Prediction Sets for High-Dimensional Mixture of Experts Models

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Abstract

Large datasets make it possible to build predictive models that can capture heterogenous relationships between the response variable and features. The mixture of high-dimensional linear experts model posits that observations come from a mixture of high-dimensional linear regression models, where the mixture weights are themselves feature-dependent. In this paper, we show how to construct valid prediction sets for an $\ell_1$-penalized mixture of experts model in the high-dimensional setting. We make use of a debiasing procedure to account for the bias induced by the penalization and propose a novel strategy for combining intervals to form a prediction set with coverage guarantees in the mixture setting. Synthetic examples and an application to the prediction of critical temperatures of superconducting materials show our method to have reliable practical performance.

1 Introduction

In traditional statistics, we imagine a universal relationship between variables that holds across an entire population; observations not following this relationship are dismissed as outliers. However, we know that reality is more complex, with numerous subpopulations likely exhibiting distinct behaviors. As datasets grow in size, we become better able to detect and properly model this heterogeneity. The mixture of regressions model (Quandt & Ramsey 1978) is an important tool for extending linear regression to this heterogeneity-aware setting. For a random response $y \in \mathbb{R}$ and a random vector of predictors $x \in \mathbb{R}^p$, we imagine a latent subgroup membership $z \in \{1, \ldots, K\}$ that determines the conditional distribution of $y$ given $x$:

$$y|x, z = k \sim N(x^T \beta_k, \sigma_k^2).$$

(1)

Making predictions with this model requires estimating for each subgroup a coefficient vector $\beta_k$, an error variance $\sigma_k^2$, and a group membership probability $\pi_k = \mathbb{P}(z = k)$. The mixture of experts model (MoE, Jordan & Jacobs 1994) is even more flexible, allowing these group membership probabilities to depend on the predictors as well:

$$z|x \sim \text{Multinomial}[\pi(x)] \quad \text{with} \quad \pi_k(x) = \frac{\exp(x^T \alpha_k)}{\sum_{\ell=1}^K \exp(x^T \alpha_\ell)}.$$  

(2)

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This model is expressive enough to capture subpopulations that change in prevalence depending on the conditions. For example, Hyun et al. (2020) develop a high-dimensional mixture of experts approach to modeling phytoplankton subpopulations as a function of environmental covariates in the ocean. The (log) diameter of the phytoplankton cells within each specific subpopulation are taken to be Gaussian with mean depending on environmental covariates (expressed through nonzero values of $\beta_1, \ldots, \beta_K$); however, the prevalence of the different subpopulations also depends on these covariates (expressed through nonzero values of $\alpha_1, \ldots, \alpha_K$).

When making predictions, it is valuable to be able to quantify one’s level of uncertainty. In this paper, we develop the machinery necessary to do so in the context of the high-dimensional mixture of the experts model described above. In particular, given a sample of $n$ observations from the model in (1)–(2), a confidence level $q \in (0,1)$, and a new predictor vector of interest $x_{\text{new}}$, we show how to form a properly calibrated prediction set $\Omega_q(x_{\text{new}})$. That is, given a new draw $(x_{\text{new}}, y_{\text{new}})$ from (1)–(2), we have that

$$\mathbb{P}(y_{\text{new}} \in \Omega_q(x_{\text{new}}) | x_{\text{new}}) \geq 1 - q.$$  (3)

As an illustration, consider the toy example shown in Figure 1. There are $K = 2$ subpopulations, one following a quadratic relation and the other being constant (for details of the construction, see Section 4). The upper panel shows that the mixture weight on the quadratic subpopulation decreases with increasing $t$. This can also be seen by inspecting the scatterplot and noting that for large $t$, most of the points are in the constant subpopulation. The solid lines show our estimated mixture of experts model fit based on the points in the scatterplot. Now suppose we are about to observe a new point $y_{\text{new}}$ at, say, $t_{\text{new}} = 0.5$. Can we form a set $\Omega_{0.95}(t_{\text{new}})$ that is guaranteed to

Figure 1: (Top left) True (dashed) and estimated (solid) class probabilities $\pi_k(t)$ and $\hat{\pi}_k(t)$. (Bottom left) Data set of $n = 100$ points $\{(t, y_t)\}$ (black dots) with true (dashed) and estimated (solid) mean functions $\mu_k(t)$ and $\hat{\mu}_k(t)$. (Middle) Prediction set at 95% confidence level $\Omega_{0.05}(t)$ for $t \in [0,1]$ (shaded area). (Right) Monte Carlo estimate of coverage and length of prediction sets $\Omega_{0.05}(t)$ across 500 training sets and 1000 $y_{\text{new}}$ per training set.
capture \( y_{\text{new}} \) at least 95% of the time? Given that we do not know which subpopulation \( y_{\text{new}} \) will be drawn from, \( \Omega_{0.95}(t_{\text{new}}) \) will be a union of two intervals. The size and location of these intervals will depend on our estimates of the subpopulation means and variances (governed by \( t_{\text{new}} \) and our estimates of \( \beta_1, \beta_2, \sigma_1, \) and \( \sigma_2 \)) as well as the estimated mixture weights (governed by \( t_{\text{new}} \) and our estimates of \( \alpha_1 \) and \( \alpha_2 \)). The gray band in the middle panel shows our constructed \( \Omega_{0.95}(t_{\text{new}}) \) as we vary \( t_{\text{new}} \) from 0 to 1. When the means of the populations are far apart, the prediction set is a union of two intervals, while the set becomes a single interval when the means are close to each other. The larger a subpopulation’s mixture weight, the wider that interval becomes. This “strategy” is reasonable because if it’s unlikely that a point will fall in a certain subpopulation, one can get away with less good coverage of that subpopulation (and thereby reduce the overall size of the prediction set). The rightmost panel shows the result of a simulation in which we generated 500 training sets, each time constructing \( \Omega_{0.95}(t) \) as a function of \( t \); then, we generated 1000 \( y_{\text{new}} \) at each \( t \) and computed the coverage rate (averaging over the 500 \( \cdot \) 1000 repetitions for each \( t \)). This verifies that our procedure approximately attains the nominal 95% coverage. The bottom panel shows the average size of the prediction set. Quite intuitively, the prediction set is smallest when the two subpopulations are very close to each other. One observes a bit of overcoverage when the subpopulations are close, which makes sense since in this situation the interval from one subpopulation can sometimes cover a point from the opposite subpopulation.

Constructing prediction sets in the context of a high-dimensional mixture of experts model is challenging. In fact, making any sort of precise statements about even the most simple mixture of regression models is nontrivial. For example, much effort has gone into understanding the convergence and estimation error of the expectation-maximization estimator (Dempster et al. 1977) used in fitting such models (Yi et al. 2014, Balakrishnan et al. 2017, Klusowski et al. 2019, Kwon et al. 2019, Kwon & Caramanis 2020) as well as being able to test whether there are two groups versus one (Zhu & Zhang 2004). Adding high dimensionality to the study of mixture of regression models brings additional challenges. Städler et al. (2010) and Yi & Caramanis (2015) proposed different \( \ell_1 \)-regularized maximum likelihood estimators with accompanying estimation error results. Wang et al. (2014) take this a step further and develop a truncation-based high-dimensional estimator with both estimation error results and the ability to construct confidence intervals for low-dimensional components of the parameter vector. While their results hold for general latent variable models, their application to mixture of regression models is more of a proof of concept, with \( K = 2, \sigma_1 = \sigma_2 \) assumed known, \( \pi_1 = \pi_2 = 0.5, \) and \( \beta_1 = -\beta_2. \) Zhang et al. (2020) provide inference for individual coefficients and differences of the form \( \beta_{1j} - \beta_{2j} \) within the context of this model using an \( \ell_1 \) penalty. They generalize to the case of unknown mixture weight \( \pi_1, \beta_1 \neq -\beta_2, \) and an unknown covariance matrix for \( X \) (which they take to be multivariate normal), but they still assume \( K = 2 \) and that the value \( \sigma_1 = \sigma_2 \) is known. While we are able to adopt in part a similar debiased approach, we will highlight later why their technique, which works in the \( K = 2 \) mixture of regression setting (which involves a single unknown mixture parameter \( \pi_1 \)) does not easily generalize to our setting of a mixture of experts model, in which mixture weights depend on the unknown parameter vectors \( \alpha_1, \ldots, \alpha_K \in \mathbb{R}^p. \)

Furthermore, our interest in forming a prediction set (3) requires the ability to make inferential statements about \( \mathbf{x}_{\text{new}}^T \beta_k, \) not just low-dimensional components of \( \beta_k. \) In this sense, Cai et al. (2021) pursue a similar goal in performing inference for individualized treatment effects \( \mathbf{x}_{\text{new}}^T (\beta_1 - \beta_2); \) however, unlike the mixture of regression setting, the group memberships are known in their context.
To summarize, to the best of our knowledge, predictive inference in mixture of expert models has not been addressed in the literature. Furthermore, we address this problem for general $K$ and in the high-dimensional setting. We make use of ideas from the debiased lasso literature. The debiasing approach for constructing confidence intervals for coefficients has been widely used in linear regression models in high-dimensional settings (Javanmard & Montanari 2014, Van de Geer et al. 2014, Javanmard & Montanari 2018). In recent years, there has been work on inference for general linear functions (Cai & Guo 2017, Guo et al. 2021, Javanmard & Lee 2020, Zhu & Bradic 2018). In terms of debiasing in the non-mixture setting, Cai & Guo (2017), Tripuraneni & Mackey (2019), Athey et al. (2018) proposed bias-corrected estimators for a single linear regression model while, as we have noted above, Cai et al. (2021) considers inference for $x_{new}^T(\beta_1 - \beta_2)$ in the case of two observed (i.e., non-latent) groups.

Interest in predictive inference has led to an active area of work on conformal prediction. These approaches are attractive for being distribution-free and providing finite-sample coverage (see, e.g., Papadopoulos et al. 2002, Vovk et al. 2005, Lei et al. 2018, Romano, Patterson & Candes 2019). They rely on very general ideas such as the exchangeability of draws from the distribution. However, the coverage that these conformal methods attain is not conditional on $x_{new}$ as in (3) but rather holds marginally over $x_{new}$:

$$P(y_{new} \in \Omega_q(x_{new})) \geq 1 - q.$$  

Indeed, it has been proven that to obtain finite length sets with conditional coverage, one needs to make stronger assumptions (Vovk 2012, Lei & Wasserman 2014). In certain applications, one specifically desires coverage of the form (3) and assuming the parametric form (1)–(2) can be a small price to pay. For example, in the oceanographic example of mixture of experts (Hyun et al. 2020), the mixture of Gaussians structure is visually well-supported. Prediction sets with conditional coverage are desirable because we would like to be able to say that for a given set of environmental conditions (e.g., at a specific temperature and salinity level) our prediction set for the phytoplankton diameters will have a 95% coverage guarantee. Marginal coverage would mean that if we make predictions over many randomly sampled environments, our coverage would average out to 95%. The latter means, for example, that a procedure could be overconfident (i.e., undercovering) at high temperatures and underconfident (i.e., overcovering) at low temperatures. Setting conditional coverage (3) as the goal guards against this undesirable property.

The rest of the paper is organized as follows. In Section 2, we describe our approach to constructing prediction sets. This involves estimating parameters using a penalized expectation-maximization approach (Section 2.1), then using a debiasing technique on the coefficient vectors from each of the component distributions (Section 2.2), and finally combining $K$ intervals into a prediction set in a fashion that maintains proper coverage (Section 2.3). In Section 3, we provide theoretical guarantees that establish the asymptotic validity of our constructed prediction sets and provide insight into the conditions under which we expect nominal coverage to hold. In Section 4 we investigate the empirical performance of our prediction sets in a variety of settings. Section 5 shows our sets and evaluates their performance empirically in predicting the critical temperatures of superconducting materials. We conclude this section with some notation.

**Notation.** Throughout the paper, we use $[p]$ for the set of integers $1, \ldots, p$. We use $e_i$ to denote the $i$-th standard basis vector. For a vector $x \in \mathbb{R}^p$, we denote $\|x\|_q = \left(\sum_{j=1}^{p} |x_j|^q\right)^{1/q}$ for $q > 0$ and
\|x\|_0 = |\text{supp}(x)|, \|x\|_\infty = \max_{j \in [p]} |x_j| . For a matrix \( A \in \mathbb{R}^{n \times n} \), we use \( |A|_\infty = \max_{1 \leq i,j \leq n} |A_{i,j}| \).

For sequences \( a_n \) and \( b_n \), we use the notation \( a_n \asymp b_n \) to indicate that \( a_n \) is bounded both above and below by \( b_n \) asymptotically, i.e., for some constants \( C_0, C_1 \) and for all \( n \geq n_0 \) we have \( C_0 \leq |a_n/b_n| \leq C_1 \). In addition, we write \( a_n = O_p(b_n) \) if for any \( \varepsilon > 0 \), there exists \( C_\varepsilon > 0 \) and large enough \( n_\varepsilon \) such that \( \mathbb{P}(|a_n/b_n| > C_\varepsilon) < \varepsilon \), for all \( n \geq n_\varepsilon \). We write \( a_n = o_p(b_n) \) if \( a_n/b_n \) converges to zero in probability, i.e., \( \lim_{n \to \infty} \mathbb{P}(|a_n/b_n| \geq \varepsilon) = 0, \forall \varepsilon > 0 \). The notation \( \Rightarrow \) indicates convergence in distribution.

We use the notation \( \| \cdot \|_{\psi_2}, \| \cdot \|_{\psi_1} \) to refer to the sub-Gaussian and sub-exponential norms respectively. Specifically, for a random variable \( X \), we let
\[
\|X\|_{\psi_1} = \sup_{q \geq 1} q^{-1}(\mathbb{E}|X|^q)^{1/q}, \quad \|X\|_{\psi_2} = \sup_{q \geq 1} q^{-1/2}(\mathbb{E}|X|^q)^{1/2} .
\]

For a random vector \( x \), its sub-Gaussian and sub-exponential norms are defined as
\[
\|x\|_{\psi_1} = \sup_{\|u\|_2 \leq 1} \|\langle x, u \rangle\|_{\psi_2}, \quad \|x\|_{\psi_1} = \sup_{\|u\|_2 \leq 1} \|\langle x, u \rangle\|_{\psi_1}. 
\]

## 2 Methodology

We begin (in Section 2.1) with a review of a penalized maximum likelihood procedure for the MoE model (1)–(2) such as is used in Hyun et al. (2020). Sections 2.2 and 2.3 then introduce our proposed methodology for forming prediction sets in this context.

### 2.1 Penalized EM-based Estimator

The expectation-maximization (EM) algorithm (Dempster et al. 1977) is a common heuristic when faced with maximum-likelihood problems involving missing data, especially in the form of latent variables. The algorithm operates in an iterative fashion, alternating between the E (expectation) step and M (maximization) step, while managing to increase the objective function.

Assume \( n \) data points \( \{(x_i, y_i)\}_{i=1}^n \) are drawn independently from the MoE model (1)–(2). The EM algorithm aims at maximizing the log-likelihood
\[
\ell(\theta) = \frac{1}{n} \sum_{i=1}^n \log \left[ \sum_{k=1}^K \pi_k(x_i) \cdot \phi_k(x_i, y_i) \right], \tag{4}
\]
where \( \theta = (\{\beta_k, \alpha_k, \sigma_k\}_{k \in [K]}) \in \mathbb{R}^{(2p+1)K} \) represents the model parameters, \( \phi_k(x_i, y_i) \) is given by
\[
\phi_k(x_i, y_i) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp \left( -\frac{(y_i - x_i^T \beta_k)^2}{2\sigma_k^2} \right), \tag{5}
\]
and \( \pi_k(x_i) \) is given in (2). The log-likelihood \( \ell(\theta) \) is not concave even as a function of \( \beta_k \), treating \( \alpha_k \) and \( \sigma_k \) as fixed. This is due to the marginalizing over the latent cluster memberships \( z_i \). The EM algorithm instead employs a minorize-maximize approach (Hunter & Lange 2004) in which a minorizer to the log-likelihood is repeatedly constructed and maximized. More specifically, given some fixed \( \hat{\theta} \) it maximizes a lower bound function \( Q(\theta; \hat{\theta}) \) over \( \theta \) to make \( \ell(\theta) - \ell(\hat{\theta}) \) large. We refer to Hastie et al. (2009) for a more detailed introduction to EM algorithm and derivation of the function \( Q(\theta; \hat{\theta}) \) and here only provide the description of the EM algorithm for the MoE model.
Let $\gamma_{i,k}(\theta)$ be the probability that $z_i = k$ conditioned on the observed variable $(x_i, y_i)$, i.e.,

$$
\gamma_{i,k}(\theta) := \mathbb{P}(z_i = k|x_i, y_i) = \frac{\pi_k(x_i) \cdot \phi_k(x_i, y_i)}{\sum_{\ell=1}^{K} \pi_{\ell}(x_i) \cdot \phi_{\ell}(x_i, y_i)}.
$$

The function $\gamma_{i,k}(\theta)$ is sometimes referred to as responsibilities in the literature (see, e.g. Hyun et al. (2020)) because it quantifies how “responsible” group $k$ is for point $i$.

Consider the function $Q(\theta|\hat{\theta})$ defined as

$$
Q(\theta|\hat{\theta}) = -\frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} \gamma_{i,k}(\hat{\theta}) \left[ \log \pi_k(x_i) + \log \phi_k(x_i, y_i) \right] + \sum_{k=1}^{K} \lambda_{\alpha} \|\alpha_k\|_1 + \sum_{k=1}^{K} \lambda_{\beta} \|\beta_k\|_1,
$$

where the regularization terms $\|\beta_k\|_1, \|\alpha_k\|_1$ are added to enforce sparsity on the estimated parameters and allow for applications in the high-dimensional sparse regime.

The EM algorithm iterates between estimating the conditional membership probabilities $\gamma_{i,k}(\hat{\theta})$, and reducing (6) by updating the parameters $\hat{\theta}$. The details of the updates are given below:

- **E step:** Estimating the conditional responsibility of membership based on the latest parameter estimate.

  $$
  \gamma_{i,k}(\hat{\theta}) = \frac{\hat{\pi}_{i,k} \exp \left(- \frac{(y_i - x_i^T \hat{\beta}_k)^2}{2\hat{\sigma}_k^2} \right)}{\sum_{\ell=1}^{K} \hat{\pi}_{i,\ell} \exp \left(- \frac{(y_i - x_i^T \hat{\beta}_\ell)^2}{2\hat{\sigma}_\ell^2} \right)}.
  $$

- **M step:** Updating $\hat{\theta}$ to lower the objective value in (6).

  - For each $k = 1, \ldots, K$, update $\hat{\beta}_k$:

    $$
    \hat{\beta}_k = \arg \min_{\beta} \sum_{i=1}^{n} \gamma_{i,k}(\hat{\theta}) \frac{(y_i - x_i^T \beta)^2}{2n} + \lambda_{\beta} \|\beta\|_1.
    $$

  - Update $\{\hat{\alpha}_k\}_{k=1}^{K}$:

    $$
    \{\hat{\alpha}_k\} = \arg \min_{\{\alpha_k\}} -\frac{1}{n} \sum_{i=1}^{n} \left( \sum_{k=1}^{K} \gamma_{i,k}(\hat{\theta}) x_i^T \alpha_k - \log \left( \sum_{\ell=1}^{K} \exp \left( x_i^T \alpha_{\ell} \right) \right) \right) + \lambda_{\alpha} \sum_{k=1}^{K} \|\alpha_k\|_1.
    $$

  - For each $k = 1, \ldots, K$, update $\hat{\sigma}_k$:

    $$
    \hat{\sigma}_k^2 = \frac{\sum_{i=1}^{n} \gamma_{i,k}(\hat{\theta})(y_i - x_i^T \hat{\beta}_k)^2}{\sum_{i=1}^{n} \gamma_{i,k}(\hat{\theta})}.
    $$

As noted in Hyun et al. (2020), this M-step update represents a decreasing in the objective but not a minimization since $(\beta_k, \sigma_k)$ would need to be jointly optimized. The algorithm terminates when the improvement in (6) is below some threshold.

In practice, we use the R package flowmix (Hyun 2022) to carry out the EM algorithm.
2.2 Debiased Prediction

From (1)–(2), we have that
\[ y_{\text{new}} | x_{\text{new}} \sim N(x_{\text{new}}^T \beta_k, \sigma_k^2) \] with probability \( \pi_k(x_{\text{new}}) \).

Because of the penalization, \( \hat{\Gamma}_k := x_{\text{new}}^T \hat{\beta}_k \) is a biased estimate of \( \Gamma_k := x_{\text{new}}^T \beta_k \), and thus would give biased predictions for \( y_{\text{new}} \) even if we knew that \( z_{\text{new}} = k \). We therefore propose a debiasing procedure. Given an arbitrary vector \( u_k \), we construct a debiased prediction
\[ \hat{\Gamma}_k^d := x_{\text{new}}^T \hat{\beta}_k + u_k^T \frac{1}{n} \sum_i \partial \ell_i(\hat{\theta}) \],
where \( \partial / \partial \beta_k \) denotes the gradient with respect to \( \beta_k \).

Our proposed choice for \( u_k \) depends on the estimated sample Fisher information matrix, which is given by
\[ \hat{I}(\hat{\theta}) = \frac{1}{n} \sum_{i=1}^n \nabla \ell_i(\hat{\theta}) \nabla \ell_i^T(\hat{\theta}) , \] where \( \ell_i(\hat{\theta}) \) are the summands in (4) evaluated at \( \hat{\theta} = \{ \hat{\beta}_k, \hat{\alpha}_k, \hat{\sigma}_k \}_{k \in [K]} \), and
\[ \nabla \ell_i = \left( \left\{ \frac{\partial \ell_i}{\partial \beta}_k \right\}_{k=1}^K, \left\{ \frac{\partial \ell_i}{\partial \alpha}_k \right\}_{k=1}^K, \left\{ \frac{\partial \ell_i}{\partial \sigma}_k \right\}_{k=1}^K \right)^T . \]

We would like a choice of \( u_k \) that will lead to a narrower interval. This intuition (which is described in greater detail below) suggests choosing \( u_k \) as the solution to the optimization problem
\[ \begin{align*}
\min_{u} & \quad u^T \hat{I}_k^{\beta}(\hat{\theta}) u \\
\text{s.t.} & \quad \sup_{w \in C} \left| \left( w, \hat{\Sigma}_k u - x_{\text{new}} \right) \right| \leq \lambda_k \| x_{\text{new}} \|_2, \| u \|_1 \leq L \| x_{\text{new}} \|_2 ,
\end{align*} \]
where we define \( \hat{\Sigma}_k := \frac{1}{n} \sum_{i=1}^n \gamma_{i,k}(\hat{\theta}) x_i x_i^T \), \( L \) is a sufficiently large constant, and \( \lambda_k \) is a tuning parameter (in Section 3, we discuss the proper rate of \( \lambda_k \) and the choice of \( L \)). In addition, \( C = \{ e_1, \ldots, e_p, x_{\text{new}}/\| x_{\text{new}} \|_2 \} \), where \( e_i \) denotes the i-th standard Euclidean basis vector. The matrix \( \hat{I}_k^{\beta}(\hat{\theta}) \) is the estimated Fisher information matrix, constrained to \( \beta_k \), which is given by
\[ \hat{I}_k^{\beta}(\hat{\theta}) = \frac{1}{n} \sum_{i=1}^n \left( \gamma_{i,k}(\hat{\theta}) y_i - x_i^T \hat{\beta}_k \right) \left( \gamma_{i,k}(\hat{\theta}) y_i - x_i^T \hat{\beta}_k \right)^T / \sigma_k^2 . \]

The above characterization follows from the definition of \( \hat{I}(\hat{\theta}) \) given by (11) along with identity (35), restricted to class \( k \).

Remark. Because \( \hat{\Sigma}_k \) and \( \hat{I}_k^{\beta}(\hat{\theta}) \) depend on both the response vector \( y \) and the covariate matrix \( X \), the solution \( u_k \) to (12) is also dependent on them. This is in contrast to the optimization problem proposed by Javanmard & Montanari (2014a) for constructing the debiasing direction, as it only
involved covariates and hence conditional on the covariate matrix \( X \), the debiasing direction was independent of the response vector \( y \).

To deal with the complications resulting from the dependence of \( u_k \) on \((X, y)\), we do sample splitting. Specifically, we split the data into two sets, \( D_1 \) and \( D_2 \), where optimization (12) is solved on \( D_1 \), and \( \hat{\beta}_k, \hat{\Gamma}_k^d \) are calculated using samples in \( D_2 \), per (10).

The above approach to construct the direction \( u_k \) is generalized from Javanmard & Montanari (2014a), Zhang & Zhang (2014), Cai & Guo (2017) and aims to find a direction that minimizes the variance while controlling the bias. However, the goal in Javanmard & Montanari (2014a), Zhang & Zhang (2014), Cai & Guo (2017) is to establish inference for coefficients, which differs from our goal of establishing inference for prediction. Closer to our aim here, we follow the proposal of Cai et al. (2021) to construct prediction intervals, under a linear regression model; however, our setting of a MoE model is more complex and requires novel methodology and analysis. In particular, our optimization problem differs from Cai et al. (2021) in that we use a constrained Fisher information matrix, \( \hat{I}_k^\beta(\hat{\theta}) \), in the objective of (12), and we allow the matrix \( \Sigma_k \) in the constraint of (12) to be different from the matrix in the objective, while Cai et al. (2021) keeps them the same.

The first constraint in (12) can be decomposed as

\[
\|\Sigma_k u - x_{\text{new}}\|_\infty \leq \lambda_k \|x_{\text{new}}\|_2 \tag{14}
\]

\[
\left|u^T \Sigma_k u - x_{\text{new}}^T \right| \leq \lambda_k \|x_{\text{new}}\|_2^2 \tag{15}
\]

Similar to the general intuition behind the quadratic optimization of Javanmard & Montanari (2014a), the objective value \( u^T \tilde{I}_k^\beta(\hat{\theta}) u_k \) is related to the variance of \( \hat{\Gamma}_k^d \), and the constraint (14) relates to its bias. So the optimization is indeed aiming to minimize the variance (and hence the length of prediction intervals which will be constructed based on \( \hat{\Gamma}_k^d \)), while controlling the bias of \( \hat{\Gamma}_k^d \). That said, in the analysis we need to show that the bias is dominated by the variance term and therefore need to establish a lower bound on the variance. The constraint (15) is added for this step. It makes the feasible set of the optimization problem smaller and makes it possible to lower bound the optimal value of the objective (see Proposition A.3 for technical arguments). This idea originates from Cai et al. (2021), which introduced the “variance-enhancement projection direction”. While the general intuition carries over to our current setting, characterizing the statistical properties of \( \hat{\Gamma}_k^d \) under the MoE requires a rather intricate and technical analysis.

We denote the estimated variance for \( \hat{\Gamma}_k^d \) as

\[
\hat{V}_k = \frac{1}{n} u_k^T \tilde{I}_k^\beta(\hat{\theta}) u_k, \quad k = 1, \ldots, K, \tag{16}
\]

and the prediction variance estimate (conditional on \( z_{\text{new}} = k \)) as

\[
b_k^2 := \hat{V}_k + \hat{\sigma}_k^2, \quad k = 1, \ldots, K. \tag{17}
\]

### 2.3 Prediction Sets

Recall that our goal is to construct a \( 100(1 - q)\% \) prediction set \( \Omega_q(x_{\text{new}}) \) satisfying (3). By the nature of the mixture, we seek a prediction set of the form

\[
\Omega_q(x_{\text{new}}) = \bigcup_{k=1}^K \mathcal{L}_k, \tag{18}
\]
where each $L_k = [l_k, u_k]$ is centered at a debiased estimator $\hat{\Gamma}_k^d$. Regarding the length of $\Omega_q(x_{\text{new}})$ as our budget it is clear at an intuitive level that we should spend more on the mixture components to which $(x_{\text{new}}, y_{\text{new}})$ is more likely to belong, i.e., to those groups $k$ with larger $\pi_k(x_{\text{new}})$. To this end, we form a probability density function using a weighted mixture of Gaussian densities:

$$f(y) = \sum_{k=1}^{K} \frac{\hat{\pi}_k(x_{\text{new}})}{b_k} \phi \left( \frac{y - \hat{\Gamma}_k^d}{b_k} \right), \quad (18)$$

where $\phi(\cdot)$ is the standard normal pdf. The particular form of this density is justified in the proof of Theorem 3.2 given in Section B. We give a schematic illustration of $f$ in Figure 2.

We seek a set of intervals $[y^-_1, y^+_1], ..., [y^-_K, y^+_K]$, such that

$$\sum_{k=1}^{K} \int_{y^-_k}^{y^+_k} f(y)dy = 1 - q, \quad (19)$$

while minimizing $\sum_{k=1}^{K} |y^+_k - y^-_k|$. For this, we start from a large cutoff (the horizontal line in the figure) and decrease that until the area under $f$ and corresponding to $y$ with $f(y)$ above the cutoff (the blue region in the figure) is $1 - q$. To approximate the area we take a discretization approach as outlined below.

Assume without loss of generality that $\hat{\Gamma}_1^d \leq ... \leq \hat{\Gamma}_K^d$. We start by considering the interval

$$Q = [\hat{\Gamma}_1^d - b_1 z_{1-q/2}, \hat{\Gamma}_K^d + b_K z_{1-q/2}],$$

which we know has probability at least $1 - q$. We then divide $Q$ into segments of size $\delta$, denoted as $Q_1, ..., Q_{|Q|}$. The area under the curve $f(y)$ confined to the segment $Q_i$ is approximately $\delta h_i$, where $h_i$ is the density $f$ evaluated at the midpoint point of $Q_i$. We next sort $h_i$’s corresponding to each segment in decreasing order, i.e.,

$$h_{(1)} \geq h_{(2)} \geq ... \geq h_{(|Q|)},$$

and find the smallest $N$ such that

$$\delta \sum_{i=1}^{N} h_{(i)} \geq 1 - q. \quad (20)$$

We return $\Omega_q(x_{\text{new}}) := \bigcup_{i=1}^{N} Q_{(i)}$ as the prediction set.

Figure 2: An illustration of the mixture density $f$, given by (18) for $K = 2$ groups. The cutoff level (indicated by the red line) is the highest level such that the region shaded in blue has area at least $1 - q$. 
Algorithm 1: Constructing prediction set $\Omega_q(x_{\text{new}})$ with $(1 - q)$ coverage

**Input:** Confidence level $1 - q$, discretization scale $\delta$, debiased estimate of each center $\hat{\Gamma}_d^k$, prediction standard error estimate $b_k$, membership probability estimate $\hat{\pi}_k(x_{\text{new}}), k = 1, \ldots, K$.

**Output:** Prediction set with $(1 - q)$ coverage

1. Form a weighted mixture of Gaussian densities

   $$f(y) = \sum_{k=1}^{K} \frac{\hat{\pi}_k(x_{\text{new}})}{b_k} \cdot \phi \left( \frac{y - \hat{\Gamma}_d^k}{b_k} \right).$$

2. Choose a large enough interval $Q$ so that the integral $\int_{Q} f(y) \geq 1 - q$, i.e.

   $$Q = [\hat{\Gamma}_1 - b_1 z_{1-q/2}, \hat{\Gamma}_K + b_K z_{1-q/2}].$$

3. Divide $Q$ into segments of size $\delta$. Let $y_i$ be the midpoint of $Q_i$ and $h_i = f(y_i)$.

4. Sort $h_i$'s in decreasing order,

   $$h_{(1)} \geq h_{(2)} \geq \ldots \geq h_{(|Q|)}.$$

5. Find the smallest $N$ such that

   $$\delta \sum_{i=1}^{N} h_{(i)} \geq 1 - q.$$

6. Return the union of the corresponding segments

   $$\Omega_q(x_{\text{new}}) = \bigcup_{i=1}^{N} Q_{(i)}. \quad (21)$$
3 Theoretical Guarantees

We consider a sequence of problems where the sample size $n \to \infty$ and covariate dimension $p = p(n) \to \infty$, while the number of groups $K$ is bounded, and we establish asymptotic validity of our prediction sets for the MoE model (1)–(2). We first lay out several technical assumptions on the estimation error of $\hat{\theta}$, the random covariate vectors $\{x_i\}_{i \in [n]}$, and the model parameters $\theta$.

- (A1) Parameter estimation $\eta_{\text{est}}$. Suppose that
  
  $\max_{k \in [K]} \|\hat{\theta}_k - \theta_k\|_1 = \max_{k \in [K]} \left(\|\hat{\beta}_k - \beta_k\|_1 + \|\hat{\alpha}_k - \alpha_k\|_1 + |\hat{\sigma}_k - \sigma_k|\right) = O_p(\eta_{\text{est}}),$

  where $\eta_{\text{est}}$ scales with $n, p$ and potentially other structure associated with the parameters (e.g. sparsity levels). We assume that
  
  $\sqrt{n} \log(np) \eta_{\text{est}}^2 = o(1).$ (22)

- (A2) Distribution of features. We have a positive-semidefinite matrix $\Sigma \in \mathbb{R}^{p \times p}$ (or more precisely a sequence of matrices of growing dimension) with bounded operator norm, $\|\Sigma\|_{op} \leq C_{\Sigma}$, for a constant $C_{\Sigma}$ as $p \to \infty$. Suppose that $\Sigma^{-1/2}x_i$ are independent sub-Gaussian vectors, with mean zero and sub-Gaussian norm $\|\Sigma^{-1/2}x_i\|_{\psi_2} = O(1)$.

- (A3) Bounded noise and signal. The noise variances $\sigma_k^2$ are strictly positive and bounded constants for $k \in [K]$. We also assume that $\max_{\ell, k \in [K]} \|\beta_k - \beta_\ell\|_2 = O(1)$.

Condition (A1) assumes an $\ell_1$-consistency rate for the estimate $\hat{\theta}$. Consistency presupposes identifiability, which in the case of the $\{\alpha_k\}$ may require additional assumptions (since $\{\alpha_k + c : k \in [K]\}$ corresponds to the same $\pi_k(x)$ as $\{\alpha_k : k \in [K]\}$). Our theoretical results apply to any estimator which satisfy condition (22). The proposed EM estimator in Section 2.1 is just one specific choice. Instead of $\ell_1$-regularization, one can follow other variants based on iterative truncation. For example, Wang et al. (2014) analyzes a mixture of regression model with two groups and proposes a truncated EM algorithm (with a gradient ascent implementation) which achieves $\eta_{\text{est}} = s \sqrt{\log(p) \log(n)/n}$, with $s$ the sparsity level of model parameters. The work Zhang et al. (2020) derives a similar $\ell_1$-consistency rate for the high-dimensional mixed linear regression with two groups, for an iterative EM procedure which performs $\ell_1$ regularization at each step. While the mixture of experts model is more complicated we conjecture that a similar rate for $\eta_{\text{est}}$ carries over to this setting. Under such conjecture, condition (22) simplifies to

$$\frac{s^2 \log(np) \log(p) \log(n)}{\sqrt{n}} = o(1).$$

Condition (A2) is on the random covariate vectors $x_i$ and is a common assumption in high-dimensional statistical estimation; see e.g. Bühlmann & Van De Geer (2011). Condition (A3) on the pairwise distances $\|\beta_k - \beta_\ell\|_2$ and noise variance $\sigma_k^2$ is to control the heterogeneity of data coming from different groups.

Our first theorem is on asymptotic normality of the bias-corrected estimators $\Gamma_k^d$ defined in (10) and involves the matrix

$$\Sigma_k = \mathbb{E} \left[ \frac{\gamma_{1k}(\theta)}{\sigma_k^2} x_1 x_1^T \right].$$
Theorem 3.1. Suppose that $\|\Sigma_k^{-1}x_{\text{new}}\|_1 = O(1)$ and $\log(p) = o(n^{1/4}/\sqrt{\log(n)})$. Let $u_k$ be the solution to the optimization problem (12) with constant $L \geq \|\Sigma_k^{-1}x_{\text{new}}\|_1 \|x_{\text{new}}\|_2$ and $\lambda_k \approx \eta_{\text{est}} \log(np) + \sqrt{\log(p)/n}$. Under Assumptions (A1), (A2), (A3), and Remark 2.2, we have

$$\sqrt{n}(\hat{\Gamma}_d - \Gamma_k) \xrightarrow{d} N(0, 1) \quad (23)$$

where $\hat{I}_k(\hat{\theta})$, given by (13), is the sample Fisher information matrix constrained to entries corresponding to $\beta_k$.

Now that we have established the asymptotic normality of our debiased estimators, we are ready to prove that our prediction sets provide proper asymptotic coverage.

Theorem 3.2. Under the assumptions of Theorem 3.1, the prediction set $\Omega_q(x_{\text{new}})$ has asymptotically valid coverage. Specifically, fix $\gamma > 0$ arbitrarily small and in Algorithm 1 set the discretization scale $\delta$ so that

$$\delta \leq 11 \sqrt{\gamma \min_{k \in [K]} (b_k)/\text{Len}(Q)},$$

with $\text{Len}(Q)$ representing the length of interval $Q$. Then, for any $x_{\text{new}}$ and its response $y_{\text{new}}$ generated according to MoE, we have

$$\lim_{n \to \infty} P(y_{\text{new}} \in \Omega_q(x_{\text{new}})|x_{\text{new}}) \geq 1 - q - \gamma.$$

Note that choosing $\gamma$ arbitrarily small we get a coverage arbitrarily close to $1 - q$. We refer to Section A for the proof of Theorems 3.1 and 3.2.

4 Numerical Study

In Section 4.1, we return to the low-dimensional example given in Section 1 and consider several variations to build greater understanding of the behavior of our intervals. In Section 4.2, we assess the performance of our procedures in a high-dimensional example.

4.1 A Low-Dimensional Example

Figure 1 shows a two-group example where the mean functions of the two groups are $\mu_1(t) = 10(t - 0.5)^2$ and $\mu_2(t) = 1$, the error variances are $\sigma_k^2 = 0.15^2$, and the log odds of being in the first group is given by

$$\log \left[ \frac{\pi_1(t)}{1 - \pi_1(t)} \right] = \log(9) - 2 \log(9) \cdot t,$$

for $n = 100$ equally spaced values of $t$ ranging from 0 to 1. This means that $\pi_1(t)$ decreases from 0.9 to 0.1. Writing this MoE model in the notation of (1)–(2), we have $x = (1, t, t^2)^T$, $\beta_1 = (2.5, -10, 10)^T$, $\beta_2 = (1, 0, 0)^T$, $\alpha_1 = (\log 9, -2 \log 9, 0)^T$, and $\alpha_2 = (0, 0, 0)^T$. This initial
setting is perfectly symmetric in the two groups other than the difference in mean functions. For example, the first group at $t = 0$ is as common as the second group is at $t = 1$. This symmetry is manifest in the width of the intervals: In the middle panel, the width of the interval around the first group at $t = 0$ matches that of the second group at $t = 1$. The symmetry is also apparent in the third panel plots.

To build our intuition, we explore the effect of breaking this symmetry between groups. For example, suppose that the error variances in the two groups are not equal. In Figure 3, we take $\sigma_1 = 0.1$ and $\sigma_2 = 0.2$. While the empirical coverage is maintained around the nominal 0.95 level, the average length of the prediction set $\Omega_{0.05}(t)$ is no longer symmetric around $t = 0.5$. This makes intuitive sense since the class imbalance means that there is more uncertainty in estimating $\beta_2$ than $\beta_1$; thus, at $t = 1$, where more of the prediction set is devoted to the second group (since $\pi_2(1) > \pi_1(1)$), the average length of $\Omega_{0.5}(1)$ will be larger compared to that of $\Omega_{0.5}(0)$.

Another way to break the symmetry would be by considering class imbalance. We again assume $\sigma_1 = \sigma_2 = 0.15$, but now suppose that overall about 60% of observations belong to the first group. In particular, we take instead $\alpha_1 = \log 10 \cdot (1, -\log 4, 0)^T$, so that $\pi_1(t)$ ranges from about 0.91 at $t = 0$ to about 0.29 at $t = 1$. Figure 4 shows the effect of this class imbalance. We see the same increasing length as in the previous example despite the error variances being equal. In this example, it is the class imbalance that leads to greater uncertainty in estimating $\beta_2$.

### 4.2 High-Dimensional Case

We consider a high-dimensional case where $K = 2$ and $p = 501$ (including the intercept). The oceanographic application in Hyun et al. (2020) has repeated observations at multiple $x_t$, and we mimic that setup with $T = 150$ feature vectors $x_t$, and $n_t = 5$ observations per $x_t$ for a total of $n = 750$ measurements. This is high-dimensional since $\theta$ has dimension $K(2p + 1) = 2002$. We take $x_{t1} = 1$ and $x_{tj}$ for $j > 1$ to be independent standard Gaussians. We generate $n_t$ responses $y_{it}$
for each $x_t$ according to the MoE model (1)–(2) with $\sigma_1 = \sigma_2 = 1$ and

$$\beta_1 = \begin{pmatrix} -2, & 4, & -2, & -4, & 6, & 2, & 0, & 0, & 0, & 0, & 0, & 0, & 1_{390}^T \end{pmatrix}^T,$$

$$\beta_2 = \begin{pmatrix} 2, & 0, & 0, & 0, & 0, & 0, & 4, & -2, & -4, & 6, & 2, & 1_{390}^T \end{pmatrix}^T,$$

and

$$\alpha_1 = \begin{pmatrix} 0_{491}, & 0, & 0, & 0, & 0, & 0, & 0.7, & 0.7, & 0.7, & 0.7 \end{pmatrix}^T,$$

$$\alpha_2 = \begin{pmatrix} 0_{491}, & -0.7, & -0.7, & -0.7, & -0.7, & -0.7, & 0, & 0, & 0, & 0, & 0, & 0 \end{pmatrix}^T.$$

We estimate the model using the penalized EM algorithm described in Section 2.1 as implemented in the \texttt{flowmix} R package (Hyun 2022). We perform five-fold cross validation to choose the parameters $(\lambda_\alpha, \lambda_\beta)$ from a $10 \times 10$ logarithmically-spaced grid. While in Section 2.2 we remark that sample splitting avoids the complications resulting from $\mathbf{u}_k$’s dependence on $(\mathbf{X}, y)$, empirically we find that coverage is attained even if we ignore this dependence. Therefore, in this and all numerical results we do not use sample splitting for the debiasing step.

To evaluate our method, we generate 100 independent $x_{\text{new}} \in \mathbb{R}^p$. For each $x_{\text{new}}$, we compute $\Omega_{0.05}(x_{\text{new}})$ and record its length. We then generate 100 independent $y_{\text{new},i}$’s for each $x_{\text{new}}$ and record the proportion of $y_{\text{new},i}$’s falling into the prediction set for that $x_{\text{new}}$.

We repeat the above procedure 500 times, keeping the 100 $x_{\text{new}}$’s the same. For each $x_{\text{new}}$, we compute

1. the average length of prediction sets (across the 500 runs), and
2. the coverage probability (proportion across the 500 runs and 100 $y_{\text{new},i}$).

In the left and middle panels of Figure 5, we plot these quantities as a function of $\pi_1(x_{\text{new}})$, the true probability of being drawn from cluster 1 for each $x_{\text{new}}$. As desired, the coverage rate
of our prediction sets meet the 95% nominal level, regardless of $\pi_1(x_{\text{new}})$. We observe that the prediction sets tend to be twice as long when $\pi_1(x_{\text{new}}) \approx 0.5$ compared to at the extremes. This is likely because at an extreme the less common group’s interval can be very narrow without hurting coverage whereas when the two groups are balanced, both intervals are needed.

In the right panel of Figure 5, we plot the average length of prediction intervals against the distances between the two group means, i.e.,

$$|x_{\text{new}}^T(\beta_1 - \beta_2)|.$$

Recall that in the low-dimensional examples (Figures 1, 3, and 4) we observed a marked decrease in the prediction set length when the means crossed each other. A similar phenomenon is apparent here. There is a linear increasing trend when $|x_{\text{new}}^T(\beta_1 - \beta_2)|$ goes from 0 to 10. As suggested in the middle panel, the individual intervals have average length around 5. Thus, this linear increase represents the two overlapping intervals gradually being pulled apart. At a distance of 10, they no longer overlap, which explains the leveling of this trend. The variability in length seen for distances greater than 10 can be explained, for example, by differing values of $\pi_1(x_{\text{new}})$.

5 Superconductivity Data Application

We apply our method to the superconductivity data provided in Hamidieh (2018). This dataset contains the critical temperature (in Kelvin) and a set of $p = 81$ attributes for about 21,000 materials. The attributes used as predictors are elemental property statistics and electronic structures of attributes. We center and scale each predictor column and we take the response to be log(1 + temperature). The log transform makes the data less skewed right and adding 1 Kelvin to each temperature can be thought of as replacing the log of extremely low temperatures (some are less than 1 mK) with 0.

We randomly split the observations into a training set of $n = 200$ (used for estimating model parameters, cross validation of $\lambda_\alpha$ and $\lambda_\beta$), and forming the prediction sets), a validation set of size 1000 (used to choose $K$), and a test set of about 20,000 observation (for measuring the coverage of
Figure 6: Plot of prediction sets for 100 randomly sampled data points in the test set. The black points are the log(1 + temperature) and the bars correspond to the prediction sets for each observation. We use red when there is only one interval and cyan when there are two intervals.

Our prediction sets. Table 1 shows the mean squared prediction error, computed on the validation set, for K ranging from 1 to 5. To make predictions at a given \( x_{\text{validation}} \), we use

\[
x_{\text{validation}}^T \hat{\beta}_k(x_{\text{validation}})
\]

where

\[
\hat{k}(x_{\text{validation}}) = \arg \max_k \hat{\pi}_k(x_{\text{validation}})
\]

is the class with highest estimated probability. The prediction errors on the validation set suggest that \( K = 2 \) may be a suitable choice.

| K  | Prediction error |
|----|------------------|
| 1  | 8.953            |
| 2  | **0.867**        |
| 3  | 0.978            |
| 4  | 1.318            |
| 5  | 0.869            |

Table 1: Prediction errors computed on a validation set for fitted models where \( K = 1, 2, 3, 4, 5 \).

For each observation \((x_{\text{new}}, y_{\text{new}})\) in the test set, we form \( \Omega_{0.05}(x_{\text{new}}) \) and note whether \( y_{\text{new}} \in \Omega_{0.05}(x_{\text{new}}) \). Figure 6 displays the prediction sets for a random subset of 100 of the 20,000 intervals formed on the test set. We see that \( \Omega_{0.05}(x_{\text{new}}) \) is often a single interval, although it also occasionally the union of two intervals. The overall coverage on the test set is 97.1%. The average length of \( \Omega_{0.05}(x_{\text{new}}) \) (after being transformed back from log-values) is around 42 Kelvin.

The 97.1% coverage is averaged over all \( x_{\text{new}} \) and yet our prediction sets are designed for conditional coverage in the sense of (3). This stronger form of coverage implies that we can get coverage on subsets of observations defined by \( x_{\text{new}} \), i.e.

\[ P(y_{\text{new}} \in \Omega_q(x_{\text{new}})|x_{\text{new}} \in S) \geq 1 - q. \]

The predictor that is most correlated with critical temperature is the weighted standard deviation of thermal conductivity. We divide the range of this variable into 5 equally-spaced sub-intervals,
and divide test data points into 5 subgroups accordingly. Table 2 confirms that our prediction sets meet the nominal level within each subgroup.

| Subgroup | Number of data | Coverage Rate |
|----------|----------------|---------------|
| 1        | 3098           | 95.9%         |
| 2        | 4039           | 97.2%         |
| 3        | 3960           | 97.1%         |
| 4        | 3999           | 95.6%         |
| 5        | 4000           | 94.8%         |

Table 2: Coverage rates of 95% prediction sets conditional on subgroups defined by the predictor “weighted standard deviation of thermal conductivity.”

6 Conclusion

We have shown how to construct prediction sets for the high-dimensional mixture of experts model. Mixture models are important for capturing the heterogeneity that is present in many real-world situations. While in small data samples it was common to dismiss deviations from the norm as outliers, in large data sets it becomes possible to use models that can identify and model these subgroups. While mixture of regression models allow for such heterogeneity-aware predictive modeling, they assume that the relative sizes of the subgroups are fixed. Importantly, mixture of experts models remove this assumption and allow the prevalence of different subgroups to depend on the features. This generalization is essential in many situations from ecology, where the relative proportions of different subpopulations depends on environmental covariates (Hyun et al. 2020), to politics, where the political composition depends on demographic and geographic variables.

Our focus on conditional coverage can be crucial in certain applications. For example, Romano, Barber, Sabatti & Candès (2019) emphasizes the importance of ensuring that all subpopulations enjoy the same coverage guarantees and cast this as a fairness issue when the subpopulations are defined based on a protected attribute.

A Proof of Main Theorems

A.1 Proof of Theorem 3.1

Before we prove the asymptotic normality, we start by presenting a proposition establishing that the optimization problem (12) is feasible. We postpone its proof to Section C.1.

Proposition A.1. (Feasibility) Under the assumptions of Theorem 3.1, there exists \( u \) such that

\[
\sup_{\omega \in \mathcal{C}} \left| \langle \omega, \tilde{\Sigma}_k u - x_{\text{new}} \rangle \right| \leq \lambda_k \| x_{\text{new}} \|_2 \quad \text{and} \quad \| u \|_1 \leq L \| x_{\text{new}} \|_2
\]

is satisfied for \( \lambda_k \asymp \eta_{\text{est}} \log(np) + \sqrt{\log(p)/n} \), \( L \geq \frac{\| \Sigma_k^{-1} x_{\text{new}} \|_1}{\| x_{\text{new}} \|_2} \), and \( \mathcal{C} = \{ e_1, \ldots, e_p, x_{\text{new}}/\| x_{\text{new}} \|_2 \} \).
We next decompose the error of the bias-corrected estimator as follows:

\[
\hat{\Gamma}_k^d - \Gamma_k = x_{\text{new}}^T \hat{\beta}_k + u_k^T \frac{1}{n} \sum_i \frac{\gamma_i,k(\theta)}{\sigma_k^2} (y_i - x_i^T \hat{\beta}_k) x_i - x_{\text{new}}^T \beta_k
\]

\[
= \left( x_{\text{new}} - \frac{1}{n} \sum_i \frac{\gamma_i,k(\theta)}{\sigma_k^2} x_i x_i^T u_k \right)^T (\hat{\beta}_k - \beta_k) + u_k^T \frac{1}{n} \sum_i \frac{\gamma_i,k(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i
\]

\[
= (x_{\text{new}} - \tilde{\Sigma}_k u_k)^T (\hat{\beta}_k - \beta_k) + u_k^T \frac{1}{n} \sum_i \frac{\gamma_i,k(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i.
\]

Recall the estimated Fisher information matrix constrained to \( \beta_k \) is given by

\[
\hat{\Gamma}_k^\beta(\theta) = \frac{1}{n} \sum_{i=1}^n \frac{\gamma_i^2(\theta)}{\sigma_k^2} \left( y_i - x_i^T \hat{\beta}_k \right)^2 x_i x_i^T,
\]

and define

\[
\hat{I}_k^\beta(\theta) = \mathbb{E} \left[ \frac{\gamma_i^2(\theta)}{\sigma_k^2} \left( y_i - x_i^T \hat{\beta}_k \right)^2 x_i x_i^T \right].
\]

We then have

\[
\frac{\sqrt{n}(\hat{\Gamma}_k^d - \Gamma_k)}{\sqrt{u_k^T \hat{\Gamma}_k^\beta(\theta) u_k}} = \frac{\sqrt{n} (x_{\text{new}} - \tilde{\Sigma}_k u_k)^T (\hat{\beta}_k - \beta_k)}{\sqrt{u_k^T \hat{\Gamma}_k^\beta(\theta) u_k}} + \frac{u_k^T \frac{1}{\sqrt{n}} \sum_i \frac{\gamma_i,k(\theta)}{\sigma_k^2} (y_i - x_i^T \hat{\beta}_k) x_i}{\sqrt{u_k^T \hat{\Gamma}_k^\beta(\theta) u_k}} + \frac{u_k^T \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{\gamma_i,k(\theta)}{\sigma_k^2} (y_i - x_i^T \hat{\beta}_k) x_i \text{ (term II)}}{\sqrt{u_k^T \hat{\Gamma}_k^\beta(\theta) u_k}} + \frac{\text{ (term III)}}{\sqrt{u_k^T \hat{\Gamma}_k^\beta(\theta) u_k}},
\]

where

\[
\text{term II} = u_k^T \frac{1}{n} \sum_i \frac{\gamma_i,k(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i - u_k^T \frac{1}{n} \sum_i \frac{\gamma_i,k(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i.
\]

We will proceed by stating three propositions which will be used to control terms I, II, and III. We defer the proof of these propositions to Section C.

The first proposition allows us to control the numerator of term I.

**Proposition A.2.** Let \( u_k \) be the solution to optimization (12) with \( \lambda_k \propto \eta_\text{est} \log(np) + \sqrt{\log(p)/n} \) and \( L \geq \| \Sigma_k^{-1} x_{\text{new}} \|_1 \). Under Assumption (A1) we have

\[
\left( x_{\text{new}} - \tilde{\Sigma}_k u_k \right)^T (\hat{\beta}_k - \beta_k) = O_p \left( \left( \eta_\text{est} \log(np) + \sqrt{\log(p)/n} \right) \eta_\text{est} \| x_{\text{new}} \|_2 \right).
\]

This proposition allows us to control the numerator of term I.
Proposition A.3. Under the assumptions of Theorem 3.1, there exist constants \( c, C > 0 \), such that
\[
\mathbf{u}_k^T \hat{I}_k^\beta(\hat{\theta}) \mathbf{u}_k \geq C \| \mathbf{x}_{\text{new}} \|_2^2.
\] (26)

Combining Propositions A.2 and A.3 we obtain
\[
\text{term I} = O_p \left( \left( \eta_{\text{est}} \sqrt{n \log(np)} + \sqrt{\log(p)} \right) \eta_{\text{est}} \right) = o_p(1),
\]
by Condition (A1), equation (22).

The next proposition controls term II.

Proposition A.4. Under the assumptions of Theorem 3.1,
\[
\left\| \frac{1}{n} \sum_{i=1}^n \left( \frac{\gamma_{i,k}(\hat{\theta})}{\sigma_k^2} - \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} \right) (y_i - x_i^T \beta_k) x_i \right\|_{\infty} = o_p(1).
\]

Therefore,
\[
\text{term II} \leq \left\| \frac{1}{n} \sum_{i=1}^n \left( \frac{\gamma_{i,k}(\hat{\theta})}{\sigma_k^2} - \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} \right) (y_i - x_i^T \beta_k) x_i \right\|_{\infty} \| \mathbf{u} \|_1 = o_p(\| \mathbf{x}_{\text{new}} \|_2).
\]

The next proposition controls the difference of the sample Fisher information at the estimated parameter \( \hat{I}_k^\beta(\hat{\theta}) \) and the true Fisher information \( I_k^\beta(\theta) \).

Proposition A.5. Under the assumptions of Theorem 3.1, and for \( \mathbf{u}_k \) the solution of optimization (12), we have
\[
\left\| \mathbf{u}_k^T \hat{I}_k^\beta(\hat{\theta}) \mathbf{u}_k - \mathbf{u}_k^T I_k^\beta(\theta) \mathbf{u}_k \right\| = o_p(\| \mathbf{x}_{\text{new}} \|_2^2). \tag{27}
\]

We next note that
\[
\nabla_{\beta_k} \ell(\theta) = \frac{1}{n} \sum_{i=1}^n \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i,
\]
and by asymptotic normality of the score functions, see e.g. Van der Vaart (2000), we have
\[
\frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i \overset{d}{\Rightarrow} N(0, I_k^\beta(\theta)).
\]

By sample splitting, \( \mathbf{u}_k \) is independent of \( \{(x_i, y_i)\} \) and therefore is also independent of \( \nabla_{\beta_k} \ell(\theta) \). By invoking Proposition A.5, and as an application of Slutsky’s Theorem, this implies that
\[
\frac{\mathbf{u}_k^T \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i}{\sqrt{\mathbf{u}_k^T \hat{I}_k^\beta(\hat{\theta}) \mathbf{u}_k}} \overset{d}{\Rightarrow} N(0, 1). \tag{28}
\]

Using the above distributional characterization, together with the bounds on terms I, II, III in decomposition (24), we obtain the desired result.
B Proof of Theorem 3.2

Let \( z_{\text{new}} \) denote the class of \( x_{\text{new}} \). Conditioning on \( z_{\text{new}} \) we have

\[
\mathbb{P}(y_{\text{new}} \in \Omega (x_{\text{new}}) | x_{\text{new}}) = \sum_{k=1}^{K} \mathbb{P}(y_{\text{new}} \in \Omega (x_{\text{new}}) | z_{\text{new}} = k, x_{\text{new}}) \mathbb{P}(z_{\text{new}} = k | x_{\text{new}})
\]

\[
= \sum_{k=1}^{K} \mathbb{P}(y_{\text{new}} \in \Omega (x_{\text{new}}) | z_{\text{new}} = k, x_{\text{new}}) \pi_k (x_{\text{new}})
\]

\[
= \sum_{k=1}^{K} \mathbb{P}(\Gamma_k + \varepsilon \in \Omega (x_{\text{new}}) | x_{\text{new}}) \pi_k (x_{\text{new}}), \tag{29}
\]

where we recall that \( \Gamma_k = x_{\text{new}}^T \beta_k \). Also \( \varepsilon \sim \mathcal{N}(0, \sigma_k^2) \) is independent of \( x_{\text{new}} \).

As shown in the proof of Theorem 3.1 we have

\[
\frac{\Gamma_k - \hat{\Gamma}_k^d}{\hat{V}_k^{1/2}} = W + \Delta,
\]

with \( W \sim \mathcal{N}(0, 1) \) and \( |\Delta| = o_p(1) \). Therefore,

\[
\frac{\Gamma_k + \varepsilon - \hat{\Gamma}_k^d}{b_k} = \frac{\hat{V}_k^{1/2}}{b_k} W + \frac{\sigma_k}{b_k} \varepsilon + \frac{\hat{V}_k^{1/2}}{b_k} \Delta
\]

\[
= c_k W' + \Delta',
\]

with \( W', \varepsilon \sim \mathcal{N}(0, 1) \) and \( |\Delta'| < |\Delta| = o_p(1) \) and \( c_k^2 := \frac{\hat{V}_k + \sigma_k^2}{b_k^2} \). Here we used the fact that \( W, \varepsilon \) are independent normal random variables.

Our procedure for constructing a prediction set returns a union of intervals: \( \Omega (x_{\text{new}}) = \bigcup_{k=1}^{K} \mathcal{L}_k(q) \) with \( \mathcal{L}_k(q) = [y_k^-, y_k^+] \). Since \( \mathcal{L}_k(q) \subseteq \Omega (x_{\text{new}}) \) we have

\[
\mathbb{P}(\Gamma_k + \varepsilon \in \Omega (x_{\text{new}})) = \mathbb{P}(\Gamma_k + \varepsilon \in \mathcal{L}_k(q))
\]

\[
= \mathbb{P} \left( \frac{\Gamma_k + \varepsilon - \hat{\Gamma}_k^d}{b_k} \in \left[ \frac{y_k^- - \hat{\Gamma}_k^d}{b_k}, \frac{y_k^+ - \hat{\Gamma}_k^d}{b_k} \right] \right)
\]

\[
= \mathbb{P} \left( c_k W' + \Delta' \in [l_k, u_k] \right), \tag{30}
\]

where we use the shorthands:

\[
l_k := \frac{y_k^- - \hat{\Gamma}_k^d}{b_k}, \quad u_k := \frac{y_k^+ - \hat{\Gamma}_k^d}{b_k}.
\]

Fix \( \gamma > 0 \) arbitrarily small. We write

\[
\mathbb{P} \left( c_k W' + \Delta' \in [l_k, u_k] \right) \geq \mathbb{P} \left( c_k W' \in [l_k + \gamma, u_k - \gamma] \right) - \mathbb{P}(|\Delta'| \geq \gamma)
\]

\[
\geq \mathbb{P} \left( W' \in [(1 + \gamma)(l_k + \gamma), (1 - \gamma)(u_k - \gamma)] \right) - \mathbb{P}(|\Delta'| \geq \gamma) - \mathbb{P} \left( \left| \frac{1}{c_k} - 1 \right| \geq \gamma \right).
\]
By taking the limit \( n \to \infty \) and using the fact that \(|\Delta'| = o_p(1)\) and \(|\hat{\sigma}_k - \sigma_k| = o_p(1)\) (Condition (A1)), we get

\[
\lim_{n \to \infty} P\left( c_k W' + \Delta' \in [l_k, u_k] \right) \geq P\left( W' \in [(1 + \gamma)(l_k + \gamma), (1 - \gamma)(u_k - \gamma)] \right) = \Phi((1 - \gamma)(u_k - \gamma)) - \Phi((1 + \gamma)(l_k + \gamma)).
\]

Since \( \gamma > 0 \) was arbitrarily small and the left-hand side does not depend on \( \gamma \), by taking \( \gamma \to 0 \), we arrive at

\[
\lim_{n \to \infty} P\left( c_k W' + \Delta' \in [l_k, u_k] \right) \geq \Phi(u_k) - \Phi(l_k). \tag{31}
\]

Using equations (30), (31) in (29) we obtain

\[
\lim_{n \to \infty} P(y_{\text{new}} \in \Omega_q(x_{\text{new}})) \geq K \sum_{k=1}^K (\Phi(u_k) - \Phi(l_k)) \pi_k(x_{\text{new}})
\]

\[
= \sum_{k=1}^K \pi_k(x_{\text{new}}) \int_{l_k}^{u_k} \phi(t) dt
\]

\[
= \sum_{k=1}^K \frac{\hat{\pi}_k(x_{\text{new}})}{b_k} \int_{y_k^-}^{y_k^+} \phi\left( \frac{y - \hat{\Gamma}_k}{b_k} \right) dy
\]

\[
= \sum_{k=1}^K \int_{y_k^-}^{y_k^+} f(y) dy
\]

\[
= \delta \sum_{i=1}^N h_{i(i)} - \text{Err}
\]

\[
\geq (1 - q) - \text{Err},
\]

where \( \text{Err} \) is the approximation error for replacing the integral with the Riemann sum. To bound \( \text{Err} \) we need to upper bound the second derivative of \( f(y) \). Define the function \( g_a(z) = \frac{1}{a^3} \phi\left( \frac{z}{a} \right) \). We have

\[
|g''(z)| = \frac{1}{a^3} \left| \frac{z^2}{a^2} - 1 \right| \phi\left( \frac{z}{a} \right) \leq 0.18 \frac{1}{a^3}.
\]

Therefore,

\[
|f''(y)| = \left| \sum_{k=1}^K \frac{\hat{\pi}_k(x_{\text{new}})}{b_k} \phi\left( \frac{y - \hat{\Gamma}_k}{b_k} \right) \right| \leq \sum_{k=1}^K \frac{0.18 \hat{\pi}_k(x_{\text{new}})}{b_k} \leq \frac{0.18}{\min_k(b_k)},
\]

where we used the observation that \( \sum_{k=1}^K \hat{\pi}_k(x_{\text{new}}) = 1 \). Therefore, the approximation error over an interval of size \( N\delta \) is bounded as

\[
\text{Err} \leq \frac{0.18}{\min_k(b_k)} \frac{(N\delta)^3}{24N^2} = 0.0075 \frac{N\delta^3}{\min_k(b_k)}. \tag{32}
\]

We also note that the returned prediction set is a subset of the initial interval \( Q \) of length \( \text{Len}(Q) \) which implies that \( N\delta \leq \text{Len}(Q) \). Hence,

\[
\text{Err} \leq 0.0075 \frac{\delta^2}{\min_k(b_k)} \leq \gamma,
\]

by our choice of \( \delta \leq 11 \sqrt{\gamma \min_k(b_k)/\text{Len}(Q)} \).
C  Proof of Propositions

C.1  Proof of Proposition A.1

We prove the feasibility of the optimization problem by showing there exists \( u \) such that

\[
\sup_{w \in C} \left| \langle w, \tilde{\Sigma}_k u - x_{\text{new}} \rangle \right| \leq \lambda_k \| x_{\text{new}} \|_2 \quad \text{and} \quad \| u \|_1 \leq L \| x_{\text{new}} \|_2
\]

is satisfied for \( \lambda_k \approx \eta_{\text{est}} \log(np) + \sqrt{\log(p)/n} \) and \( C = \{ e_1, \ldots, e_p, x_{\text{new}}/\| x_{\text{new}} \|_2 \} \).

Recall the following quantities:

\[
\tilde{\Sigma}_k = \frac{1}{n} \sum_{i=1}^{n} \gamma_{ik}(\hat{\theta}) x_i x_i^T,
\]

\[
\Sigma^*_k = \frac{1}{n} \sum_{i=1}^{n} \gamma_{ik}(\theta) x_i x_i^T,
\]

\[
\Sigma_k = \mathbb{E} \left[ \frac{\gamma_{1k}(\theta)}{\sigma_k^2} x_1 x_1^T \right].
\]

Take \( u = \Sigma_k^{-1} x_{\text{new}} \). By the assumption on \( L \) stated in the statement of the proposition, we have \( \| u \|_1 \leq L \| x_{\text{new}} \|_2 \). To show that the other constraint is satisfied we leverage Lemma D.6 for the set \( C \) which implies that

\[
\sup_{\xi \in C} \left\| (\tilde{\Sigma}_k - \Sigma^*_k) \xi \right\|_\infty = O_p \left( \eta_{\text{est}} \log(np) \right),
\]

\[
\sup_{\xi \in C} \left\| (\Sigma_k - \Sigma^*_k) \xi \right\|_\infty = O_p \left( \sqrt{\log(p)/n} \right).
\]

Combining the above two inequalities we get

\[
\sup_{\xi \in C} \left\| (\tilde{\Sigma}_k - \Sigma_k) \xi \right\|_\infty = O_p \left( \eta_{\text{est}} \log(np) + \sqrt{\log(p)/n} \right). \tag{33}
\]

For any \( w \in C \),

\[
\langle w, \tilde{\Sigma}_k u - x_{\text{new}} \rangle = \langle w, \tilde{\Sigma}_k u - \Sigma_k u \rangle \\
\leq \left\| (\tilde{\Sigma}_k - \Sigma_k) w \right\|_\infty \| u \|_1 \\
\leq O_p \left( \eta_{\text{est}} \log(np) + \sqrt{\log(p)/n} \right) L \| x_{\text{new}} \|_2 \\
\leq \lambda_k \| x_{\text{new}} \|_2,
\]

where in the second inequality we used (33). This completes the proof of the feasibility claim.
C.2 Proof of Proposition A.2

As proved in Proposition A.1, for the choice of \( \lambda_k \approx \eta_{\text{est}} \log(np) + \sqrt{\log(p)/n} \) and \( L \geq \frac{\|\Sigma_k^{-1}x_{\text{new}}\|_2}{\|x_{\text{new}}\|_2} \), optimization problem (12) is feasible. The claim follows readily from the constraints of this optimization problem. Specifically,

\[
\left| \left( x_{\text{new}} - \hat{\Sigma}_k u_k \right)^T (\hat{\beta}_k - \beta_k) \right| \leq \|x_{\text{new}} - \hat{\Sigma}_k u_k\|_\infty \|\hat{\beta}_k - \beta_k\|_1 \\
\leq \lambda_k \|x_{\text{new}}\|_2 \|\hat{\beta}_k - \beta_k\|_1 \\
\leq O_p \left( \left( \eta_{\text{est}} \log(np) + \sqrt{\log(p)/n} \right) \eta_{\text{est}} \|x_{\text{new}}\|_2 \right)
\]

where the first inequality follows from Hölder’s inequality (duality of \( \ell_1 - \ell_\infty \) norms).

C.3 Proof of Proposition A.3

We will use the proof strategy of Javanmard & Montanari (2014a, Lemma 3.1), which was also used in Cai et al. (2021, Lemma 1) and modified to account for the additional constraint (15). However, before doing that we need to deal with the challenge that in optimization (12) the objective function is based on \( \tilde{I}_{\beta} (\hat{\theta}) \), while the constraints are in terms of \( \tilde{\Sigma}_k \). We first relate \( u_k^T \tilde{I}_{\beta}(\hat{\theta}) u_k \) to \( u_k^T \tilde{\Sigma}_k u_k \).

We denote the first term in (6) by \( \tilde{Q}(\theta|\hat{\theta}) \), i.e.,

\[
\tilde{Q}(\theta|\hat{\theta}) = -\frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} \gamma_{i,k}(\hat{\theta}) \left[ \log \pi_{k}(x_i) + \log \phi_{k}(x_i, y_i) \right].
\]  
(34)

We restate a lemma from Wang et al. (2014) that allows us to connect the derivatives of the function \( \tilde{Q}(\theta|\hat{\theta}) \) with the derivatives of the log-likelihood \( \ell(\theta) \).

**Lemma C.1.** (Wang et al. 2014, Lemma 2.1) For the true parameter \( \theta \) and any \( \hat{\theta} \), it holds that

\[
\nabla_1 \tilde{Q}(\theta|\hat{\theta}) = \nabla_1 \ell(\hat{\theta}),
\]

\[
\mathbb{E}[\nabla^2_{1,1} \tilde{Q}(\theta|\theta) + \nabla^2_{1,2} \tilde{Q}(\theta|\theta)] = -\mathbf{I}(\theta),
\]

(36)

where \( \mathbf{I}(\theta) = -\mathbb{E}[\nabla^2 \ell(\theta)] \) is the Fisher information matrix and \( \nabla_1 \) and \( \nabla_2 \) denote differentiation with respect to \( \beta_k \) in the first and second arguments of \( \tilde{Q}(\cdot|\cdot) \), respectively.

Following the same argument as in the proof of (Zhang et al. 2020, Lemma 3), we have

\[
-\nabla^2_{1,2} \tilde{Q}(\theta|\theta) = -\frac{\partial^2}{\partial \beta_k \partial \beta'_k} \tilde{Q}(\theta|\theta')_{\theta' = \theta} \geq 0.
\]

(37)

Combining (36) and (37) we get

\[
\mathbf{I}^\beta_k(\theta) = -\mathbb{E}[\nabla^2_{1,1} \tilde{Q}(\theta|\theta) + \nabla^2_{1,2} \tilde{Q}(\theta|\theta)] \\
\geq -\mathbb{E}[\nabla^2_{1,1} \tilde{Q}(\theta|\theta)] \\
= \mathbb{E} \left[ \frac{\gamma_{1k}(\theta)}{\sigma_k^2} x_1 x_1^T \right] =: \Sigma_k,
\]

(38)
where in the last step we used the notations defined in Lemma D.6.

We next write the following chain of terms:
\[
\begin{align*}
  u_k^T T_k^g(\hat{\theta}) u_k &= u_k^T \tilde{\Sigma}_k u_k + u_k^T (I_k^g(\hat{\theta}) - \Sigma_k) u_k \\
  &+ u_k^T (\Sigma_k - \Sigma_k^t) u_k + u_k^T (\Sigma_k^t - \tilde{\Sigma}_k) u_k \\
  &+ u_k^T (I_k^g(\hat{\theta}) - I_k^g(\theta)) u_k \\
  &\geq u_k^T \tilde{\Sigma}_k u_k + u_k^T (I_k^g(\hat{\theta}) - \Sigma_k) u_k - O_p \left( \|x_{new}\|_2^2 \left\{ \log(p) \sqrt{\log p \over n} + \eta_{est} \log^3(p) \log(nK) \right\} \right) \\
  &\geq u_k^T \tilde{\Sigma}_k u_k - o_p(\|x_{new}\|_2^2),
\end{align*}
\]

where in the first inequality we used Lemma D.6 and Proposition A.5, together with the fact that \(\|u\|_1 \leq L\|x_{new}\|_2\). The last step in (39) follows from the condition \(\sqrt{n} \log(np) \eta_{est} = o(1)\) according to Assumption (A1), and the assumption \(\log(p) = o(n^{1/4}/\sqrt{\log(n)})\).

We next lower bound \(u_k^T \tilde{\Sigma}_k u_k\). For any feasible solution \(u\) of optimization (12) we have:
\[
  u^T \tilde{\Sigma}_k u \geq u^T \tilde{\Sigma}_k u + t((1 - \lambda_k)\|x_{new}\|_2^2 - x_{new}^T \tilde{\Sigma}_k x_{new}),
\]

for any \(t > 0\). The last inequality holds true because by the constraint of optimization (12), we have:
\[
  \|x_{new}\|_2^2 - x_{new}^T \tilde{\Sigma}_k x_{new} \leq \left| x_{new}^T \tilde{\Sigma}_k u - \|x_{new}\|_2^2 \right| \leq \|x_{new}\|_2^2 \lambda_k.
\]

Minimizing over all feasible \(u\) gives
\[
u_k^T \tilde{\Sigma}_k u_k \geq \min_u \left\{ u^T \tilde{\Sigma}_k u + t((1 - \lambda_k)\|x_{new}\|_2^2 - x_{new}^T \tilde{\Sigma}_k x_{new}) \right\}.
\]

The minimizer \(u^*\) satisfies \(\tilde{\Sigma}_k u^* = {\gamma(\hat{\theta}) \over 2} \Sigma_k x_{new}\). Substituting for \(u^*\), we obtain
\[
u_k^T \tilde{\Sigma}_k u_k \geq -t^2 \over 4 x_{new}^T \tilde{\Sigma}_k x_{new} + t(1 - \lambda_k) \|x_{new}\|_2^2.
\]

Optimizing this bound over \(t\), we get
\[
u_k^T \tilde{\Sigma}_k u_k \geq \left( 1 - \lambda_k \right)^2 \|x_{new}\|_2^4 \over x_{new}^T \Sigma_k x_{new},
\]

with the optimal choice \(t^* = 2(1 - \lambda_k)\|x_{new}\|_2^2 \over x_{new}^T \Sigma_k x_{new} > 0\).

Similar to the proof of Lemma D.6, D.7, we have \(\left| x_{new}^T \Sigma_k x_{new} - 1 \right| = O_p(\sqrt{\log p \over n})\), and hence \(u_k^T \tilde{\Sigma}_k u_k \geq C \|x_{new}\|_2^2\), which in conjunction with equation (39) gives the desired result.

### C.4 Proof of Proposition A.4

By the triangle inequality we have
\[
\left| \gamma_{i,k}(\hat{\theta}) - \gamma_{i,k}(\theta) \right| \leq \left| \gamma_{i,k}(\hat{\theta}) - \gamma_{i,k}(\hat{\theta}) \right| + \left| \gamma_{i,k}(\hat{\theta}) - \gamma_{i,k}(\hat{\theta}) \right|.
\]

(41)
The first term can be bounded as follows by recalling Condition (A1) on the error term \(|\tilde{\sigma}_k - \sigma_k|\):

\[
\left| \frac{\gamma_{i,k}(\tilde{\theta})}{\tilde{\sigma}_k^2} - \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} \right| = \left| \frac{\gamma_{i,k}^2(\tilde{\theta})}{\tilde{\sigma}_k^2} \cdot \frac{\sigma_k^2}{\sigma_k^2} - 1 \right| \leq \frac{1}{\sigma_k^2} \cdot \left| \frac{\sigma_k^2}{\sigma_k^2} - 1 \right| = O\left( |\sigma_k - \tilde{\sigma}_k| \right) = O_p(\eta_{est}),
\]

uniformly over all \(i \in [n]\), \(k \in [K]\). For the second term, by using Lemma D.3 together with Assumption (A1) on the error term \(\|\tilde{\theta} - \theta\|_1\) we get

\[
\sup_{i \in [n], k \in [K]} \left| \frac{\gamma_{i,k}(\tilde{\theta}) - \gamma_{i,k}(\theta)}{\sigma_k^2} \right| = O_p\left( \sqrt{\log(np)} \log(nK)\eta_{est} \right).
\]

Combining the above two bounds into (41) we get that

\[
\sup_{i \in [n], k \in [K]} \left| \frac{\gamma_{i,k}(\tilde{\theta})}{\sigma_k^2} - \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} \right| = O_p\left( \sqrt{\log(np)} \log(nK)\eta_{est} \right).
\]

Next, we observe that

\[
\| (y_i - x_i^T \beta_k)x_i \|_\infty \leq \max_{i,k} \| y_i - x_i^T \beta_k \| \cdot \max_i \| x_i \|_\infty = O_p\left( \sqrt{\log(nK)} \cdot \sqrt{\log(np)} \right)
\]

by Lemma D.2. Using this result combined with (42) gives the bound

\[
\left\| \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\gamma_{i,k}(\tilde{\theta})}{\sigma_k^2} - \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} \right) (y_i - x_i^T \beta_k)x_i \right\|_\infty
\leq \sup_{i \in [n], k \in [K]} \left| \frac{\gamma_{i,k}(\tilde{\theta})}{\sigma_k^2} - \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} \right| \cdot \frac{1}{n} \sum_{i=1}^{n} \| (y_i - x_i^T \beta_k)x_i \|_\infty
\]

\[
= O_p\left( \log(np) \log(nK)\eta_{est} \right)
\]

\[
= o_p\left( \sqrt{\log(np)} \cdot \log(nK) \cdot n^{-1/4} \right),
\]

where the last line follows from our assumption on the estimation rate \(\eta_{est}\), cf. equation (22). Finally note that by invoking the assumption \(\log(p) = o(n^{1/4}/\sqrt{\log(n)})\), the last term is \(o_p(1)\).

### C.5 Proof of Proposition A.5

Note that for a matrix \(A\) and a vector \(u\) we have

\[
|u^T Au| = \left| \sum_{ij} A_{ij} u_j u_j \right| \leq |A|_\infty \sum_{ij} |u_i||u_j| = |A|_\infty \|u\|_1^2.
\]

From Lemma D.7, \(\tilde{I}_k^\beta(\tilde{\theta}) - I_k^\beta(\theta)\|_\infty = O_p\left( \sqrt{\log^2(np) \log(nK)\eta_{est} + \log(np) \sqrt{\log(p)/n}} \right)\).

Given that \(\|u_k\|_1 \leq L\|x_{new}\|_2\) for a constant \(L\), and \(\sqrt{n} \log(np)\eta_{est}^2 = o(1)\) according to Assumption (A1) we have

\[
|u_k^T I_k^\beta(\tilde{\theta}) u_k - u_k^T I_k^\beta(\theta) u_k| = \|x_{new}\|_2^2 O_p\left( \log(np) \sqrt{\log(nK)n^{-1/4} + \log(np) \sqrt{\log(p)/n}} \right) = o_p(\|x_{new}\|_2^2),
\]

where the last step follows from the assumption \(\log(p) = o(n^{1/4}/\sqrt{\log(n)})\).
D Intermediate Lemmas and Proofs

This section summarizes several technical lemmas that were used in establishing our theoretical results.

The first lemma is a classical maximal inequality for sub-Gaussian random variables.

**Lemma D.1. (Maximal Inequality for Sub-Gaussians)** Let \( x = (x_1, \ldots, x_n) \) be a vector of zero-mean sub-Gaussian random variables with variances \( \nu_1^2, \ldots, \nu_n^2 \), respectively. Then, for any constant \( c > 0 \) we have

\[
\sup_{i=1, \ldots, n} |x_i| \leq v_{\max} \sqrt{2c \log n},
\]

with probability at least \( 1 - 2n^{1-c} \), where \( v_{\max} = \max_{i \in [n]} \nu_i \).

The above result is obtained by using the tail bound of sub-Gaussian variables, followed by a simple union bound, and therefore it does not require the random variables to be independent.

Our next lemma is a simple corollary of the above maximal inequality.

**Lemma D.2.** Define the following probability events:

\[
\mathcal{E}_1 := \left\{ \max_{i \in [n]} \|x_i\|_\infty \leq C \sqrt{\log(np)} \right\},
\]

\[
\mathcal{E}_2 := \left\{ \max_{i \in [n], k \in [K]} |y_i - x_i^T \beta_k| \leq C \sqrt{\log(nK)} \right\},
\]

and let \( \mathcal{E} := \mathcal{E}_1 \cap \mathcal{E}_2 \). Then, under Assumptions (A2)–(A3) we have \( \mathbb{P}(\mathcal{E}) \geq 1 - \frac{4}{n^2} \), for large enough constant \( C > 0 \).

**Proof.** we write \( x_{ir} = (\Sigma^{1/2} e_r, \Sigma^{-1/2} x_i) \). Therefore,

\[
\|x_{ir}\|_\psi^2 \leq \left\| \Sigma^{1/2} e_r \right\|_2 \left\| \Sigma^{-1/2} x_i \right\|_\psi \leq C_{\Sigma}^{1/2} \left\| \Sigma^{-1/2} x_i \right\|_\psi < \kappa,
\] (43)

for all \( r \in [p], i \in [n] \) and some constant \( \kappa < \infty \) by Assumption (A2). By Lemma D.1, and for sufficiently large constant \( C > 0 \), we get \( \mathbb{P}(\mathcal{E}_1) \geq 1 - \frac{2}{n^2} \).

To bound probability of \( \mathcal{E}_2 \), suppose that sample \( i \) belongs to group \( \ell \), by which we can write

\[
y_i - x_i^T \beta_k = x_i^T (\beta_\ell - \beta_k) + \varepsilon_i.
\]

We then have

\[
\|y_i - x_i^T \beta_k\|_\psi \leq \max_{\ell \in [K]} \|x_i^T (\beta_\ell - \beta_k) + \varepsilon_i\|_\psi \\
\leq \max_{\ell \in [K]} \left( \|x_i^T (\beta_\ell - \beta_k)\|_\psi + \|\varepsilon_i\|_\psi \right) \\
\leq \max_{\ell \in [K]} \left( \left\| \Sigma^{1/2} (\beta_\ell - \beta_k) \right\|_2 \left\| \Sigma^{-1/2} x_i \right\|_\psi + \sigma_\ell \right) \\
\leq \max_{\ell \in [K]} \left( C_{\Sigma} \left\| \beta_\ell - \beta_k \right\|_2 \left\| \Sigma^{-1/2} x_i \right\|_\psi + \sigma_\ell \right).
\]
Taking maximum over \(i,k\) from both sides, we get

\[
\sup_{i \in [n], k \in [K]} \| y_i - x_i^T \beta_k \|_{\psi_2} \leq C_{\Sigma} \left( \max_{i \in [n]} \| \Sigma^{-1/2} x_i \|_{\psi_2} \right) \left( \max_{k \in [K]} \| \beta_k \|_2 \right) + \max_{k \in [K]} \sigma_k. \tag{44}
\]

Recalling Assumptions (A2) and (A3), we get \(\sup_{i \in [n], k \in [K]} \| y_i - x_i^T \beta_k \|_{\psi_2} \leq \kappa'\), for some constant \(\kappa' < \infty\). Therefore, by another application of Lemma D.1, and for sufficiently large constant \(C > 0\), we get \(\mathbb{P}(E_2) \geq 1 - \frac{2}{n^2}\).

Combining the two probability bounds we get \(\mathbb{P}(E) \geq 1 - \mathbb{P}(E_1) - \mathbb{P}(E_2) \geq 1 - \frac{1}{n^2}\). \hfill \Box

While Assumption (A1) concerns the estimation error \(\| \hat{\theta} - \theta \|_1\), in our analysis we often need to control the perturbation of different functions of \(\theta\). A useful step for these bounds is a control on the Lipschitz factor of \(\gamma_{i,k}(\theta)\), which is the subject of the next lemma.

**Lemma D.3.** (Lipschitzness of \(\gamma_{i,k}(\theta)\)) On event \(\mathcal{E}\), defined in Lemma D.2, the Lipschitz factor of \(\gamma_{i,k}(\theta)\) with respect to the \(\ell_1\) norm is \(O_p(\log(np))\), uniformly over all \(i \in [n], \ k \in [K]\). As a result, we have

\[
\sup_{i \in [n], k \in [K]} \left\| \frac{\partial \gamma_{i,k}}{\partial \beta_k} \right\|_{\infty} \leq O_p(\sqrt{\log(np) \log(nK)}). \tag{45}
\]

**Proof.** To prove the claim, it suffices to show that

\[
\sup_{i \in [n], k \in [K]} \left( \left\| \frac{\partial \gamma_{i,k}}{\partial \beta_k} \right\|_{\infty}, \left\| \frac{\partial \gamma_{i,k}}{\partial \alpha_k} \right\|_{\infty}, \left\| \frac{\partial \gamma_{i,k}}{\partial \sigma_k} \right\|_{\infty} \right) = O_p(\sqrt{\log(np) \log(nK)}). \nonumber
\]

Recall that \(\gamma_{i,k}(\theta) = \frac{\pi_k(x_i) \phi_k(x_i, y_i)}{\sum_{\ell=1}^K \pi(\ell) \phi(\ell, y_i)}\), with \(\phi_k\) given by (5). A simple algebraic calculation shows that for a function of form \(f_k(z) = \sum_{\ell=1}^K c_{\ell} e^{\ell z}\), we have

\[
\frac{\partial}{\partial z_k} f_k(z) = f_k(z) - f_k^2(z). \tag{45}
\]

Applying this result, we obtain

\[
\frac{\partial \gamma_{i,k}}{\partial \beta_k} = (\gamma_{i,k} - \gamma_{i,k}^2) \frac{1}{\sigma_k^2} (y_i - x_i^T \beta_k) x_i. \nonumber
\]

Therefore, on the event \(\mathcal{E}\) we have

\[
\left\| \frac{\partial \gamma_{i,k}}{\partial \beta_k} \right\|_{\infty} \leq \frac{1}{\sigma_k^2} \left\| \gamma_{i,k} - \gamma_{i,k}^2 \right\| \left\| y_i - x_i^T \beta_k \right\| \left\| x_i \right\|_{\infty} \nonumber
\]

\[
\leq \frac{1}{\sigma_k^2} C^2 \sqrt{\log(np) \log(nK)} = O(\sqrt{\log(np) \log(nK)}), \nonumber
\]

where we used the definition of \(\mathcal{E}\) and the fact that since \(0 \leq \gamma_{i,k} \leq 1\), \(\gamma_{i,k}(1 - \gamma_{i,k}) \leq \frac{1}{4}\).

Similarly, we can bound the partial derivative with respect to \(\alpha_k\). By another application of (45), we obtain
\[
\frac{\partial \gamma_{i,k}}{\partial \alpha_k} = (\gamma_{i,k} - \gamma_{i,k}^2)x_i,
\]
\[
\left\| \frac{\partial \gamma_{i,k}}{\partial \alpha_k} \right\|_\infty \leq |\gamma_{i,k} - \gamma_{i,k}^2| \left\| x_i \right\|_\infty \leq \frac{1}{4} \left\| x_i \right\|_\infty = O(\sqrt{\log(np)}) \,
\]
\[
\sup_{i \in [n], k \in [K]} \left\| \frac{\partial \gamma_{i,k}}{\partial \alpha_k} \right\|_\infty \leq \sup_i \left\| x_i \right\|_\infty \leq O(\sqrt{\log(np)}).
\]

Finally, we bound the partial derivative with respect to \(\sigma_k\). By another application of (45), we obtain
\[
\left| \frac{\partial \gamma_{i,k}}{\partial \sigma_k} \right| = \frac{\gamma_{i,k} - \gamma_{i,k}^2}{\sigma_k^2} \left( y_i - x_i^T \beta_k \right)^2 = O(\log(nK)).
\]

This completes the proof. \(\square\)

**Lemma D.4.** (Mixture Estimation Error) On the event \(\mathcal{E}\), defined in Lemma D.2, we have
\[
\sup_{i \in [n], k \in [K]} \frac{\gamma_{i,k}(\hat{\theta}) - \gamma_{i,k}(\theta)}{\sigma_k^2} = O_p \left( \sqrt{\log(np) \log(nK)^\eta_{est}} \right).
\]

**Proof.** We have that
\[
\sup_{i \in [n], k \in [K]} \frac{\gamma_{i,k}(\hat{\theta}) - \gamma_{i,k}(\theta)}{\sigma_k^2} \leq \sup_{i,k} \frac{\gamma_{i,k}(\hat{\theta})}{\sigma_k^2} - \frac{\gamma_{i,k}(\theta)}{\sigma_k^2} \leq \sup_{i,k} \frac{1}{\sigma_k^2} - \frac{1}{\sigma_k^2} + \sup_{i,k} \frac{\gamma_{i,k}(\hat{\theta}) - \gamma_{i,k}(\theta)}{\sigma_k^2} \leq (a) + (b).
\]

For (a), we have
\[
(a) \leq \sup_k \left| \frac{1}{\sigma_k^2} - \frac{1}{\sigma_k^2} \right| = \sup_k \left| \sigma_k - \sigma_k \right| \sigma_k^2 + \sigma_k = O_p(\eta_{est}),
\]
by Assumption (A1) and (A3). For (b), as shown in Lemma D.3 we have
\[
\sup_{i,k} \left| \frac{\gamma_{i,k}(\hat{\theta}) - \gamma_{i,k}(\theta)}{\sigma_k^2} \right| \leq \frac{1}{\sigma_k^2} O_p \left( \sqrt{\log(np) \log(nK)^\eta_{est}} \right),
\]
where in the last step we used Assumption (A1) and (A3). \(\square\)

The next lemma is a concentration result on the covariate vectors \(x_i\) which will be used in our analysis.

**Lemma D.5.** Let \(\{x_i\}_{i=1}^n\) satisfy Assumption (A2). Then for any fixed unit vector \(\xi\) we have
\[
P \left\{ \sup_{\ell \in [p]} \left| \frac{1}{n} \sum_{i=1}^n x_{i,\ell}(x_i, \xi) - \mathbb{E}[x_{i,\ell}(x_i, \xi)] \right| \geq t \right\} \leq 2p \exp \left( -c \min \left( \frac{nt^2}{C^2}, \frac{nt}{C} \right) \right),
\]
and
\[
\mathbb{E}[x_{i,\ell}(x_i, \xi)] \leq C,
\]
for some positive constant \(C\).
Proof. To obtain the first result, we first note that $|x_i,\ell(x_i, \xi)|$ is a product of two sub-Gaussian random variables and thus is a sub-exponential variable. Applying Theorem 2.8.1 of Vershynin (2018) to a fixed $\ell \in [p]$, we get that for $C \geq \max_{i \in [n]} \|x_i,\ell(x_i, \xi)\|_{\psi_1}$,

$$
P\left\{ \left| \frac{1}{n} \sum_{i=1}^{n} |x_i,\ell(x_i, \xi)| - \mathbb{E}|x_i,\ell(x_i, \xi)| \right| \geq t \right\} \leq 2 \exp \left( -c \min\left( \frac{nt^2}{C^2}, \frac{nt}{C} \right) \right),$$

(46)

where $\| \cdot \|_{\psi_1}$ is the sub-exponential norm of a random variable and $c > 0$ is an absolute constant.

To obtain our intended bound, we compute the sub-exponential norms $\|x_i,\ell(x_i, \xi)\|_{\psi_1}$. By Lemma 2.7.7 of Vershynin (2018), we have

$$
\|x_i,\ell(x_i, \xi)\|_{\psi_1} \leq \|x_i,\ell\|_{\psi_2} \|x_i, \xi\|_{\psi_2} = \left\| (\Sigma^{1/2} e_{\ell}, \Sigma^{-1/2} x_i) \right\|_{\psi_2} \left\| (\Sigma^{1/2} \xi, \Sigma^{-1/2} x_i) \right\|_{\psi_2} \leq C' C_{\Sigma} =: C,
$$

(47)

where we used that $\|\Sigma\|_{op} \leq C_{\Sigma}$ and $\|\Sigma^{-1/2} x_i\|_{\psi_2} \leq C'$, for some constants $C', C_{\Sigma}$, per Assumption (A2).

To prove the second part of the lemma, we note that by definition

$$
\|x_i,\ell(x_i, \xi)\|_{\psi_1} = \sup_{q \geq 1} q^{-1} \mathbb{E}|x_i,\ell(x_i, \xi)|^q \right|^{1/q},
$$

by which we have

$$
\mathbb{E}|x_i,\ell(x_i, \xi)| \leq \|x_i,\ell(x_i, \xi)\|_{\psi_1} \leq C,
$$

for all $\ell \in [p]$.

\[\square\]

Lemma D.6. (Covariance Matrix Estimation Error) Let

$$
\hat{\Sigma}_k = \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\hat{\theta})}{\hat{\sigma}_k^2} x_i x_i^T, \\
\Sigma^*_k = \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\theta)}{\sigma_k^2} x_i x_i^T, \\
\Sigma_k = \mathbb{E}\left[ \frac{\gamma_{1k}(\theta)}{\sigma_k^2} x_1 x_1^T \right].
$$

Consider a set of unit-norm vectors $C = \{\xi_1, \ldots, \xi_m\}$, for a fixed integer $m \geq 1$. Under Assumption (A2), and on the event $E$ defined in Lemma D.2, we have

$$
\sup_{\xi \in C} \left\| (\hat{\Sigma}_k - \Sigma^*_k) \xi \right\|_\infty = O_p \left( \eta_{\text{est}} \sqrt{\log(np) \log(nK)} \right),
$$

and

$$
\sup_{\xi \in C} \left\| (\Sigma_k - \Sigma^*_k) \xi \right\|_\infty = O_p \left( \sqrt{\frac{\log p}{n}} \right).
$$
Proof. We have
\[
\sup_{\xi \in C} \| (\hat{\Sigma}_k - \Sigma_k^*) \xi \|_\infty \leq \sup_{\ell \in [p], \xi \in C} \frac{1}{n} \sum_{i=1}^{n} \left| \frac{\gamma_{ik}(\hat{\theta})}{\sigma_k^2} - \frac{\gamma_{ik}(\theta)}{\sigma_k^2} \right| |x_{i,\ell}| \| (x_i, \xi) \|.
\]

For the first component, we leverage Lemma D.4, which proves a $O_p(\eta_{est} \sqrt{\log(np) \log(nK)})$ bound. For the second component, we use Lemma D.5 with $t = C \sqrt{\frac{2m \log(p)}{cn}}$ and union bound over the set $C$, which gives

\[
\sup_{\ell \in [p], \xi \in C} \frac{1}{n} \sum_{i=1}^{n} |x_{i,\ell}| \| (x_i, \xi) \| = O_p \left( 1 + \sqrt{\frac{\log p}{n}} \right) = O_p(1).
\]

Putting them together, we have
\[
\sup_{\xi \in C} \| (\hat{\Sigma}_k - \Sigma_k^*) \xi \|_\infty = O_p \left( \eta_{est} \sqrt{\log(np) \log(nK)} \right).
\]

To prove the second result, we have
\[
\sup_{\ell \in [p], \xi \in C} \| (\Sigma_k^* - \Sigma_k) \xi \|_\infty \leq \sup_{\ell \in [p], \xi \in C} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{\gamma_{ik}(\theta)}{\sigma_k^2} x_{i,\ell} (x_i, \xi) - \mathbb{E} \left[ \frac{\gamma_{ik}(\theta)}{\sigma_k^2} x_{i,\ell} (x_i, \xi) \right] \right\} \right|.
\]

As shown in (47), $x_{i,\ell} (x_i, \xi)$ have bounded sub-exponential norm and since $\frac{\gamma_{ik}(\theta)}{\sigma_k^2}$ is bounded, we have that $\frac{\gamma_{ik}(\theta)}{\sigma_k^2} x_{i,\ell} (x_i, \xi)$ has bounded sub-exponential norm. Therefore, by Theorem 2.8.1 of Vershynin (2018) (similar to Lemma D.5) and a union bound over $\ell \in [p]$ and $\xi \in C$, we obtain,
\[
\sup_{\ell \in [p], \xi \in C} \left| \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{\gamma_{ik}(\theta)}{\sigma_k^2} x_{i,\ell} (x_i, \xi) - \mathbb{E} \left[ \frac{\gamma_{ik}(\theta)}{\sigma_k^2} x_{i,\ell} (x_i, \xi) \right] \right\} \right| = O_p \left( \sqrt{\frac{\log p}{n}} \right),
\]

which completes the proof of the second part. \qed

Lemma D.7. (Fisher Information Estimation Error) Let
\[
\tilde{I}_k(\hat{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\hat{\theta})}{\sigma_k^2} \left( y_i - x_i^T \hat{\beta}_k \right)^2 x_i x_i^T,
\]
\[
\tilde{I}_k^*(\theta) = \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\theta)}{\sigma_k^2} \left( y_i - x_i^T \beta_k \right)^2 x_i x_i^T,
\]
\[
\tilde{I}_k(\theta) = \mathbb{E} \left[ \frac{\gamma_{ik}(\theta)}{\sigma_k^2} \left( y_i - x_i^T \beta_k \right)^2 x_i x_i^T \right].
\]

Under Assumptions (A1), (A2) and (A3), We have
\[
\left| \tilde{I}_k^*(\hat{\theta}) - \tilde{I}_k^*(\theta) \right|_\infty = O_p \left( \sqrt{\log^3(np) \log(nK)} \eta_{est} \right).
\]
and

\[ |\hat{I}_k^\beta(\theta) - I_k^\beta(\theta)|_\infty = O_p\left(\log(np)\sqrt{\frac{\log(p)}{n}}\right). \]

**Proof.** We have

\[ |\hat{I}_k^\beta(\theta) - I_k^\beta(\theta)|_\infty \leq \sup_{\ell, r \in [p]} \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\gamma^2_{ik}(\theta)}{\sigma^2_k} \left( y_i - x_i^T \hat{\beta}_k \right)^2 - \frac{\gamma^2_{ik}(\theta)}{\sigma^2_k} \left( y_i - x_i^T \beta_k \right)^2 \right) \left| x_{i, \ell} \right| |x_{i, r}| \]

\[ \leq \left( \sup_{i \in [n]} \left| \frac{\gamma^2_{ik}(\theta)}{\sigma^2_k} \left( y_i - x_i^T \hat{\beta}_k \right)^2 \right| \right) \left( \sup_{\ell, r \in [p]} \frac{1}{n} \sum_{i=1}^{n} |x_{i, \ell}| |x_{i, r}| \right) \]

\[ \leq \left( \sup_{i \in [n]} \left| \frac{\gamma^2_{ik}(\theta)}{\sigma^2_k} \left( y_i - x_i^T \hat{\beta}_k \right)^2 \right| \right) \left( \sup_{i \in [n]} \left| \frac{1}{\sigma^2_k} \left( y_i - x_i^T \beta_k \right)^2 \right| \right) \left( \sup_{i \in [n]} \left| \frac{1}{\sigma^2_k} \left( y_i - x_i^T \hat{\beta}_k \right)^2 \right| \right) \]

\[ \cdot \left( \sup_{\ell, r \in [p]} \frac{1}{n} \sum_{i=1}^{n} |x_{i, \ell}| |x_{i, r}| \right). \]

On the event \( E \) we have that

\[ \sup_{i \in [n], k \in [K]} |y_i - x_i^T \beta_k| \leq \sup_{i \in [n], k \in [K]} |y_i - x_i^T \beta_k| + \sup_{i \in [n], k \in [K]} |x_i^T (\beta_k - \hat{\beta}_k)| \]

\[ \leq C \sqrt{\log(nK)} + \left( \sup_{i \in [n]} \|x_i\|_\infty \right) \left( \sup_{k \in [K]} \|\beta_k - \hat{\beta}_k\|_1 \right) \]

\[ \leq C \left( \sqrt{\log(nK)} + \sqrt{\log(np)\eta_{est}} \right) \]

\[ = O \left( \sqrt{\log(np)} \right). \tag{48} \]

Therefore part (a) can be bounded as follows:

\[ \sup_{i \in [n]} \left| \frac{\gamma^2_{ik}(\theta)}{\sigma^2_k} \left( y_i - x_i^T \hat{\beta}_k \right)^2 \right| \left( \sup_{i \in [n]} \left| \frac{1}{\sigma^2_k} \left( y_i - x_i^T \beta_k \right)^2 \right| \right) \left( \sup_{i \in [n]} \left| \frac{1}{\sigma^2_k} \left( y_i - x_i^T \hat{\beta}_k \right)^2 \right| \right) \]

\[ = O_p\left(\eta_{est} \log(np)\right), \]

where we used that \( \gamma_{i,k}(\hat{\theta}) \leq 1 \) and \( |\hat{\sigma}_k - \sigma_k| = O_p(\eta_{est}) \) per Assumption (A1).
For (b), we write

$$
\sup_{i \in [n]} \frac{1}{\sigma_k} \left| \gamma^{2}_{ik}(\hat{\theta}) \left( y_i - x_i^T \hat{\beta}_k \right) \right| - \gamma^{2}_{ik}(\theta) \left( y_i - x_i^T \beta_k \right)^2 \\
= \sup_{i \in [n]} \frac{1}{\sigma_k} \left| \gamma^{2}_{ik}(\hat{\theta}) \left( y_i - x_i^T \hat{\beta}_k \right) \right| - \gamma^{2}_{ik}(\theta) \left( y_i - x_i^T \beta_k \right)^2 + \gamma^{2}_{ik}(\hat{\theta}) \left( y_i - x_i^T \beta_k \right)^2 - \gamma^{2}_{ik}(\theta) \left( y_i - x_i^T \beta_k \right)^2 \\
\leq \sup_{i \in [n]} \frac{1}{\sigma_k} \left| \gamma^{2}_{ik}(\hat{\theta}) - \gamma^{2}_{ik}(\theta) \right| \left( y_i - x_i^T \beta_k \right)^2 + \sup_{i \in [n]} \frac{1}{\sigma_k} \left| \gamma^{2}_{ik}(\hat{\theta}) \left( x_i^T \hat{\beta}_k \right) \right| \left( y_i - x_i^T \beta_k + y_i - x_i^T \hat{\beta}_k \right) \\
\leq \sup_{i \in [n]} \frac{2}{\sigma_k} \left| \gamma^{2}_{ik}(\hat{\theta}) - \gamma^{2}_{ik}(\theta) \right| \left( y_i - x_i^T \beta_k \right)^2 + \sup_{i \in [n]} \frac{1}{\sigma_k} \left\| x_i \right\| \left\| \hat{\beta}_k - \beta_k \right\| \left( y_i - x_i^T \beta_k + y_i - x_i^T \hat{\beta}_k \right) \\
= O(\log^{3/2}(np) \sqrt{\log(nK)\eta_{\text{test}}}) + O(\sqrt{\log(nK)} \log(np)\eta_{\text{test}}) \\
= O(\log^{3/2}(np) \sqrt{\log(nK)\eta_{\text{test}}}).
$$

where in the penultimate step, we bounded the first term using Lemma D.3 together with Assumption (A1) and we bounded the second term using definition of event $E$ along with (48).

Finally, for (c), we use Lemma D.5 with $\xi = e_r$ for $r \in [p]$ followed by a union bound over $r$ to get

$$
\sup_{\ell, r \in [p]} \frac{1}{n} \sum_{i=1}^{n} |x_{i, \ell}||x_{i, r}| = O_p(1).
$$

Putting (a), (b), and (c) together, we have

$$
\left| \hat{I}_k^{\beta}(\theta) - \hat{I}_k^{\beta}(\theta) \right|_{\infty} = O_p(\log^{3/2}(np) \sqrt{\log(nK)\eta_{\text{test}}}).
$$

To prove the second result, we have

$$
\mathbb{P} \left( \left| \hat{I}_k^{\beta}(\theta) - \hat{I}_k^{\beta}(\theta) \right|_{\infty} \geq t \right) \leq \mathbb{P} \left( \left| \hat{I}_k^{\beta}(\theta) - \hat{I}_k^{\beta}(\theta) \right|_{\infty} \geq t; E \right) + \mathbb{P}(E^c) \\
\leq \mathbb{P} \left( \left| \hat{I}_k^{\beta}(\theta) - \hat{I}_k^{\beta}(\theta) \right|_{\infty} \geq t; E \right) + \frac{4}{n^2},
$$

(49)
where we used the result of Lemma D.2 to bound $P(E^c)$. We next write

$$P\left(\left|\mathbf{I}_k^\beta(\theta) - \mathbf{I}_k^\beta(\theta)\right|_\infty \geq t; E\right)$$

$$= P\left(\sup_{\ell,r \in [p]} \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\theta)}{\sigma_k^2} (y_i - x_i^T \beta_k)^2 x_{i,\ell} x_{i,r} - \mathbb{E} \left[\frac{\gamma_{ik}(\theta)}{\sigma_k^4} (y_i - x_i^T \beta_k)^2 x_{i,\ell} x_{i,r}\right] \geq t; E\right)$$

$$\leq P\left(\sup_{i \in [n]} (y_i - x_i^T \beta_k)^2 \sup_{\ell,r \in [p]} \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r} - \mathbb{E} \left[\frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r}\right] \geq t; E\right)$$

$$\leq P\left(\sup_{\ell,r \in [p]} \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r} - \mathbb{E} \left[\frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r}\right] \geq \frac{t}{C^2 \log(np)}; E\right)$$

$$\leq P\left(\sup_{\ell,r \in [p]} \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r} - \mathbb{E} \left[\frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r}\right] \geq \frac{t}{C^2 \log(np)}\right), \quad (50)$$

where the second last step follows from definition of event $E$.

Now by using equation (47) with $\boldsymbol{\xi} = \mathbf{e}_r$, we have that $x_{i,\ell} x_{i,r}$ is sub-exponential and since $\frac{\gamma_{ik}(\theta)}{\sigma_k^4}$ is bounded, we get that $\frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r}$ is a sub-exponential random variable. Thus, by Bernstein’s inequality (see e.g. (Vershynin 2018, Theorem 2.8.1)) and union bound over the $p^2$ choices of $\ell, r$, we obtain,

$$P\left(\sup_{\ell,r \in [p]} \frac{1}{n} \sum_{i=1}^{n} \frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r} - \mathbb{E} \left[\frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r}\right] \geq \frac{t}{C^2 \log(np)}\right) \leq 2p^2 \exp\left(-c \frac{n t^2}{\log^2(np)}\right).$$

Therefore by choosing $t = 2 \sqrt{\frac{\log(p)}{cn}} \log(np)$ we obtain

$$P\left(\sup_{\ell,r \in [p]} \frac{1}{n} \sum_{i=1}^{n} \left|\frac{\gamma_{ik}(\theta)}{\sigma_k^4} x_{i,\ell} x_{i,r}\right| \geq \frac{2}{C^2} \sqrt{\frac{\log(p)}{cn}}\right) \leq 2p^{-2}. \quad (51)$$

Combining equations (49), (50) and (51) we arrive at

$$\left|\mathbf{I}_k^\beta(\theta) - \mathbf{I}_k^\beta(\theta)\right|_\infty = O_p \left(\log(np) \sqrt{\frac{\log(p)}{n}}\right),$$

which completes the proof of the second claim.

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