assume that two steps are conducted on independent samples of size $n$ each, which is obtained, for example, by sample splitting in practice. This simplifies the analysis while keeping the statistical rate unchanged. We note that the local linear regression is just one way to estimate the nonparametric component in index models. See Liu et al. (2013) for a robust estimator as an alternative.

To unify the presentation, we consider a more general heteroscedastic index model:

$$y \mid x = f(\langle \beta^\star, x \rangle) + \tilde{g}(x) \epsilon,$$

(A.1)

where $\mathbb{E}[\epsilon|x] = 0$, $\mathbb{E}[\epsilon^2|x] = 1$. By setting $\tilde{g}(x) = g(\langle \gamma^\star, x \rangle)$ we obtain the single index volatility model and $\tilde{g}(x) = g(G^{T} x)$ would lead to multiple index volatility model. The estimator $\tilde{\beta}$ in Yang et al. (2017a) is defined as

$$\tilde{\beta} = \phi_{\lambda} \left( \frac{1}{n} \sum_{i=1}^{n} \Psi_{\tau}(y_i)\Psi_{\tau}(S(x_i)) \right),$$

(A.2)

where $\lambda$ and $\tau$ are tuning parameters. This Lasso-type estimator comes from the first-order Stein’s identity applied on the response $y$. Here $\tau$ is the truncation threshold and $\lambda$ controls the sparsity of $\hat{\beta}$. Note that $\tilde{\beta}$ can be computed without the knowledge of $f$. Its convergence rate is presented in the following theorem.

**Theorem A.1** ($\beta^\star$ estimation). Suppose Assumption 2.5 with $p \geq 4$ holds and $f(\langle \beta^\star, x \rangle)$ together with $x$ satisfies the first-order regularity condition. Furthermore, suppose $\|\beta^\star\|_0 \leq s$. Then, for any $0 < \delta < 1$, the estimator $\tilde{\beta}$ with $\lambda \approx \sqrt{\log(d/\delta)/n}$ and $\tau \approx (n/\log(d/\delta))^{1/4}$ in (A.2) for $\beta^\star$ in model (A.1) satisfies

$$P \left( \| \tilde{\beta} - \beta^\star \|_2 \geq \sqrt{\frac{s \log d/\delta}{n}} \right) \leq \delta.$$

Theorem 4.2 in Yang et al. (2017a) proves the above result for a high-dimensional homoscedastic single index model. Theorem A.1 states a more general result that is valid for a heteroscedastic single index model. The proof is omitted as the proof strategy of Yang et al. (2017a) is directly applicable, since

$$\mathbb{E}[yS(x)] = \mathbb{E}[f(\langle \beta^\star, x \rangle)S(x)] + \mathbb{E}[\tilde{g}(x)S(x)] = \mathbb{E}[f(\langle \beta^\star, x \rangle)S(x)] + c\beta^\star.$$

With $\tilde{\beta}$ defined above, we use a local linear regression estimator to estimate $f(\cdot)$. The results borrows from Fan (1993) and requires the following assumption (see Condition 1 in Fan (1993) for comparison). The assumption is specifically required for estimation using local linear regression and would need to be modified if other estimators are used.
Assumption A.2. For any fixed estimator $\hat{\beta}$ with the rate of convergence as in Theorem A.1, we assume

(a) (smoothness) $f \in C^2(\mathbb{R})$ with $|f'(x)| \vee |f''(x)| \leq L_1, \forall x \in \mathbb{R}$.
(b) (6th moment projection) $\max_{|v| \leq 1} \mathbb{E}[|x^Tv|^6] \leq L_2$.
(c) (4th moment function) $r_{\hat{\beta}}(x) = \mathbb{E}[\tilde{g}^4(x) | \hat{\beta}^T x = x]$ is continuous and bounded.
(d) (density) $\hat{\beta}^T x$ has bounded positive density $q_{\hat{\beta}}$ with $|q_{\hat{\beta}}(x) - q_{\hat{\beta}}(y)| \leq L_3|x - y|^\alpha$ for $\alpha \in (0, 1)$.
(e) (tail) there exists a constant $L_4 > 0$ such that $|f(x)|^4/q_{\hat{\beta}}^2(x)$, $r_{\hat{\beta}}(x)/q_{\hat{\beta}}(x)$, and $|f'(x)|^4/q_{\hat{\beta}}(x)$ are integrable on $(-\infty, -L_4) \cup (L_4, \infty)$.

With these assumptions, we define the local linear estimator to be

$$\tilde{f}(t) = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i + (nh)^{-2}},$$

where $w_i = K_h(x_i^T \hat{\beta} - t)(s_{n2} - (x_i^T \hat{\beta} - t) \cdot s_{n1})$ with $s_{n2} = \sum_{i=1}^{n} K_h(x_i^T \hat{\beta} - t)(x_i^T \hat{\beta} - t)$ for $l = 0, 1, 2$, $h$ is the bandwidth, and $K_h(\cdot) = K(\cdot/h)$ for a kernel function $K(\cdot)$. With a Gaussian kernel, we have the following rate of convergence for the local estimator.

**Theorem A.3 (Mean estimation).** Suppose $\hat{\beta}$ is estimated from the sample $D_1$ and satisfies the rate as in Theorem A.1. Given $\hat{\beta}$, let $\tilde{f}$, defined in (A.3), be a local linear regression estimator of the link function $f$ in model (A.1) based on samples $D_2 = \{y_i, \hat{\beta}^T x_i\}_{i=1}^{n}$ independent from $D_1$. Suppose Assumption 2.5 with $p \geq 4$ and Assumption A.2 (a-d) hold and the bandwidth $h$ satisfies $h \to 0$ and $nh \to \infty$. Then there exist $N$ and $\Upsilon_1$ such that $\forall n \geq N$,

$$\mathbb{E}[|\tilde{f}(x^T \hat{\beta}) - f(x^T \beta^*)|^4 | x, D_1] \leq \Upsilon_1 \left(h^8 + \frac{r_{\hat{\beta}}(x^T \hat{\beta})}{n^2 h^2 q_{\hat{\beta}}^2(x^T \hat{\beta})} + \frac{\|\hat{\beta} - \beta^*\|^4 \cdot |f'(x^T \hat{\beta})|^4}{h^2 q_{\hat{\beta}}^3(x^T \hat{\beta})} + \frac{|x^T \beta^* - x^T \hat{\beta}|^4 + |f(x^T \hat{\beta})|^4}{n^{16} h^{16} q_{\hat{\beta}}^{10}(x^T \hat{\beta})}\right).$$

Furthermore, suppose Assumption A.2 (e) holds as well and $h = n^{-1/5}$, then there exists a constant $\Upsilon_2$ such that

$$P\left(\mathbb{E}[|\tilde{f}(x^T \hat{\beta}) - f(x^T \beta^*)|^2 \cdot W(x) | D_1, D_2] \right) \geq \frac{\sqrt{\mathbb{E}[T_2]}}{\delta} \frac{\mathcal{Y}_2 n^{-4/5}}{\mathcal{Y}_2(n, 1)} \leq 2\delta,$$

where $W(x)$ is either the first-order score variable $S(x)$ or the second-order score variable $H(x)$.

We see that equation (A.4) gives an explicit form for $\tilde{e}_f(\hat{\beta}^T x, n, 1)$. We explicitly write out higher-order terms in (A.4) to clarify the difference between a high-dimensional single index model and a nonparametric model. In a low-dimensional setting with $x$ being in a compact set and $q_{\hat{\beta}}$...
lower bounded away from zero (Zhu and Xue, 2006; Van Keilegom and Wang, 2010; Wang et al., 2010; Lian et al., 2015), the last two terms can be ignored.

As discussed in Section 2, estimation of \( \mathbf{G}^* \) is possible under a heavy-tailed design if condition (10) holds. Assumption A.2 (e) implies that expectation of the right hand side of (A.4), conditional on \( \tilde{\mathbf{\beta}} \), is bounded on the tails; while within the interval \([-L_4, L_4]\), we can make use of continuity so that the integral is bounded naturally. In particular, the assumption imposes conditions on the decay rate of \( |f(x)|, |f'(x)| \), and \( r_{\mathbf{\beta}}(x) \), and holds for any random variables that have compact support. Taking conditional expectation for \( \tilde{e}_f(\tilde{\mathbf{\beta}}^T \mathbf{x}, n, 1) \) and ignoring all smaller order terms, we have

\[
\tilde{e}_f(\tilde{\mathbf{\beta}}, n, 1) \leq h^8 + \frac{1}{n^2 h^2} + \frac{\|\tilde{\mathbf{\beta}} - \mathbf{\beta}^*\|_2^4}{h^2}.
\]

Moreover, using the fact that \( \|\tilde{\mathbf{\beta}} - \mathbf{\beta}^*\|_2 \leq 1/\sqrt{n} \), we can set the bandwidth \( h \asymp n^{-1/5} \) to obtain \( \tilde{e}_{f,\delta}(n, 1) \leq n^{-4/5} \).

We also point out that \( L_3 \) and \( L_4 \) in Assumption A.2 (c-d) do not depend on \( \tilde{\mathbf{\beta}} \) as long as it is close to \( \mathbf{\beta}^* \), which is assumed in Zhang (2018). An equivalent statement would be to assume \( q_{\mathbf{\beta}}, r_{\mathbf{\beta}} \) satisfy conditions (c-d) and further add some continuity conditions on \( q_{\mathbf{\beta}}, r_{\mathbf{\beta}} \) with respect to \( \mathbf{\beta} \), such that \( |q_{\mathbf{\beta}} - q_{\mathbf{\beta}^*}| \) and \( |r_{\mathbf{\beta}} - r_{\mathbf{\beta}^*}| \) are small enough. For example, suppose \( |q_{\mathbf{\beta}}(x) - q_{\mathbf{\beta}^*}(x)| \leq L_3 \|\mathbf{\beta} - \mathbf{\beta}^*\|_2 \) and sup \( L_x \) then by triangle inequality we have \( \forall x, y \)

\[
\begin{align*}
|q_{\mathbf{\beta}}(x) - q_{\mathbf{\beta}}(y)| &\leq |q_{\mathbf{\beta}}(x) - q_{\mathbf{\beta}^*}(x)| + |q_{\mathbf{\beta}^*}(x) + q_{\mathbf{\beta}^*}(y)| + |q_{\mathbf{\beta}}(y) - q_{\mathbf{\beta}^*}(y)| \\
&\leq 2 \sup_x L_x \|\mathbf{\beta} - \mathbf{\beta}^*\|_2 + L_3 |x - y|^\alpha \lesssim L_3' |x - y|^\alpha.
\end{align*}
\]

Assumption A.2 (b) is used for bounding \( \mathbb{E}[|f(x^T \tilde{\mathbf{\beta}})|^4 \mid \tilde{\mathbf{\beta}}] \).

## B Proofs of Main Theorems and Lemmas

Throughout this section we write \( M \), omitting the subscript from \( M_p \), since the moment degree \( p \) is clear from the statement of theorem. For simplicity, we replace the truncation function \( \Psi_\tau \) by notation \( \bar{\Psi}_\tau \) where the truncation threshold \( \tau \) is contained implicitly. In particular, we have \( \Psi_\tau(v) = \bar{\Psi}_\tau \). We use \( \Upsilon > 0 \) to denote a generic constant, which may take different values for each appearance. For Theorem 3.2, 3.3, 3.4, 3.5, 4.1, 4.2, we only prove the first part of statement since the second part is trivial to obtain by plugging in \( \tilde{e}_{f,\delta}(n, 1) \asymp n^{-4/5} \).

### B.1 Proof of Theorem 2.6

We prove the result for \( W(x) = S(x) \) as the other case is shown analogously. For any \( j \in [d] \),

\[
\mathbb{E}_f[|\hat{f}_j(x) - f(x)|^2 \cdot |S(x)_j|] \leq \sqrt{\mathbb{E}_f[|\hat{f}(x) - f(x)|^4]} \sqrt{\mathbb{E}[|S(x)_j|^2]} \leq \sqrt{M} \sqrt{\mathbb{E}_f[|\hat{f}(x) - f(x)|^4]}.
\]

Therefore, we have

\[
\|\mathbb{E}_f[|\hat{f}(x) - f(x)|^2 \cdot S(x)]\|_\infty \leq \sqrt{M} \sqrt{\mathbb{E}_f[|\hat{f}(x) - f(x)|^4]}.
\]
By Markov’s inequality, for any $0 < \delta < 1$, with probability $1 - \delta$, we have
\[
\sqrt{\mathbb{E}_f[|\hat{f}(x) - f(x)|^4]} \leq \sqrt{\frac{\mathbb{E}[|\hat{f}(x) - f(x)|^4]}{\delta}} \leq \frac{\varepsilon_f(n,d)}{\delta}.
\]
Combining the above two inequalities completes the proof.

\section*{B.2 Proof of Corollary 2.7}

Similar to the proof of Theorem 2.6, we have for any $j \in [d],$
\[
\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^2 \cdot |S(x)_j|] \leq \sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]} \mathbb{E}[|S(x)_j|^2] \\
\leq \sqrt{M} \sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]}
\]
and
\[
\|\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^2 \cdot |S(x)_j|]\|_{\infty} \leq \sqrt{M} \sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]}.
\]
By Markov’s inequality, for any $0 < \delta < 1$ and any sample set $\mathcal{D}_1$,
\[
P\left(\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4] \leq \frac{\mathbb{E}_{\tilde{\beta}}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]}{\delta} \bigg| \mathcal{D}_1\right) \geq 1 - \delta, \tag{B.1}
\]
where the probability is taken over randomness in $\mathcal{D}_2$. By the definition in (9), we have
\[
P\left(\sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]} \leq \sqrt{\varepsilon_f(\tilde{\beta},n,1)/\delta} \bigg| \mathcal{D}_1\right) \geq 1 - \delta.
\]
Under the condition (10), we have
\[
P\left(\|\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^2 \cdot |S(x)_j|]\|_{\infty} \geq \sqrt{M} \cdot \varepsilon_f,\delta(n,1)/\delta\right) \\
\leq P\left(\sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]} \geq \varepsilon_f,\delta(n,1)/\delta\right) \\
\leq P\left(\sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]} \geq \varepsilon_f(\tilde{\beta},n,1)/\delta \text{ or } \sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]} \geq \varepsilon_f(\tilde{\beta},n,1)/\delta\right) \\
\leq P\left(\sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]} \geq \varepsilon_f(\tilde{\beta},n,1)/\delta\right) + P\left(\sqrt{\mathbb{E}_{\tilde{\beta},j}[|\hat{f}(x^T\tilde{\beta}) - f(x^T\beta^*)|^4]} \geq \varepsilon_f(\tilde{\beta},n,1)/\delta \bigg| \mathcal{D}_1\right) \\
\leq \frac{2\delta}{\delta} \\
\leq 2\delta.
\]
Here the last inequality uses the fact that $\mathcal{D}_1$ and $\mathcal{D}_2$ are independent, so (B.1) holds uniformly for any $\mathcal{D}_1$. 

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B.3 Proof of Theorem 3.2

Since the samples we use for estimating $\hat{\gamma}$ are independent from $\hat{f}, \hat{\beta}$, we have

$$\mathbb{E}_{\hat{f},\hat{\beta}}[(y - \hat{f}(x^T\hat{\beta}))^2 \cdot S(x)] = \mathbb{E}_{\hat{f},\hat{\beta}}[(y - f(x^T\beta^*) + f(x^T\beta^*) - \hat{f}(x^T\hat{\beta}))^2 \cdot S(x)]$$

$$= \mathbb{E}[y^2(x^T\gamma^*)S(x)] + \mathbb{E}_{\hat{f},\hat{\beta}}[(f(x^T\beta^*) - \hat{f}(x^T\hat{\beta}))^2 \cdot S(x)]$$

$$\geq (13) \hat{\gamma} + \mathbb{E}_{\hat{f},\hat{\beta}}[(f(x^T\beta^*) - \hat{f}(x^T\hat{\beta}))^2 \cdot S(x)]. \quad \text{(B.2)}$$

For the second term, according to (11), for any $\delta > 0$

$$P\left(\left\|\mathbb{E}_{\hat{f},\hat{\beta}}[\langle\hat{\beta}, x\rangle - f(\langle\beta^*, x\rangle)]^2 \cdot S(x)\right\|_{\infty} \geq \frac{\sqrt{\mathbb{M}} \cdot \epsilon_{f,\delta}(n, 1)}{\delta}\right) \leq 2\delta, \quad \text{(B.3)}$$

since $\sqrt{\mathbb{M}_2} \leq \sqrt{\mathbb{M}_6}$. Next, we bound the error that occurs when using $\hat{\gamma}_1$ to approximate the left hand side term in (B.2). We apply the Lemma C.2. Based on Assumption 2.5 ($p \geq 6$) we know that for some constant $\Upsilon_1$

$$\mathbb{E}[|y|^6] \vee \mathbb{E}[|S(x)_j|^6] \vee \mathbb{E}[|f(X^T \beta)|^6] \leq \Upsilon_1 M, \quad \forall j \in [d].$$

Furthermore, for any $\delta > 0$, we have

$$\mathbb{E}_{\hat{f},\hat{\beta}}[|\hat{f}(x^T\hat{\beta})|^6] \leq \frac{32}{\delta} \mathbb{E}[|\hat{f}(x^T\hat{\beta}) - f(x^T\beta)|^6] + 32\mathbb{E}_{\hat{f}}[|f(x^T\beta)|^6]$$

with probability $1 - \delta$. Note that the first term goes to zero as $n \to \infty$ and it only attributes to the higher order error. Furthermore, there exists $N_\delta$ such that $\forall n \geq N_\delta$,

$$\frac{32\mathbb{E}[|\hat{f}(x^T\hat{\beta}) - f(x^T\beta)|^6]}{\delta} \leq \frac{\Upsilon_1 M}{2}.$$ 

Roughly, we only require $\frac{1}{\delta M^p} \leq M$, which implies $n \geq (\frac{1}{\delta M^p})^{\frac{1}{p}} := N_\delta$ for some $p > 1$. Also, by Lemma C.1, we have $\mathbb{E}_{\hat{f}}[|f(x^T\beta)|^6] \leq 64 M$ for a sufficiently large $N$ (not depending on $\delta$). Combining them together, we have $\mathbb{E}_{\hat{f},\hat{\beta}}[|\hat{f}(x^T\beta)|^6] \leq \Upsilon_1 M$ with probability $1 - \delta$. Based on the definition in (15), we have

$$\left\|\hat{\gamma}_1 - \mathbb{E}_{\hat{f},\hat{\beta}}[\hat{y}^2S(x)]\right\|_{\infty}$$

$$\leq \frac{1}{n} \left\|\sum_{i=1}^{n} y_i^2 S(x_i) - \mathbb{E}_{\hat{f},\hat{\beta}}[y^2S(x)]\right\|_{\infty} + 2\frac{1}{n} \left\|\sum_{i=1}^{n} y_i \hat{f}(x_i^T \hat{\beta}) S(x_i) - \mathbb{E}_{\hat{f},\hat{\beta}}[y \hat{f}(x^T \beta) S(x)]\right\|_{\infty}$$

$$+ \frac{1}{n} \left\|\sum_{i=1}^{n} \hat{f}(x_i^T \hat{\beta})^2 S(x_i) - \mathbb{E}_{\hat{f},\hat{\beta}}[\hat{f}(x^T \hat{\beta}) S(x)]\right\|_{\infty}.\quad \text{(B.4)}$$

We set $\tau = (\frac{n\Upsilon_1 M}{\log(2d/\delta)}{\frac{1}{2}}$, apply Lemma C.2 and take the union bound over $d$ indices to get

$$P\left(\left\|\hat{\gamma}_1 - \mathbb{E}_{\hat{f},\hat{\beta}}[\hat{y}^2S(x)]\right\|_{\infty} \leq 28\frac{\Upsilon_1 M \log(2d/\delta)}{n} \right) \geq 1 - 4\delta.
Combining (B.2), (B.3), and (B.4) together and replacing $6\delta$ by $\delta$, there exists $\Upsilon$ such that

$$\|\hat{\gamma}_1 - \gamma\|_\infty \leq \|\hat{\gamma}_1 - E_{\hat{\beta}} f((y - \hat{f}(x^T \hat{\beta}))^2 S(x))\|_\infty + \|E_{\hat{\beta}, f}[(f(x^T \beta^*) - \hat{f}(x^T \hat{\beta}))^2 S(x)]\|_\infty$$

$$\leq \Upsilon\left(\sqrt{\frac{M \log(12d/\delta)}{n}} + \frac{\sqrt{M \cdot \delta_\delta(n_1, 1)}}{\delta}\right)$$

(B.5)

with probability at least $1 - \delta$. Since $\|\hat{\gamma}_1 - \gamma\|_2 \leq \sqrt{d} \|\hat{\gamma}_1 - \gamma\|_\infty$, we get that, for some constant $\Upsilon$, if $\tau = \Upsilon\left(\frac{nM}{\log(12d/\delta)}\right)^{\frac{1}{5}}$ then for all $n \geq N_\delta$

$$P\left(\|\hat{\gamma}_1 - \gamma\|_2 \leq \Upsilon\left(\sqrt{\frac{Md \log(12d/\delta)}{n}} + \frac{\sqrt{M \cdot \delta_\delta(n_1, 1)}}{\delta}\right)\right) \geq 1 - \delta.$$

(B.6)

This completes the first part of proof. For the second part, we plug in $\delta_\delta(n_1, 1) \approx n^{-4/5}$ and see that the nonparametric rate is negligible. For completeness, we will show $\text{dist}(\hat{\gamma}_1, \gamma^*) \leq \frac{1}{\mu_1} \|\hat{\gamma}_1 - \gamma\|_2^2$.

In fact, we have

$$\text{dist}(\hat{\gamma}_1, \gamma^*) = 1 - \frac{\|\hat{\gamma}_1^T \gamma^*\|}{\|\hat{\gamma}_1\|_2} = 1 - \frac{1}{2\mu_1\|\hat{\gamma}_1\|_2} \left(\|\gamma\|_2^2 + \|\hat{\gamma}_1\|_2^2 - \|\hat{\gamma}_1 - \gamma\|_2^2\right)$$

$$\leq \left(1 - \frac{\|\mu_1\|}{2\|\gamma\|_2} - \frac{\|\hat{\gamma}_1\|}{2\mu_1}\right) + \frac{1}{2\mu_1\|\hat{\gamma}_1\|_2} \cdot \|\hat{\gamma}_1 - \gamma\|_2^2$$

$$\leq \frac{1}{2\mu_1^2} \cdot \|\hat{\gamma}_1 - \gamma\|_2^2 \cdot \|\mu_1\|_{\|\hat{\gamma}_1\|_2}. \quad \text{(B.7)}$$

Note that

$$|\mu_1 - \|\hat{\gamma}_1 - \gamma\|_2| \leq \|\hat{\gamma}_1 - \gamma\|_2 \leq |\mu_1| + \|\hat{\gamma}_1 - \gamma\|,$$

so that

$$1 - \frac{\|\hat{\gamma}_1 - \gamma\|_2}{|\mu_1|} \leq \frac{|\mu_1|}{\|\hat{\gamma}_1\|_2} \leq 1 + \frac{\|\hat{\gamma}_1 - \gamma\|_2}{|\mu_1|}.$$

Plugging back into (B.7) and concludes the proof.

### B.4 Proof of Theorem 3.3

We start from the definition (16). From the basic inequality, we know

$$\frac{1}{2}\|\hat{\gamma}_2\|_2^2 - \langle \hat{\gamma}_2, \hat{\gamma}_1 \rangle + \lambda \|\hat{\gamma}_2\|_1 \leq \frac{1}{2}\|\gamma\|_2^2 - \langle \gamma, \hat{\gamma}_1 \rangle + \lambda \|\gamma\|_1.$$

Define $\Delta = \hat{\gamma}_2 - \gamma$ and $\omega = \text{supp}(\hat{\gamma}) = \text{supp}(\gamma^*)$, then we have

$$\frac{1}{2}\|\hat{\gamma}_2 - \gamma\|_2^2 \leq \langle \Delta, \hat{\gamma}_1 - \gamma \rangle + \lambda (\|\hat{\gamma}_1\|_1 - \|\hat{\gamma}_2\|_1)$$

$$\leq \|\Delta\|_1 \|\hat{\gamma}_1 - \gamma\|_\infty + \lambda \|\hat{\gamma}_1\|_1 - \|\Delta\|_1 \|\Delta\omega\|_1 - \lambda \|\Delta\Delta\|_1$$

From (B.5) we have $\|\hat{\gamma} - \hat{\gamma}_1\|_\infty \leq \lambda/2$ with probability at least $1 - \delta$. Therefore

$$\frac{1}{2}\|\Delta\|_2^2 \leq \frac{3\lambda}{2}\|\Delta\omega\|_1 - \frac{\lambda}{2}\|\Delta\Delta\|_1 \Rightarrow \|\Delta\|_2 \leq 3\sqrt{3}\lambda,$$

(B.8)

$$\|\Delta\|_1 \leq 4\|\Delta\omega\|_1 \leq 4\sqrt{3}\|\Delta\|_2 \leq 12s\lambda.$$

For bounding $\text{dist}(\hat{\gamma}_2, \gamma^*)$, we follow the same derivation as for (B.7).
B.5 Proof of Theorem 3.4

We apply the one-dimensional sin($\theta$) theorem in Lemma C.5. By equation (17), $U^* = 2\mu_2\gamma^*\gamma^T$. Then

$$\|\hat{U} - U^*\|_{\infty,\infty} \leq \|\hat{U} - \mathbb{E}_{\hat{\beta},f}[(y - \hat{f}(x^T\hat{\beta}))2H(x)]\|_{\infty,\infty} + \|\mathbb{E}_{\hat{\beta},f}[(y - \hat{f}(x^T\hat{\beta}))^2H(x)] - U^*\|_{\infty,\infty}. \tag{B.9}$$

For the second term, note that

$$\|\mathbb{E}_{\hat{\beta},f}[(y - \hat{f}(x^T\hat{\beta}))^2H(x)] - U^*\|_{\infty,\infty} = \|\mathbb{E}_{\hat{\beta},f}[(f(x^T\hat{\beta}^*) - \hat{f}(x^T\hat{\beta}))^2H(x)]\|_{\infty,\infty}. \tag{B.9}$$

By condition (11), we have

$$P\left(\|\mathbb{E}_{\hat{\beta},f}[(y - \hat{f}(x^T\hat{\beta}))^2H(x)] - U^*\|_{\infty,\infty} \geq \frac{\sqrt{M} \cdot \bar{e}_{f,\delta}(n,1)}{\delta}\right) \leq 2\delta. \tag{B.10}$$

For the first term, we proceed as in (B.4) and apply the Lemma C.2. For any $\delta > 0$, there exist constants $N_\delta, T_1$ such that if $n \geq N_\delta$ and $\tau = T_1(nM \log(2d^2/\delta),\hat{\beta})$, we have

$$P\left(\|\hat{U} - \mathbb{E}_{\hat{\beta},f}[(y - \hat{f}(x^T\hat{\beta}))^2H(x)]\|_{\infty,\infty} > \frac{8}{\delta} \sqrt{M \log(2d^2/\delta)}\right) < 4\delta. \tag{B.11}$$

Combining (B.9), (B.10), (B.11) and replacing $6\delta$ by $\delta$, we have for some constant $\Upsilon$

$$P\left(\|\hat{U} - U^*\|_{\infty,\infty} \leq \Upsilon\left(\sqrt{\frac{M \log(12d^2/\delta)}{n}} + \frac{\sqrt{M} \cdot \bar{e}_{f,\delta}(n,1)}{\delta}\right)\right) \geq 1 - \delta. \tag{B.12}$$

Since $\|\hat{U} - U^*\|_2 \leq d\|\hat{U} - U^*\|_{\infty,\infty}$, by setting $\tau = \Upsilon\left(nM \log(12d^2/\delta),\hat{\beta}\right)$, we have

$$P\left(\|\hat{U} - U^*\|_2 \leq \Upsilon\left(\sqrt{\frac{M \log(12d^2/\delta)}{n}} + \frac{\sqrt{M} \cdot \bar{e}_{f,\delta}(n,1)}{\delta}\right)\right) \geq 1 - \delta. \tag{B.12}$$

Without loss of generality, we assume $\mu_2 > 0$. If $\mu_2 < 0$, we can simply replace $U^*$ by $-U^*$ and $\hat{U}$ by $-\hat{U}$, but the estimator in (18) does not change, since we extract the eigenvector of $\hat{U}$ corresponding to the eigenvalue with the largest magnitude. To use Lemma C.5, we need the leading eigenvalue of $\hat{U}$ to be positive. Note that $\lambda_{\text{max}}(U^*) = 2\mu_2 > 0$ and for $n$ large enough Lemma C.6 gives us

$$\lambda_{\text{max}}(\hat{U}) \geq 2\mu_2 - \|\hat{U} - U^*\|_2 > 0.$$

From Lemma C.5, we finally have

$$\min_{\iota = \pm 1} \|\widehat{\gamma}_3 - \gamma^*\|_2 \leq \frac{\sqrt{2\Upsilon}}{\mu_2} \left(\sqrt{\frac{M \log(12d^2/\delta)}{n}} + \frac{\sqrt{M} \cdot \bar{e}_{f,\delta}(n,1)}{\delta}\right),$$

with probability at least $1 - \delta$, which completes the proof.
B.6 Proof of Theorem 3.5

Let \( V^* = \gamma^* \gamma^{*T} \) and \( U^* = 2\mu_2 V^* \). Since \( V^* \) is feasible for the optimization program (19), from the basic inequality we have

\[
\langle \hat{V}, \hat{U} \rangle - \lambda \| \hat{V} \|_{1,1} \geq \langle V^*, \hat{U} \rangle - \lambda \| V^* \|_{1,1}.
\]

This is equivalent to

\[
\langle \hat{V} - V^*, \hat{U} - U^* \rangle - \lambda \| \hat{V} \|_{1,1} + \lambda \| V^* \|_{1,1} \geq \langle U^*, V^* - \hat{V} \rangle.
\]

For the right hand side term, we can assume \( \mu_2 > 0 \) without loss of generality. Otherwise we replace \( U^* \) by \(-U^*\). We apply Lemma C.7 and get

\[
\langle U^*, V^* - \hat{V} \rangle \geq \mu_2 \| V^* - \hat{V} \|_F^2.
\]

Applying the elementwise Holder’s inequality we get

\[
\| \hat{V} - V^* \|_{1,1} \| \hat{U} - U^* \|_{\infty, \infty} - \lambda \| \hat{V} \|_{1,1} + \lambda \| V^* \|_{1,1} \geq \mu_2 \| V^* - \hat{V} \|_F^2.
\]  \( \text{(B.13)} \)

Define \( \Delta = \hat{V} - V^* \) and \( \omega = \text{supp}(\gamma^*) \times \text{supp}(\gamma^*). \) By (B.12), we have \( \| \hat{U} - U^* \|_{\infty, \infty} \leq \lambda \) with probability at least \( 1 - \delta \). The left hand side of (B.13) can upper bounded as

\[
\lambda(\| \Delta \|_{1,1} - \| \hat{V} \|_{1,1} + \| V^* \|_{1,1}) = \lambda(\| \Delta \omega \|_{1,1} - \| \hat{V} \omega \|_{1,1} + \| V^* \omega \|_{1,1}) \leq 2\lambda \| \Delta \omega \|_{1,1} \leq 2s\lambda \| \Delta \|_F.
\]

Plugging back into (B.13), we have

\[
\| \Delta \|_2 \leq \| \Delta \|_F \leq \frac{2s\lambda}{\mu_2}.
\]

By Lemma C.5 and C.6, we know when \( n \) large enough such that \( \hat{V} \) has positive leading eigenvalue, then

\[
\min_{i=\pm 1} \| \gamma_i - \gamma^* \|_2 \leq \frac{4\sqrt{2s\lambda}}{\mu_2},
\]

which completes the proof.

B.7 Proof of Theorem 3.6

We proceed as in the proof of Theorem 3.3. We set \( \lambda \geq 2\| \hat{w} - \langle \hat{\beta}, \hat{w} \rangle \cdot \hat{\beta} - \hat{\gamma} \|_\infty \). Let \( \hat{\gamma} = \hat{w} - \langle \hat{\beta}, \hat{w} \rangle \cdot \hat{\beta} \). By (21) we have

\[
\| \hat{\gamma} - \hat{\gamma} \|_\infty \leq \| \hat{w} - E[y^2 S(x)] \|_\infty + \| \langle \hat{\beta}, \hat{w} \rangle \cdot \hat{\beta} - 2\eta_1 \beta^* \|_\infty \\
\leq \| \hat{w} - E[y^2 S(x)] \|_\infty + 2\| \hat{\beta} - \beta^* \|_\infty + \| \langle \hat{\beta}, \hat{w} \rangle - 2\eta_1 \|.
\]  \( \text{(B.14)} \)

For the first term, we can apply Lemma C.2. By setting \( \tau = \left( \frac{nM}{\log(2d/\delta)} \right)^{\frac{1}{2}} \), we have

\[
P \left( \| \hat{w} - E[y^2 S(x)] \|_\infty \leq 7\sqrt{\frac{M \log(2d/\delta)}{n}} \right) \geq 1 - \delta.
\]  \( \text{(B.15)} \)
The second term has the same rate as in Theorem A.1. For the third term, we have
\[
|\langle \beta, \hat{w} \rangle - 2\eta_1| = |\langle \hat{\beta}, \hat{w} \rangle - \langle \beta^*, \mathbb{E}[y^2S(x)] \rangle| \\
\leq |\langle \hat{\beta}, \hat{w} \rangle - \langle \beta^*, \hat{w} \rangle| + |\langle \beta^*, \hat{w} \rangle - \langle \beta^*, \mathbb{E}[y^2S(x)] \rangle| \\
\leq \|\hat{\beta} - \beta^*\|_x \|\hat{w}\|_1 + \|\beta^*\|_1 \|\hat{w} - \mathbb{E}[y^2S(x)]\|_x \\
\leq \|\hat{\beta} - \beta^*\|_x \|\hat{w} - \mathbb{E}[y^2S(x)]\|_1 + \|\mathbb{E}[y^2S(x)]\|_1 \|\hat{\beta} - \beta^*\|_x + \|\beta^*\|_1 \|\hat{w} - \mathbb{E}[y^2S(x)]\|_x.
\]
(B.16)

As in the proof of Theorem 3.3, if \( \kappa = 14 \sqrt{\frac{M \log(2d/\delta)}{n}} \geq 2 \|\hat{w} - \mathbb{E}[y^2S(x)]\|_x \), then
\[
\|\hat{w} - \mathbb{E}[y^2S(x)]\|_1 \leq 24 \kappa, \\
\|\hat{w} - \mathbb{E}[y^2S(x)]\|_\infty \leq \|\hat{w} - \hat{w}\|_\infty + \|\hat{w} - \mathbb{E}[y^2S(x)]\|_\infty \leq \frac{3}{2} \kappa.
\]
The first inequality is due to cone condition (note that \( \|\mathbb{E}[y^2S(x)]\|_0 \leq 2s \)) and the second inequality is due to the fact that \( \|v - \phi_\kappa(v)\|_\infty \leq \kappa, \forall v \in \mathbb{R}^d \). Plugging back into (B.16) and noting that \( \|\mathbb{E}[y^2S(x)]\|_1 \leq 2|\eta_1| \cdot \|\beta^*\|_1 + |\mu_1| \cdot \|\gamma^*\|_1 \), we get
\[
|\langle \hat{\beta}, \hat{w} \rangle - 2\eta_1| \leq 24 \kappa |\beta - \beta^*\|_x + 2|\eta_1| \cdot \|\beta^*\|_1 + |\mu_1| \cdot \|\gamma^*\|_1 |\|\hat{\beta} - \beta^*\|_x + \frac{3}{2} \|\beta^*\|_1 \kappa.
\]
(B.17)
Combining (B.14), (B.15), (B.17), Theorem A.1 and noting that \( \|\hat{\beta} - \beta^*\|_x \approx \kappa \), we have
\[
\|\gamma - \tilde{\gamma}\|_\infty \leq \left( |\eta_1| + 1 \right) \cdot \|\beta^*\|_1 + |\mu_1| \cdot \|\gamma^*\|_1 \kappa.
\]
\( C_{|\eta_1|, |\mu_1|, \|\beta^*\|_1, \|\gamma^*\|_1} \)

The proof now follows as in Theorem 3.3

B.8 Proof of Theorem 3.7

From the proof of Theorem 3.5 (see (B.13)), we require \( \lambda \geq \|\hat{U} - U^*\|_{x, \infty} \). Then
\[
\min_{i=\pm 1} \|\xi_6 - \gamma^*\|_2 \leq \frac{4\sqrt{2s} \lambda}{\mu_2}.
\]

Note that by equation (17) we have
\[
\|\hat{U} - U^*\|_{x, \infty} \leq \|\hat{U} - \mathbb{E}[y^2H(x)]\|_{x, \infty} + \|\hat{\beta}^T \hat{U}\hat{\beta} - 2\eta_2 \beta^* \beta^T\|_{x, \infty}.
\]
By Lemma C.2, with \( \tau = \left( \frac{nM \log(2d/\delta)}{\log(2d/\delta)} \right)^{\frac{1}{2}} \), we have
\[
P(\|\hat{U} - \mathbb{E}[y^2H(x)]\|_{x, \infty} > \tau \sqrt{\frac{M \log(2d/\delta)}{n}}) < \delta.
\]
(B.18)
For the second term, we have
\[
\|\hat{\beta}^T \hat{U}\hat{\beta} - 2\eta_2 \beta^* \beta^T\|_{x, \infty} \leq \|\hat{\beta}^T \hat{U}\hat{\beta} - 2\eta_2\|_1 + 2|\eta_2| \cdot \|\hat{\beta}^T - \beta^* \beta^T\|_{x, \infty} \\
\leq \|\hat{\beta}^T \hat{U}\hat{\beta} - 2\eta_2\|_1 + 4|\eta_2| \cdot \|\hat{\beta} - \beta^*\|_{x, \infty}.
\]
Furthermore,
\[
|\hat{\beta}^T \hat{U} - 2\eta_2| = |\hat{\beta}^T \hat{U} - \beta^T \mathbb{E}[y^2 H(x)]\beta| = \left|\left\langle \hat{U}, \hat{\beta}^T \hat{\beta}\right\rangle - \langle \hat{U}, \hat{\beta}^T \beta\rangle\right|
\leqslant \left|\langle \hat{U}, \mathbb{E}[y^2 H(x)]\beta - \hat{\beta}\rangle\right| + \left|\langle \mathbb{E}[y^2 H(x)]\beta - \hat{\beta}, \hat{\beta}^T \beta\rangle\right|
\leqslant \left\| \hat{U} - \mathbb{E}[y^2 H(x)]\beta \right\|_{\infty,\infty} \left\| \hat{\beta}^T \beta \right\|_{1,1} + \left\| \mathbb{E}[y^2 H(x)]\beta - \hat{\beta}, \hat{\beta}^T \beta\right\|_{\infty,\infty}
\leqslant 2\left\| \hat{U} - \mathbb{E}[y^2 H(x)]\beta \right\|_{\infty,\infty} \left\| \hat{\beta}^T \beta - \beta^T \beta\right\|_{\infty,\infty} + 2\left\| \beta^T \beta\right\|_{1,1} \left\| \hat{U} - \mathbb{E}[y^2 H(x)]\beta \right\|_{\infty,\infty}.
\]

Combining (B.18) and Theorem A.1, we have
\[
P\left( |\hat{\beta}^T \hat{U} - 2\eta_2| \leqslant \Upsilon((\eta_2 + 1) \cdot \left\| \beta^T \beta \right\|_{1,1} + \left\| \mu_2 \cdot \gamma^* \right\|_{1,1}^2) \sqrt{\frac{M \log(2d^2/\delta)}{n}} \right) \geqslant 1 - 2\delta
\]
and
\[
P\left( \left\| \hat{U} - U^* \right\|_{\infty,\infty} \leqslant \Upsilon((\eta_2 + 1) \cdot \left\| \beta^T \beta \right\|_{1,1} + \left\| \mu_2 \cdot \gamma^* \right\|_{1,1}^2) \sqrt{\frac{M \log(2d^2/\delta)}{n}} \right) \geqslant 1 - 3\delta.
\]

This concludes the proof.

### B.9 Proof of Theorem 4.1

From (26), \( \hat{G}_1 \in \mathbb{R}^{d \times v} \) is a matrix whose columns are eigenvectors of \( \hat{U} \) corresponding to the \( v \) largest eigenvalues. Based on (25), \( U^* = 2G^* \Lambda G^{*T} \). Suppose \( 2\Lambda = P \Pi P^T \) is the eigenvalue decomposition, so \( U^* = G^* \Pi P^T G^{*T} \). From (B.12) in the proof of Theorem 3.4, we have that for any \( \delta > 0 \), there exist \( N_\delta, \Upsilon \) such that \( \forall n \geqslant N_\delta \) with probability at least \( 1 - \delta \),
\[
\left\| \hat{U} - U^* \right\|_2 \leqslant \Upsilon(d \sqrt{\frac{M \log(12d^2/\delta)}{n}} + \frac{\sqrt{M} \cdot \bar{c}_f \delta(n, 1)}{\delta}),
\]
\[
\left\| \hat{U} - U^* \right\|_F \leqslant \Upsilon(d \sqrt{\frac{Md \log(12d^2/\delta)}{n}} + \frac{d \sqrt{Md} \cdot \bar{c}_f \delta(n, 1)}{\delta}).
\]

Let \( \lambda_v(\hat{U}) \) be the \( v \)-th largest eigenvalue of \( \hat{U} \). Based on Lemma C.6, when \( n \) large enough,
\[
\lambda_v(\hat{U}) \geqslant 2\mu_3 - \left\| \hat{U} - U^* \right\|_2 > \frac{3\mu_3}{2},
\]
\[
\lambda_{v+1}(\hat{U}) \leqslant \left\| \hat{U} - U^* \right\|_2 < \frac{\mu_3}{2},
\]
with probability at least \( 1 - \delta \). Therefore the problem (26) has a unique solution up to orthonormal transformation. Let \( F = G^* P \) and note that \( F^T F = I_v \). Then
\[
\left\langle \hat{U}, FF^T \right\rangle \leqslant \left\langle \hat{U}, \hat{G}_1 \hat{G}_1^T \right\rangle.
\]
By Lemma C.4 and C.8, we have
\[
\inf_{Q \in \mathbb{Q}^{u \times u}} \| \hat{G}_1 - G^* Q \|_F = \inf_{Q \in \mathbb{Q}^{u \times v}} \| \hat{G}_1 - G^* PQ \|_F \leq \sqrt{2} \| \sin(\angle(\hat{G}_1, F)) \|_F
\]
\[
\leq \frac{1}{\mu_3}\|\hat{U} - U^*\|_F^{(B.19)} \leq \frac{\gamma}{\mu_3} \left( d \sqrt{\frac{d \log(12d^2 / \delta)}{n}} + d \sqrt{M d \cdot \tilde{e}_{f, \delta}(n, 1)} \right),
\]
which concludes the proof.

B.10 Proof of Theorem 4.2

Define \( V^* = G^* G^{*T} \) to be the projection matrix. Since \( V^* \) is feasible for (19), we have
\[
\langle \hat{V}, \hat{U} \rangle - \lambda \| \hat{V} \|_{1,1} \geq \langle V^*, \hat{U} \rangle - \lambda \| V^* \|_{1,1}.
\]
This implies
\[
\langle \hat{V} - V^*, \hat{U} - U^* \rangle - \lambda \| \hat{V} \|_{1,1} + \lambda \| V^* \|_{1,1} \geq \langle U^*, V^* - \hat{V} \rangle.
\]
For the right hand side term, we apply Lemma C.7 and get
\[
\langle U^*, V^* - \hat{V} \rangle \geq \mu_3 \| V^* - \hat{V} \|_F^2.
\]
Same as (B.13), in the proof of Theorem 3.5, as long as
\[
\lambda \geq \gamma \left( \sqrt{\frac{M d \log(12d^2 / \delta)}{n}} + \sqrt{M d \cdot \tilde{e}_{f, \delta}(n, 1)} \right)^{(B.12)} \geq \| \hat{U} - U^* \|_{\infty, \infty},
\]
we have
\[
\| \hat{V} - V^* \|_F \leq \frac{2s \sqrt{\tilde{v} \lambda}}{\mu_3}.
\]
Using Lemma C.6, we see that \( \hat{G}_2 \) is unique up to orthonormal transformation and
\[
\langle \hat{V}, G^* G^{*T} \rangle \leq \langle \hat{V}, \hat{G}_2 \hat{G}_2^{T} \rangle.
\]
From Lemma C.4 and C.8, we have
\[
\inf_{Q \in \mathbb{Q}^{u \times v}} \| \hat{G}_2 - G^* Q \|_F \leq \sqrt{2} \| \sin(\angle(\hat{G}_2, G^*)) \|_F \leq 2 \| \hat{V} - V^* \|_F \leq \frac{4s \sqrt{\tilde{v} \lambda}}{\mu_3}.
\]

B.11 Proof of Theorem 4.3

As in the proof of Theorem 4.2, if \( \| \hat{U} - U^* \|_{\infty, \infty} \leq \lambda \), we have
\[
\| \hat{V} - G^* G^{*T} \|_F \leq \frac{2s \sqrt{\tilde{v} \lambda}}{\mu_3}.
\]
For the estimator $\hat{G}_3$, we know the columns of $\hat{G}_3$ are the orthonormal basis of the subspace spanned by the eigenvectors of $\bar{V}$ corresponding to the $v$ largest eigenvalues. Therefore

$$\inf_{Q \in \mathbb{Q}^{r \times u}} \|\hat{G}_3 - G^*Q\|_F \leq \sqrt{2}\sin(\angle(\hat{G}_3, G^*))\|_F \leq 2\|\bar{V} - G^*G^{*T}\|_F \leq \frac{4\sqrt{v}\lambda}{\mu_3}.$$  

From the proof of Theorem 3.7, we can set

$$\lambda \geq \mathcal{Y}((|\eta_2| + 1) \cdot \|\beta^*\|_1^2 + |\mu_2| \cdot \|\gamma^*\|_1^2)\sqrt{M\log(6d^2/\delta)}.$$  

This concludes the proof.

C Auxiliary Lemmas

We collect lemmas used in Section B. Some of the proofs are given in Section D.

**Lemma C.1** (Boundedness of $f(x^T \hat{\beta})$). Suppose Assumption A.2 (a,b) hold and $\hat{\beta}$ is a consistent estimator of $\beta^*$. If $\mathbb{E}[|f(x^T \beta^*)|^6] \leq M$, then

$$\mathbb{E}_{\hat{\beta}}[|f(x^T \hat{\beta})|^6] \leq 64M$$  

for any $n \geq N_M$, where $N_M$ depends on $M$ only.

**Lemma C.2.** Suppose $\{x_i, y_i, z_i, w_i\}_{i=1}^n$ is a sequence of $n$ i.i.d. samples distributed as $x_i \sim x$, $y_i \sim y$, $z_i \sim z$, and $w_i \sim w$. Suppose there exists a constant $M$ such that

$$\mathbb{E}[|x|^{2(p+q+r+s)}] \vee \mathbb{E}[|y|^{2(p+q+r+s)}] \vee \mathbb{E}[|z|^{2(p+q+r+s)}] \vee \mathbb{E}[|w|^{2(p+q+r+s)}] \leq M$$  

for some integers $p, q, r, s$ with $p^2 + q^2 + r^2 + s^2 \geq 1$. Then $\forall \delta > 0$ and $\tau = \left(\frac{nM}{\log(2/\delta)}\right)^{1/(p+q+r+s)}$, we have

$$\left|\frac{1}{n} \sum_{i=1}^n \tilde{x}_i^p \tilde{y}_i^q \tilde{z}_i^r \tilde{w}_i^s - \mathbb{E}[x^p y^q z^r w^s]\right| \leq 7\sqrt{\frac{M\log(2/\delta)}{n}}$$  

with probability at least $1 - \delta$.

**Definition C.3** (Principal angles between two spaces). Let $A, B \in \mathbb{R}^{d \times r}$ such that $A^T A = B^T B = I_r$ and $A^T B = U\Sigma V^T$ is the singular value decomposition. Let $\angle(A, B) \in \mathbb{R}^{r \times r}$ be the diagonal matrix with $(\angle(A, B))_{ii} = \arccos(\Sigma_{ii})$. We call $\angle(A, B)$ the $r$ principal angles between two subspaces $\text{Im}(A)$ and $\text{Im}(B)$.

**Lemma C.4.** Suppose $A, B \in \mathbb{R}^{d \times r}$ have orthonormal columns. Then

$$\inf_{Q \in \mathbb{Q}^{r \times r}} \|A - BQ\|_F^2 \leq 2\|\angle(A, B)\|_F^2 = \|AA^T - BB^T\|_F^2,$$

where the principal angles $\angle(A, B)$ are defined in Definition C.3.
Lemma C.5 (One-dimensional Davis-Kahan sin(θ) theorem, Theorem 5.9 in Vershynin (2012)). Suppose $A \in \mathbb{R}^{d \times d}$ is a positive semidefinite matrix. Let $(\lambda_1, \gamma_1), \ldots, (\lambda_d, \gamma_d)$ denote the pairs of eigenvalues-eigenvectors of $A$ ordered such that $\lambda_1 \geq \ldots \geq \lambda_d$. For any $d \times d$ matrix $B$ such that the leading eigenvalue is positive, let $\mu_1 \in \arg \max |\mu|_2 \leq 1 \mu^T B \mu$. Then

$$\min_{\delta = \pm 1} \| \delta \mu_1 - \gamma_1 \|_2 \leq \sqrt{2} \sin(\angle(\mu_1, \gamma_1)) \leq \frac{2\sqrt{2}}{\lambda_1 - \lambda_2} \| A - B \|_2,$$

where $\angle(\mu_1, \gamma_1) = \arccos(|\mu_1^T \gamma_1|)$.

Lemma C.6 (Weyl’s inequality, Weyl (1912)). Suppose we have $A = B + C$ for symmetric matrices $A, B, C \in \mathbb{R}^{d \times d}$, and their eigenvalues are denoted as $a_i, b_i, c_i$ in descending order. Then we have

$$b_i \leq c_n \leq a_i \leq b_i + c_1.$$

Lemma C.7 (Curvature, Lemma 3.1 in Vu et al. (2013)). Let $A$ be a symmetric matrix and $E$ be the projection matrix that projects onto the subspace spanned by the eigenvectors of $A$ corresponding to its $d$ largest eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$. If $\delta_A = \lambda_d - \lambda_{d+1} > 0$, then

$$\frac{\delta_A}{2} \| E - F \|_F^2 \leq \langle A, E - F \rangle$$

for all $F$ satisfying $0 \leq F \leq I$ and $\text{Trace}(F) = d$.

Lemma C.8 (Variational sin(θ) theorem, Corollary 4.1 in Vu and Lei (2013)). Let $A \in \mathbb{R}^{p \times p}$ be a positive semidefinite matrix and suppose its eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$ satisfy $\delta_A = \lambda_d - \lambda_{d+1} > 0$ for some $d < p$. Let $Q_1 \in \mathbb{R}^{p \times d}$ be the matrix whose columns are the eigenvectors of $A$ corresponding to the $d$ largest eigenvalues. We denote $E = Q_1 Q_1^T$. Furthermore, suppose matrix $Q_2 \in \mathbb{R}^{p \times d}$ has orthonormal columns and let $F = Q_2 Q_2^T$. Then for any symmetric matrix $B$, if it satisfies

$$\langle B, E \rangle \leq \langle B, F \rangle,$$

we have

$$\| \sin(\angle(Q_1, Q_2)) \|_F \leq \frac{\sqrt{2}}{\delta_A} \| A - B \|_F.$$

Here $\sin(\angle(Q_1, Q_2))$ is defined in Definition C.3.

D Proofs of Other Theorems and Lemmas

This section collects proofs for results in the appendix and Section C.

D.1 Proof of Theorem A.3

The proof for classical nonparametric regression has been established in Theorem 1 in Fan (1993). For completeness, we present a proof for index model (A.1), which additional care. Our starting point is

$$\mathbb{E}_{\tilde{\beta} x}[|\tilde{f}(x^T \tilde{\beta}) - f(x^T \beta^*)|^4] \leq 8 \mathbb{E}_{\tilde{\beta} x}[|\tilde{f}(x^T \tilde{\beta}) - f(x^T \beta)|^4] + 8 |f(x^T \beta) - f(x^T \beta^*)|^4. \quad (D.1)$$
For the second term, by Assumption A.2 (a) we have
\[ |f(x^T \hat{\beta}) - f(x^T \beta^*)|^4 \leq L_1^4 |x^T \beta^* - x^T \hat{\beta}|^4. \]  
(D.2)

Next, we deal with the first term. We first introduce some additional notations. Let \( t = x^T \hat{\beta}, \) \( t_i = x_i^T \hat{\beta}, \forall i \in [n], \) \( Y = (y_1; \ldots; y_n), \) \( Y_0 = (f(x_1^T \beta^*); \ldots; f(x_n^T \beta^*)), \) \( Y_1 = (f(t_1); \ldots; f(t_n)), \) \( r = Y - Y_0 = (\tilde{g}(x_1) \epsilon_1; \ldots; \tilde{g}(x_n) \epsilon_n), \) and
\[
X_t = \begin{pmatrix}
1 & t_1 - t \\
1 & t_2 - t \\
& \ddots \\
1 & t_n - t
\end{pmatrix}, \quad W_t = \begin{pmatrix}
K_h(t_1 - t) & \cdots & K_h(t_n - t)
\end{pmatrix},
\]
for \( K_h(\cdot) = K(\cdot/h)/h \) where \( K(\cdot) \) is Gaussian kernel. For \( l = 0, 1, 2, \ldots, \) we define
\[
S_{nl} = \sum_{j=1}^n (t_j - t)^l K_h(t_j - t), \quad \Xi_{nl} = \sum_{j=1}^n (t_j - t)^l K_h^2(t_j - t) \sqrt{r^2_\beta(t_j)},
\]
and also use \( a_l, b_l \) to denote integral without absolute value. Note that taking expectation conditional on \( \hat{\beta}, x \) means \( t \) is fixed and randomness comes from \( \{x_i, \epsilon_i\}_{i \in [n]}, \) which are independent from \( \hat{\beta}, x. \)

We will drop the subscript of matrix \( X \) and \( W \) and let \( E_t[\cdot] = \mathbb{E}_{\hat{\beta}, x}[\cdot]. \) We define the 2-by-2 matrix
\[
H = \begin{pmatrix}
S_{n2} & -S_{n1} \\
-S_{n1} & S_{n0}
\end{pmatrix}, \quad S_n = S_{n2}S_{n0} - S_{n1}^2 + \frac{1}{n^2 \pi^2},
\]
and vector \( l = W X H e_1/S_n \in \mathbb{R}^n, \) where \( e_1 \in \mathbb{R}^2 \) is the first canonical basis of \( \mathbb{R}^2. \) With this notation, the estimator proposed in Fan (1993) can be written as \( \hat{f}(t) = l^T Y. \) We have the following decomposition
\[
\hat{f}(t) - f(t) = e_1^T H X^T W Y/S_n - f(t)
\]
\[
= e_1^T H X^T W (Y - Y_0)/S_n + e_1^T H X^T W (Y_0 - Y_1)/S_n + e_1^T H X^T W Y_1/S_n - f(t)
\]
\[
:= I_1 + I_2 + I_3. \quad \text{(D.3)}
\]

We proceed to bound \( E_t[I_1^4], E_t[I_2^4], E_t[I_3^4]. \) Since \( I_1 = l^T r, \) we have
\[
E_t[I_1^4] = E_t[\sum_{i \in [n]} l_i r_i^4] = E_t[\sum_{i,j,s,r \in [n]} l_i l_j l_s l_r \tilde{g}(x_i) \tilde{g}(x_j) \tilde{g}(x_s) \tilde{g}(x_r) \epsilon_i \epsilon_j \epsilon_s \epsilon_r]
\]
\[
= E[\epsilon^4] \cdot \sum_{i \in [n]} E_t[\tilde{g}(x_i)^4] + 6(E[\epsilon^2])^2 \sum_{i \neq j \in [n]} E_t[l_i^2 l_j^2 \tilde{g}(x_i)^2 \tilde{g}(x_j)^2]
\]
\[
\leq 6E[\epsilon^4] \left( \sum_{i \in [n]} E_t[l_i^4 r_\beta(t_i)] + \sum_{i \neq j \in [n]} E_t[l_i^2 l_j^2 \sqrt{r_\beta(t_i) r_\beta(t_j)}] \right)
\]
\[
= 6E[\epsilon^4] E_t[(l^T D_1 l)^2], \quad \text{(D.4)}
\]
where \( D_1 = \text{diag}(\sqrt{r_\beta(t_1)}, \ldots, \sqrt{r_\beta(t_n)}). \) For the term \( l^T D_1 l, \) we have
\[
l^T D_1 l = \frac{1}{S_n^2} (S_{n2}^2 \Xi_{n0} - 2S_{n1} S_{n2} \Xi_{n1} + S_{n1}^2 \Xi_{n2}). \quad \text{(D.5)}
\]
For any random variable $Z_n$ and integer $r$, we write $Z_n = O_r(a_n)$, if $E[|Z_n|^r] = O(a_n^r)$, and define $o_r(a_n)$ similarly. Note that $Z_n = E[Z_n] + O_r((E[|Z_n - E[Z_n]|^r]^{1/r})$ and, by Cauchy-Schwarz inequality, we have $O_r(a_n)O_r(b_n) = O_{r/2}(a_n b_n)$. We show how to control $S_{nl}$ in (D.5), while the other terms are bounded in a similar way. We have

$$E_t\left[\frac{1}{nh^t}S_{nl}\right] = \frac{1}{n} \sum_{j=1}^{n} E_t\left[\left(\frac{t_j - t}{h}\right)^l K_h(t_j - t)\right] = \int x^l K(x)q_\beta(t + hx) \, dx = a_l \cdot q_\beta(t) + O(h^\alpha).$$

For any even integer $r \geq 2$,

$$E_t\left[\left|\frac{1}{nh^t}S_{nl} - E_t\left[\frac{1}{nh^t}S_{nl}\right]\right|^r\right] = E_t\left[\left|\frac{1}{n} \sum_{j=1}^{n} \frac{(t_j - t)^l}{h} K_h(t_j - t) - E_t\left[\frac{(t_j - t)^l}{h} K_h(t_j - t)\right]\right|^r\right].$$

For any positive integer $\tilde{r}$, we know

$$E_t[|\xi_j|^r] \leq 2^{\tilde{r}} E_t[\left|\frac{t_j - t}{h}\right|^\tilde{r} K_h(t_j - t)] \leq C_{\tilde{r}, l} 2^{\tilde{r}} \frac{h^{r-1}}{h^{r-1}},$$

where $C_{\tilde{r}, l}$ is a constant depending on $\tilde{r}, l$ and upper boundedness of $q_\beta$. Expanding the summation term and combining with above inequality, we have

$$E_t\left[\left|\frac{1}{nh^t}S_{nl} - E_t\left[\frac{1}{nh^t}S_{nl}\right]\right|^r\right] \leq \frac{1}{n^r} E_t\left[\left(\sum_{j=1}^{n} \xi_j\right)^r\right]$$

$$= \frac{1}{n^r} \sum_{k=1}^{r/2} \sum_{c_1 + \ldots + c_k = r, c_i \geq 2, \forall i} E_t\left[\left|\xi_{j1}\right|^{c_1} \left|\xi_{j2}\right|^{c_2} \ldots \left|\xi_{jk}\right|^{c_k}\right]$$

$$\leq \frac{1}{n^r} \sum_{k=1}^{r/2} \binom{n}{k} \binom{r - k - 1}{k - 1} \frac{2^r}{h^{r-k}}$$

$$\leq \max_{x \in \{2, 3, \ldots, r/2\}} \binom{r - x - 1}{x - 1} \frac{2^r}{(nh)^{r/2}}.$$
By (D.5), (D.7), (D.8), there exists constant $\Upsilon_1$ such that
\[
(I^T D_1 l)^2 = \Upsilon_1 \left( \frac{b_0^2 r_{\beta}(t)}{n^2 h^2 q_{\beta}^2(t)} + \frac{o_1(1)}{n^2 h^2} \right) \left( 1 + O_r(h^\alpha + \frac{1}{\sqrt{nh}}) \right).
\]

Combine with (D.4) and let $n$ sufficient large to ignore the smaller order term, we have
\[
E_t[I_1^4] \lesssim E_t[(I^T D_1 l)^2] \lesssim \frac{r_{\beta}(t)}{n^2 h^2 q_{\beta}^2(t)}.
\]

Here we use the condition $h \to 0$ and $nh \to \infty$. For the term $I_2$, by Taylor expansion
\[
Y_0 - Y_1 = (f'(t_1)x_1^T(\beta^* - \hat{\beta}); \ldots; f'(t_n)x_n^T(\beta^* - \hat{\beta}))
\]
\[
+ \left( \frac{f''(\xi)}{2}(x_1^T(\beta^* - \hat{\beta}))^2; \ldots; f''(\xi)(x_n^T(\beta^* - \hat{\beta}))^2 \right)
\]
\[
:= b_1 + b_2,
\]

where random variable $\xi_j \in (x_j^T \beta^*, x_j^T \hat{\beta})$. Therefore
\[
E_t[I_2^2] = E_t[(I^T b_1 + I^T b_2)^2] \leq 8E_t[(I^T b_1 b_1^T l)^2] + 8E_t[(I^T b_2 b_2^T l)^2].
\]

We bound the first term, while the second term can be easily shown to have smaller order error using the boundedness of $f''$. We have
\[
(I^T b_1)^4 = \left( \sum_{i \in [n]} l_i f'(t_i)x_i^T(\beta^* - \hat{\beta}) \right)^4 \leq \left( \sum_{i \in [n]} l_i^2 (f'(t_i))^2 \right)^2 \left( \sum_{i \in [n]} (x_i^T(\beta^* - \hat{\beta}))^2 \right)^2
\]
\[
:= n^2 (I^T D_2 l)^2 \cdot \left( \frac{1}{n} \sum_{i \in [n]} (x_i^T(\beta^* - \hat{\beta}))^2 \right)^2,
\]

where $D_2 = \text{diag}([|f'(t_1)|^2, \ldots, |f'(t_n)|^2])$. By Assumption A.2 (b), we know
\[
\frac{1}{n} \sum_{i \in [n]} (x_i^T(\beta^* - \hat{\beta}))^2 = O_3(\|\hat{\beta} - \beta^*\|_2^2).
\]

Moreover, we can use the same step of bounding $(I^T D_1 l)^2$ to get
\[
(I^T b_1)^4 = \Upsilon_2 \left( \frac{b_0^2 (f'(t))^4 O_{1.5}(\|\hat{\beta} - \beta^*\|_2^4)}{h^2 q_{\beta}^2(t)} + \frac{o_1(1)}{h^2} \right) \left( 1 + O_r(h^\alpha + \frac{1}{\sqrt{nh}}) \right).
\]

Using the convergence rate of $\hat{\beta}$, which implies $E_t[o_1(\|\hat{\beta} - \beta^*\|_2^4)/h^2] \to 0$, and ignoring the smaller order terms, we have
\[
E_t[I_2^2] \lesssim E_t[(I^T b_1)^4] \lesssim \frac{\|\hat{\beta} - \beta^*\|_2^4 f'(t))^4}{h^2 q_{\beta}^2(t)}.
\]
Lastly, we deal with $\mathcal{I}_3$ term. A simple observation is that

$$Y_1 = f(t)Xe_1 + f'(t)Xe_2 + u,$$

where $u \in \mathbb{R}^n$ with $u_j = f(t_j) - f(t) - f'(t)(t_j - t) = \frac{f''(\xi_j)}{2}(t_j - t)^2$. Based on this, we have

$$\mathcal{I}_3 = e_1^T HX^TY_1/S_n - f(t) = -\frac{f(t)}{n^2 \hat{h}^2 S_n} + e_1^T HX^TWu/S_n$$

$$= -\frac{f(t)}{n^2 \hat{h}^2 S_n} + \frac{1}{2S_n} \sum_{j \in [n]} f''(\xi_j)(t_j - t)^2 K_h(t_j - t) - S_{n1} \sum_{j \in [n]} f''(\xi_j)(t_j - t)^3 K_h(t_j - t))$$

$$\leq \frac{f(t)}{n^2 \hat{h}^2 S_n} + \frac{L_1}{2S_n} (S_{n2} + S_{n1} \sum_{j \in [n]} |t_j - t|^3 K_h(t_j - t))$$

We can obtain that

$$\sum_{j \in [n]} |t_j - t|^3 K_h(t_j - t) = n\hat{h} \beta q_{\hat{h}}(t)(1 + O_r(h^\alpha + \frac{1}{\sqrt{nh}})).$$

Combine with (D.6) and (D.8), we have

$$E_t[\mathcal{I}_3^2] \leq h^8 + \frac{|f(t)|^4}{n^{16} h^{16} q_{\beta}^8(t)}.$$

(D.11)

Based on results in (D.1), (D.2), (D.3), (D.9), (D.10), and (D.11), we know there exists a constant $\Upsilon$ such that

$$E_t[|\hat{f}(t) - f(t)|^4] \leq \Upsilon \left(h^8 + \frac{r_{\beta}(t)}{n^2 \hat{h}^2 q_{\beta}^2(t)} + \frac{\|\beta - \beta^*\|_2^4 \cdot |f'(t)|^4}{h^2 q_{\beta}^2(t)} + |x^T \beta^* - x^T \hat{\beta}|^4 + \frac{|f(t)|^4}{n^{16} h^{16} q_{\beta}^8(t)}\right)$$

for a sufficiently large $n$. This concludes the first part of the proof and also gives an explicit formula for $\tilde{e}_f(\hat{\beta}^T x, n, 1)$.

For the second part of proof, we will use the result in Corollary 2.7. According to Assumption A.2 (e), we directly have that for another constant $\Upsilon'$

$$\tilde{e}_f(\hat{\beta}, n, 1) = E_{\beta}[e(\hat{\beta}^T x, n, 1)] \leq \Upsilon' \left(h^8 + \frac{1}{n^2 \hat{h}^2} + \frac{\|\beta - \beta^*\|_2^2}{h^2} \right).$$

Plugging in the rate in Theorem A.1, we get

$$P \left(\sqrt{\tilde{e}_f(\hat{\beta}, n, 1)} \geq \left(h^4 + \frac{s \log(d/\delta)}{nh}\right)^{1/4}\right) \leq \delta, \quad \forall 0 < \delta < 1.$$

Therefore, setting the bandwidth $h$ as $h \asymp n^{-1/5}$ we get $\tilde{e}_f(\hat{\beta}, n, 1) \approx n^{-4/5}$. Here we assume $s \log(d/\delta)$ is constant and negligible, otherwise we can choose the optimal bandwidth to be $h \asymp (s \log(d/\delta)/n)^{1/5}$ and get

$$\tilde{e}_f(\hat{\beta}, n, 1) = \left(\frac{s \log(d/\delta)}{n}\right)^{4/5}.$$
D.2 Proof of Lemma C.1
For any fixed $\hat{\beta}$, we have

$$E_{\hat{\beta}}[|f(x^T\hat{\beta}) - f(x^T\beta^*)|^6] \leq L_4^6\|\hat{\beta} - \beta^*\|_2^6$$

and

$$|f(x^T\hat{\beta})|^6 \leq 32|f(x^T\hat{\beta}) - f(x^T\beta^*)|^6 + 32|f(x^T\beta^*)|^6.$$  

Use the consistency of $\hat{\beta}$ and note that $E_{\hat{\beta}}[|f(x^T\beta^*)|^6] = E[|f(x^T\beta^*)|^6] \leq M$ to obtain

$$E_{\hat{\beta}}[|f(x^T\hat{\beta})|^6] \leq 32L_4^6\|\hat{\beta} - \beta^*\|_2^6 + 32M \leq 64M,$$

for sufficient large $n$.

D.3 Proof of Lemma C.2
We apply the Bernstein’s inequality in Corollary 2.11 in Boucheron et al. (2013). We have

$$\left|\frac{1}{n} \sum_{i=1}^{n} \tilde{x}_i^p \tilde{y}_i^q z_i^r \tilde{w}_i^s - E[x^p y^q z^r w^s]\right|$$

$$\leq \frac{1}{n} \sum_{i=1}^{n} \tilde{x}_i^p \tilde{y}_i^q z_i^r \tilde{w}_i^s - E[\tilde{x}_i^p \tilde{y}_i^q z_i^r \tilde{w}_i^s] + |E[\tilde{x}_i^p \tilde{y}_i^q z_i^r \tilde{w}_i^s] - E[x^p y^q z^r w^s]|$$

$$:= |I_1| + |I_2|.$$ (D.12)

For the $I_2$ term, we have

$$|I_2| \leq E[|x^p y^q z^r w^s|1_{|x|>\tau} \text{ or } |y|>\tau \text{ or } |z|>\tau \text{ or } |w|>\tau]$$

$$\leq \sqrt{E[x^{2p}y^{2q}z^{2r}w^{2s}]} \cdot \sqrt{P(|x|>\tau) + P(|y|>\tau) + P(|z|>\tau) + P(|w|>\tau)}$$

$$\leq \sqrt{E[x^{2p}y^{2q}z^{2r}w^{2s}]} \cdot \sqrt{\frac{P(\tau+x^{p+q+r+s})}{\tau^{p+q+r+s}} \cdot \frac{P(\tau+y^{p+q+r+s})}{\tau^{p+q+r+s}} \cdot \frac{P(\tau+z^{p+q+r+s})}{\tau^{p+q+r+s}} \cdot \frac{P(\tau+w^{p+q+r+s})}{\tau^{p+q+r+s}} \cdot \sqrt{4M}}$$

$$\leq \frac{2M}{\tau^{p+q+r+s}}.$$ (D.13)

The third inequality is due to the generalized Hölder’s inequality. For the $I_1$ term, we have

$$|\tilde{x}_i^p \tilde{y}_i^q z_i^r \tilde{w}_i^s| \leq \tau^{p+q+r+s},$$

$$V_n = \sum_{i=1}^{n} \text{Var}(\tilde{x}_i^p \tilde{y}_i^q z_i^r \tilde{w}_i^s) \leq nE[\tilde{x}_i^{2p} \tilde{y}_i^{2q} \tilde{z}_i^{2r} \tilde{w}_i^{2s}] \leq nM.$$  

By Bernstein’s inequality we have $\forall t > 0$,

$$P(|I_1| > t) \leq 2 \exp\left(-\frac{nt^2}{2M + 4t\tau^{p+q+r+s}}\right).$$ (D.14)
For any $\delta > 0$, we let $t = \frac{1}{\log(2/\delta)} = \sqrt{\log(2/\delta)}$. Plug in (D.14) and combine with (D.12) and (D.13), we can get

$$\frac{1}{n} \sum_{i=1}^{n} \tilde{x}_i^\top \tilde{y}_i^\top \tilde{z}_i^\top \tilde{w}_i^\top = \mathbb{E}[x^\top y^\top z^\top w^\top] \leq 7 \sqrt{\frac{M \log(2/\delta)}{n}}$$

with probability at least $1 - \delta$. This concludes our proof.

### D.4 Proof of Lemma C.4

Suppose $A^T B = U \cos(\angle(A, B)) V^T$. Then

$$\inf_{Q \in \mathbb{R}^{r \times r}} \|A - BQ\|_F^2 = \inf_{Q \in \mathbb{R}^{r \times r}} (\|A\|_F^2 + \|B\|_F^2 - 2\text{Trace}(A^T B Q))$$

$$= 2(r - \sup_{Q \in \mathbb{R}^{r \times r}} \text{Trace}(A^T B Q))$$

$$= 2(r - \sup_{Q \in \mathbb{R}^{r \times r}} \text{Trace}(U \cos(\angle(A, B)) V^T Q))$$

$$= 2(r - \sup_{Q \in \mathbb{R}^{r \times r}} \text{Trace}(\cos(\angle(A, B)) V^T Q U))$$

Minimum is attained for $Q = VU^T$, so

$$\inf_{Q \in \mathbb{R}^{r \times r}} \|A - BQ\|_F^2 = 2(r - \sum_{i=1}^{r} \cos(\angle(A, B)_i))$$

$$\leq 2(r - \sum_{i=1}^{r} \cos^2(\angle(A, B)_i))$$

$$= 2 \sum_{i=1}^{r} \sin^2(\angle(A, B)_i) = 2\|\sin(\angle(A, B))\|_F^2.$$

Furthermore

$$\|\sin(\angle(A, B))\|_F^2 = r - \|\cos(\angle(A, B))\|_F^2$$

$$= \frac{1}{2} (\|AA^T\|_F^2 + \|BB^T\|_F^2 - 2\|A^T B\|_F^2)$$

$$= \frac{1}{2} (\|AA^T\|_F^2 + \|BB^T\|_F^2 - 2\langle AA^T, BB^T \rangle)$$

$$= \frac{1}{2} \|AA^T - BB^T\|_F^2.$$

Combining the two equations together, we finish the proof.

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