Aggregation of supports along the Lasso path

Pierre C. Bellec

Ensa-Crest

Abstract: In linear regression with fixed design, we propose two procedures that aggregate a data-driven collection of supports. The collection is a subset of the $2^p$ possible supports and both its cardinality and its elements can depend on the data. The procedures satisfy oracle inequalities with no assumption on the design matrix. Then we use these procedures to aggregate the supports that appear on the regularization path of the Lasso in order to construct an estimator that mimics the best Lasso estimator. If the restricted eigenvalue condition on the design matrix is satisfied, then this estimator achieves optimal prediction bounds. Finally, we discuss the computational cost of these procedures.

1. Introduction

Let $n, p$ be two positive integers. We consider the mean estimation problem

$$Y_i = \mu_i + \xi_i, \quad i = 1, \ldots, n,$$

where $\mu = (\mu_1, \ldots, \mu_n)^T \in \mathbb{R}^n$ is unknown, $\xi = (\xi_1, \ldots, \xi_n)^T$ is a subgaussian vector, that is,

$$\mathbb{E}[\exp(v^T \xi)] \leq \exp \frac{\sigma^2 |v|^2}{2} \quad \text{for all } v \in \mathbb{R}^n,$$

(1.1)

where $\sigma > 0$ is the noise level and $| \cdot |_2$ is the Euclidean norm in $\mathbb{R}^n$. We only observe $y = (Y_1, \ldots, Y_n)^T$ and wish to estimate $\mu$. A design matrix $X$ of size $n \times p$ is given and $p$ may be larger than $n$. We do not require that the model is well-specified, i.e., that there exists $\beta^* \in \mathbb{R}^p$ such that $\mu = X \beta^*$. Our goal is to find an estimator $\hat{\mu}$ such that the prediction loss $\|\hat{\mu} - \mu\|^2$ is small, where $\| \cdot \|^2$ is the empirical loss defined by

$$\|u\|^2 = \frac{1}{n} |u|^2 = \frac{1}{n} \sum_{i=1}^n u_i^2, \quad u = (u_1, \ldots, u_n)^T \in \mathbb{R}^n.$$

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In a high-dimensional setting where \( p > n \), the Lasso is known to achieve good prediction performance. For any tuning parameter \( \lambda > 0 \), define the Lasso estimate \( \hat{\beta}_\lambda \) as any solution of the convex minimization problem

\[
\hat{\beta}_\lambda \in \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2n} |y - \mathbb{X}\beta|^2 + \lambda |\beta|_1,
\]

(1.2)

where \( |\beta|_1 = \sum_{j=1}^n |\beta_j| \) is the \( \ell_1 \)-norm. If \( \mathbb{X}^T\mathbb{X}/n = I_{p \times p} \) where \( I_{p \times p} \) is the identity matrix of size \( p \), then an optimal choice of the tuning parameter is \( \lambda_{\text{univ}} \sim \sigma \sqrt{\log(p)/n} \), up to a numerical constant. If the Restricted Eigenvalue condition holds (cf. Definition 1 below), then the universal tuning parameter \( \lambda_{\text{univ}} \sim \sigma \sqrt{\log(p)/n} \) leads to good prediction performance [Bickel et al., 2009]. However, if the columns of \( \mathbb{X} \) are correlated and the Restricted Eigenvalue condition is not satisfied, the question of the optimal choice of the tuning parameter \( \lambda \) is still unanswered, even if the noise level \( \sigma^2 \) is known. Empirical and theoretical studies [van de Geer and Lederer, 2013, Hebiri and Lederer, 2013, Dalalyan et al., 2014] have shown that if the columns of \( \mathbb{X} \) are correlated, the Lasso estimate with a tuning parameter substantially smaller than the universal parameter leads to a prediction performance which is substantially better than that of the Lasso estimate with the universal parameter. To summarize, these papers raise the following question:

**Problem 1** (Data-driven selection of the tuning parameter). Find a data-driven quantity \( \hat{\lambda} \) such that the prediction loss \( \| \mathbb{X}\hat{\beta}_\lambda^L \|_2^2 \) is small with high probability.

In this paper, we focus on a different problem, namely:

**Problem 2** (Lasso Aggregation). Construct an estimator \( \hat{\mu} \) that mimics the prediction performance of the best Lasso estimator, that is, construct an estimator \( \hat{\mu} \) such that with high probability,

\[
\| \hat{\mu} - \mu \|^2 \leq C \min_{\lambda > 0} \left( \| \mathbb{X}\hat{\beta}_\lambda^L - \mu \|^2 + \Delta(\hat{\beta}_\lambda^L) \right),
\]

(1.3)

where \( C \geq 1 \) is a constant and \( \Delta(\hat{\beta}_\lambda^L) \) is a small quantity.

1 and 2 have the same goal, that is, to achieve a small prediction loss with high probability. In 1, the goal is to select a Lasso estimate that has small prediction loss. In 2, we look for an estimator \( \hat{\mu} \) such that the prediction performance of \( \hat{\mu} \) is almost as good as the prediction performance of any Lasso estimate. The estimator \( \hat{\mu} \) may be of a different form than \( \hat{\beta}_\lambda^L \) for some data-driven parameter \( \hat{\lambda} \).
Our motivation to consider \( M \) instead of \( J \) is the following. Let \( \mu_1, \ldots, \mu_M \) be deterministic vectors \( \mathbb{R}^n \). If the goal is to mimic the best approximation of \( \mu \) among \( \mu_1, \ldots, \mu_M \), it is well known in the literature on aggregation problems that an estimator of the form \( \hat{\mu} = f \hat{k} \) for some data-driven integer \( \hat{k} \) is suboptimal (cf. Theorem 2.1 in Rigollet and Tsybakov [2012], Section 2 of Juditsky et al. [2008] and Proposition 6.1 in Gerchinovitz [2011]). Thus, an optimal procedure cannot be valued in the discrete set \( \{ \mu_1, \ldots, \mu_M \} \). Optimal procedures for this problem are valued in the convex hull of the set \( \{ \mu_1, \ldots, \mu_M \} \). Examples are the Exponential Weights procedures proposed in Leung and Barron [2006], Dalalyan and Salmon [2012] or the Q-aggregation procedure of Dai et al. [2014].

Although a lot of progress has been made for various aggregation problems, to our knowledge no previous work deals with the problem of aggregation of nonlinear estimators such as the collection \( (X\hat{\beta}_\lambda)_{\lambda>0} \) based on the sample. In the setting of the present paper, the observation \( y \) and the Lasso estimates are not independent: no data-split is performed and the same data is used to construct the Lasso estimators and to aggregate them.

We will show that aggregation of nonlinear estimators of the form \( X\hat{\beta} \) is possible, for any nonlinear estimators \( \hat{\beta} \) and without any assumption on \( X \). For instance, an estimator \( \hat{\mu} \) that achieves (1.3) with

\[
\Delta(\beta) \simeq \frac{\sigma^2 |\beta|_0}{n} \log \left( \frac{ep}{|\beta|_0 \lor 1} \right)
\]

is given in Section 3. Here, \( |\beta|_0 \) denotes the number of nonzero coefficients of \( \beta \) and \( a \lor b = \max(a, b) \).

Given a design matrix \( X \), we call support any subset \( T \) of \( \{1, \ldots, p\} \). The cardinality of \( T \) is denoted by \( |T| \) and for \( \beta \in \mathbb{R}^p \), \( \text{supp}(\beta) \) is the set of indices \( k = 1, \ldots, p \) such that \( \beta_k \neq 0 \). Given a support \( T \), we denote by \( \Pi_T \) the square matrix of size \( n \) which is the orthogonal projection on the linear span of the columns of \( X \) whose indices belong to \( T \). Denote by \( \mathcal{P}\{1, \ldots, p\} \) the set of all subsets of \( \{1, \ldots, p\} \). We will consider the following problem.

**Problem 3** (Aggregation of a data-driven collection of supports). Let \( \hat{F} \) be a data-driven collection of supports, that is, an estimator valued in \( \mathcal{P}\{1, \ldots, p\} \). Construct an estimator \( \hat{\mu} \) such that with high probability,

\[
\| \hat{\mu} - \mu \|^2 \leq \min_{T \in \hat{F}} \left( \| \Pi_T \mu - \mu \|^2 + \Delta(T) \right),
\]

where \( \Delta(\cdot) \) is a function that takes small values.
The set $\hat{F}$ is a family of supports. Let us emphasize that both its cardinality and its elements can depend on the data $y$. Note that for any support $T$, $\Pi_T \mu = X_\beta^T$ where $\beta^T$ minimizes $|X\beta - \mu|^2$ subject to $\beta_k = 0$ for all $k \notin T$. In Section 3, we construct an estimator $\hat{\mu}$ that satisfies (1.4) with $\Delta(T) \simeq \sigma^2 |T| \log(p/|T|)/n$ for all nonempty supports $T$. In the literature on aggregation problems, one is given a collection of estimators $\{\hat{\mu}_1, ..., \hat{\mu}_M\}$ where $M \geq 1$ is a deterministic integer and the goal is to mimic the best estimator in this collection, cf. Tsybakov [2014] and the references therein. A novelty of the present paper is to consider aggregation of a collection of estimators, where the cardinality of the collection depends on the data.

The main contributions of the present paper are the following.

- In Section 2, we propose an estimator $\hat{\mu}_{\hat{F}, \hat{\sigma}^2}$ that satisfies the oracle inequality (1.4) with $\Delta(T) \simeq \hat{\sigma}^2 |T| \log(p/|T|)/n$ for all nonempty supports $T$, where $\hat{\sigma}^2$ is an estimator of the noise level. This estimator solves 3. We explain in Corollary 1 how Section 2 can be used to construct a procedure that aggregates nonlinear estimators of the form $X\hat{\beta}$.
- Section 3 is devoted to 2. Using the result from Section 2, we construct an estimator $\hat{\mu}$ that satisfies (1.3) with $\Delta(\beta) \simeq \sigma^2 |\beta|_0 \log(p/|\beta|_0)$. The computational complexity of the procedure is the sum of the complexity of the regularization path of the Lasso and the complexity of a convex quadratic program.

The proofs can be found in the appendix.

2. Aggregation of a data-driven family of supports

Throughout this section, let $\hat{F}$ be a data-driven collection of supports and let $\hat{\sigma}^2 \geq 0$ be a real valued estimator. Let $M$ be the cardinality of $\hat{F}$, and let $(\hat{T}_j)_{j=1, \ldots, M}$ be supports such that

$$\hat{F} = \{\hat{T}_1, \ldots, \hat{T}_M\}. \quad (2.1)$$

For all supports $T \subset \{1, \ldots, p\}$, define the weights [Rigollet and Tsybakov, 2012]

$$\pi_T := \left( H_p \left( \frac{p}{|T|} \right)^{e^{|T|}} \right)^{-1}, \quad H_p := \frac{e - e^{-p}}{e - 1}. $$

Note that by construction, the constant $H_p$ is greater than 1 and $\sum_{T \in \mathcal{P}(\{1, \ldots, p\})} \pi_T = 1$ where $\mathcal{P}(\{1, \ldots, p\})$ is the set of all subsets of $\{1, \ldots, p\}$. Given a support $T$,
the Least Squares estimator on the linear span of the covariates indexed by \( T \) is \( \Pi_T y \).

We will consider two estimators of \( \mu \) based on \( \hat{F} \) and \( \hat{\sigma}^2 \). The first estimator is defined as follows. Define the criterion

\[
\text{Crit}_{\hat{\sigma}^2}(T) = |y - \Pi_T y|^2 + 18\hat{\sigma}^2 \log \frac{1}{\pi_T}.
\]

We have

\[
|T| \leq \log \frac{1}{\pi_T} \leq \frac{1}{2} + 2|T| \log(ep/|T|) \quad (2.2)
\]

for any support \( T \). The lower bound is a direct consequence of \( H_p > 1 \) and the upper bound is proved in [Rigollet and Tsybakov, 2012, (5.4)]. As (2.2) holds, the above criterion is of the same nature as \( C_p \), AIC, BIC and their variants, cf. Birgé and Massart [2001]. Define the estimator

\[
\Pi_{T_{\hat{F},\hat{\sigma}^2}}(y) \quad \text{where} \quad T_{\hat{F},\hat{\sigma}^2} \in \text{argmin}_{T \in \hat{F}} \text{Crit}_{\hat{\sigma}^2}(T). \quad (2.3)
\]

The estimator (2.3) is the orthogonal projection of \( y \) onto the linear span of the columns of \( X \) whose indices are in \( T_{\hat{F},\hat{\sigma}^2} \). If \( \hat{F} \) is not data-dependent, the procedure \( \Pi_{T_{\hat{F},\hat{\sigma}^2}}(y) \) is close to the one studied in Birgé and Massart [2001].

We now define a second estimator valued in the convex hull of \( (\Pi_T y)_{T \in \hat{F}} \). Let \( \hat{M} \) be the cardinality of \( \hat{F} \), and let \( (\hat{T}_j)_{j=1,..,\hat{M}} \) be supports such that (2.1) holds. For any \( j = 1, ..., \hat{M} \), let \( \hat{\mu}_j = \Pi_{\hat{T}_j} y \). Define a simplex in \( \mathbb{R}^{\hat{M}} \) as follows:

\[
\Lambda^{\hat{M}} = \{ \theta \in \mathbb{R}^{\hat{M}}, \quad \sum_{j=1}^{\hat{M}} \theta_j = 1, \quad \forall j = 1, ..., \hat{M}, \quad \theta_j \geq 0 \}.
\]

For any \( \theta \in \mathbb{R}^{\hat{M}} \), define \( \hat{\mu}_\theta = \sum_{j=1}^{\hat{M}} \theta_j \hat{\mu}_j \). For all \( \theta \in \Lambda^{\hat{M}} \), let

\[
H_{F,\hat{\sigma}^2}(\theta) := |\hat{\mu}_\theta - y|^2 + \frac{1}{2} \text{pen}_Q(\theta) + 26\hat{\sigma}^2 \sum_{j=1}^{\hat{M}} \theta_j \log \frac{1}{\pi_{\hat{T}_j}}. \quad (2.4)
\]

where

\[
\text{pen}_Q(\theta) := \sum_{j=1}^{\hat{M}} \theta_j |\hat{\mu}_j - \hat{\mu}_\theta|^2. \quad (2.5)
\]

The penalty (2.5) is inspired by recent works on the \( Q \)-aggregation procedure [Dai et al., 2012], and it was used to derive sharp oracle inequalities for aggregation of linear estimators [Dai et al., 2014, Bellec, 2014a].
and density estimators [Bellec, 2014b]. The penalty pushes $\hat{\mu}_\theta$ towards the points $\{\hat{\mu}_1, ..., \hat{\mu}_M\}$. Finally, the term $\sum_{j=1}^M \theta_j \log \frac{1}{\pi_j}$ is another penalty that pushes the coordinate $\theta_j$ to 0 if the size of the support $\hat{T}_j$ is large.

Define the estimator $\hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2}$ as any minimizer of the function $H_{\hat{F}, \hat{\sigma}^2}$ defined in (2.4):

$$\hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2} := \hat{\mu}_{\hat{\theta}}, \quad \hat{\theta} \in \arg\min_{\theta \in \Lambda^M} H_{\hat{F}, \hat{\sigma}^2}(\theta).$$ (2.6)

**Theorem 1.** Let $n, p$ be positive integers and let $\sigma > 0$. Let $\mu \in \mathbb{R}^n$ and $X$ be any matrix of size $n \times p$. Let $\hat{F}$ be any data-driven collection of subsets of $\{1, ..., p\}$. Assume that the noise $\xi$ satisfies (1.1). Let $\hat{\sigma}^2$ be any real valued estimator and let $\delta := \mathbb{P}(\hat{\sigma}^2 < \sigma^2)$. Then for all $x > 0$, the estimator $\hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2}$ defined in (2.6) satisfies with probability greater than $1 - \delta - 2\exp(-x)$,

$$\|\hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2} - \mu\|^2 \leq \min_{T \in \hat{F}} \left( \|\Pi_T \mu - \mu\|^2 + \hat{\sigma}^2 \left( 24 + 96|T| \log \left( \frac{ep}{|T|} \sqrt[4]{1} \right) \right) + \frac{22\sigma^2 x}{n} \right).$$ (2.7)

Furthermore, the estimator $\Pi_{\hat{F}, \hat{\sigma}^2}(y)$ satisfies with probability greater than $1 - \delta - 2\exp(-x)$,

$$\|\Pi_{\hat{F}, \hat{\sigma}^2}(y) - \mu\|^2 \leq \min_{T \in \hat{F}} \left( 3\|\Pi_T \mu - \mu\|^2 + \frac{\hat{\sigma}^2}{n} \left( 26 + 104|T| \log \left( \frac{ep}{|T|} \sqrt[4]{1} \right) \right) + \frac{28\sigma^2 x}{n} \right).$$ (2.8)

In previously studied aggregation problems, one is given a collection of estimators $\{\hat{\mu}_1, ..., \hat{\mu}_M\}$ where $M \geq 1$ is a deterministic integer and the goal is to construct an estimator $\hat{\mu}$ such that with high probability,

$$\|\hat{\mu} - \mu\|^2 \leq \min_{j=1, ..., M} \|\hat{\mu}_j - \mu\|^2 + \Delta_n(M),$$

where $\Delta_n(M)$ is a small error term that increases with $M$, cf. Tsybakov [2014] and the references therein. Theorem 1 is of a different nature for several reasons. First, the set $\hat{F}$ is random, its cardinality can depend on the observed data $y$. Second, the error term that appears inside the minimum of (2.7) does not depend on the cardinality of $\hat{F}$.

The estimator $\hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2}$ of Theorem 1 with $\hat{\sigma}^2 = \sigma^2$ and $\hat{F}$ being the set of all subsets of $\{1, ..., p\}$ was previously studied as the Exponential Screening estimator [Rigollet and Tsybakov, 2011] or as the Sparsity Pattern Aggregate [Rigollet and Tsybakov, 2012]. In this special case, $\hat{F}$ is deterministic and contains all the $2^p$ possible supports. Because of this exponential number
of supports, computing the sparsity pattern aggregate in practice is hard. An MCMC algorithm is developed in Rigollet and Tsybakov [2011] to compute an approximate solution of the sparsity pattern aggregate, but to our knowledge there is no theoretical guarantee that this MCMC algorithm will converge to a good approximation in polynomial time. The Sparsity Pattern Aggregate satisfies (2.7) with $\hat{\sigma}^2 = \sigma^2$ and $\hat{F} = \mathcal{P}(\{1,...,p\})$. This sharp oracle inequality yields the minimax rate over all $\ell_q$ balls for all $0 < q \leq 1$, under no assumption on the design matrix $\mathbf{X}$ [Dai et al., 2014, Tsybakov, 2014].

To construct the estimator $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$, one has to solve the optimization problem (2.6). This is a convex quadratic program of size $|\hat{F}|$ with a simplex constraint. The complexity of computing $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$ is polynomial in the cardinality of $\hat{F}$. Thus, if $\hat{F}$ is small then it is possible to construct $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$ efficiently.

As the cardinality of $\hat{F}$ decreases, the prediction performance of the estimator $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$ becomes worse, but computing $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$ becomes easier.

**Problem 4.** Construct a data-driven set of supports $\hat{F}$ such that with high probability, there exists a support $T \in \hat{F}$ for which, simultaneously, the bias $\|\Pi_T \mu - \mu\|^2$ and the size $|T|$ are small.

If we can construct such a set $\hat{F}$, by (2.7) the prediction loss of the estimator $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$ will be small. Note that Theorem 1 needs no assumption on the data-driven set $\hat{F}$ and the design matrix $\mathbf{X}$.

In the following Corollary, we perform aggregation of a family of nonlinear estimators of the form $(\mathbf{X}\hat{\beta}_j)_{j \in J}$ for some set $J$. All estimators in the family share the same design matrix $\mathbf{X}$ and this matrix is deterministic.

**Corollary 1.** Let $n, p$ be positive integers and let $\sigma > 0$. Let $\mu \in \mathbb{R}^n$ and $\mathbf{X}$ be any matrix of size $n \times p$. Let $\hat{F}$ be any data-driven collection of subsets of $\{1,...,p\}$. Assume that the noise $\xi$ satisfies (1.1). Let $(\hat{\beta}_j)_{j \in J}$ be a family of estimators valued in $\mathbb{R}^p$. Both the cardinality of the family and its elements can depend on the data. Let $\hat{\sigma}^2$ be any real valued estimator and let $\delta := \mathbb{P}(\hat{\sigma}^2 < \sigma^2)$. Define $\hat{F} = \{\text{supp}(\hat{\beta}_j), j \in J\}$ and let $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$ be the estimator (2.6). Then for all $x > 0$, the estimator $\hat{\mu}_q^{\hat{F},\hat{\sigma}^2}$ satisfies with probability greater than $1 - \delta - 2\exp(-x)$,

$$
\|\hat{\mu}_q^{\hat{F},\hat{\sigma}^2} - \mu\|^2 \leq \min_{j \in J} \left( \|\mathbf{X}\hat{\beta}_j - \mu\|^2 + \frac{\hat{\sigma}^2}{n} \left( 24 + 96|\hat{\beta}_j|_0 \log \left( \frac{ep}{|\hat{\beta}_j|_0 \vee 1} \right) \right) + \frac{22\sigma^2 x}{n} \right).
$$

Using (2.8), a similar result can be readily obtained for the estimator
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Let us recall some properties of the Lasso path [Efron et al., 2004]. For a given observation $y$, there exists a positive integer $K$ and a finite sequence

$$\lambda_0 > \lambda_1 > ... > \lambda_K = 0$$

such that $\hat{\beta}_\lambda^l = 0$ for all $\lambda > \lambda_0$, and such that

$$\forall \lambda \in (\lambda_{k+1}, \lambda_k), \quad \text{supp}(\hat{\beta}_\lambda^l) = \text{supp}(\hat{\beta}_\lambda^l).$$

Thus, there is a finite number of supports on the Lasso path. In this section, we study the estimator of Theorem 1 in the special case $\hat{F} = \{\text{supp}(\hat{\beta}_\lambda^l), k = 0, ..., K\}$, that is, we aggregate all the supports that appear on the Lasso path.

**Theorem 2.** Let $n, p$ be positive integers and let $\sigma > 0$. Let $\mu \in \mathbb{R}^n$ and $X$ be any matrix of size $n \times p$. Assume that the noise $\xi$ satisfies (1.1). Let $\hat{\sigma}^2$ be any real valued estimator and let $\delta := \mathbb{P}(\hat{\sigma}^2 < \sigma^2)$. Let $\lambda_0 > ... > \lambda_K$ be the knots of the Lasso path. Let $\hat{F} = \{\text{supp}(\hat{\beta}_{\lambda_j}^l), j = 0, ..., K\}$ be the family of all supports that appear on the Lasso path and let $\hat{\mu}_{\hat{F}, \hat{\sigma}^2}^0$ be the estimator (2.6). Then for all $x > 0$, the estimator $\hat{\mu}_{\hat{F}, \hat{\sigma}^2}^0$ satisfies with probability greater than $1 - \delta - 2 \exp(-x)$,

$$\|\hat{\mu}_{\hat{F}, \hat{\sigma}^2}^0 - \mu\|^2 \leq \min_{\lambda > 0} \left( \|X\hat{\beta}_\lambda^l - \mu\|^2 + \frac{\hat{\sigma}^2}{n} \left( 24 + 96|\hat{\beta}_\lambda^l|_0 \log \left( \frac{ep}{|\hat{\beta}_\lambda^l|_0 \vee 1} \right) \right) \right) + \frac{22\sigma^2x}{n},$$

(3.1)

where for all $\lambda > 0$, $\hat{\beta}_\lambda^l$ is the Lasso estimator (1.2).

Using (2.8), a similar result can be readily obtained for the estimator $\Pi_{\hat{F}, \hat{\sigma}^2}(y)$ with the leading constant 3.

The computational complexity of the procedure of Theorem 2 is polynomial in the number of knots of the Lasso path. This will be further discussed in Section 4. In the rest of this section, we assume that $\hat{\sigma}^2 = \sigma^2$ and $\delta = 0$. We will come back to the estimation of the noise level in Section 5 below.

Interestingly, Theorem 2 does not need any assumption on the design matrix $X$. The estimators $\hat{\mu}_{\hat{F}, \hat{\sigma}^2}^0$ and $\Pi_{\hat{F}, \hat{\sigma}^2}(y)$ have a good performance as soon as for some possibly unknown $\lambda > 0$, both the support of $\hat{\beta}_\lambda^l$ and the loss $\|X\hat{\beta}_\lambda^l - \mu\|^2$ are small.
3.1. Prediction guarantees under the restricted eigenvalue condition

The goal of this section is to study the prediction performance of the procedure defined in Theorem 2 under the Restricted Eigenvalue condition on the design matrix $X$.

**Definition 1.** For any $s \in \{1, \ldots, p\}$ and $c_0 > 0$, condition $RE(s, c_0)$ is satisfied if

$$\kappa(s, c_0) := \min_{T \subset \{1, \ldots, p\}} \min_{|T| \leq s} \frac{|X\delta|_2}{\sqrt{n} |\delta_T|_2} > 0.$$

The following result is a reformulation of Bickel et al. [2009, Theorem 6.2].

**Theorem 3 (Bickel et al. [2009]).** Let $X$ be such that the diagonal elements of $X^TX/n$ are all equal to 1. Assume that $\mu = X\beta^*$ and let $s := |\beta^*|_0$. Assume that $\xi \sim N(0, \sigma^2 I_{n \times n})$ and that condition $RE(s, 3)$ is satisfied. Let $x_0 > 0$. There is an event $\Omega(x_0)$ of probability greater than $1 - e^{-x_0}$ on which the Lasso estimator (1.2) with tuning parameter $\lambda_{x_0} = \sigma \sqrt{8(x_0 + \log p)/n}$ satisfies simultaneously

$$|\hat{\beta}^l_{\lambda_{x_0}}|_0 \leq \frac{64 \phi_{\text{max}}}{\kappa^2(s, 3)} s,$$

$$\|X(\hat{\beta}^l_{\lambda_{x_0}} - \beta^*)\|_2 \leq \frac{128 \sigma^2 s(x_0 + \log p)}{\kappa^2(s, 3)n},$$

where $\phi_{\text{max}}$ is the largest eigenvalue of the matrix $X^TX/n$.

Thus, if the restricted eigenvalue condition is satisfied, the Lasso estimator with the universal parameter $\lambda_{x_0} = \sigma \sqrt{8(x_0 + \log p)/n}$ enjoys simultaneously an $\ell_0$ norm of the same order as the true sparsity (cf. (3.2)), and a prediction loss of order $s \log(p)/n$ (cf. (3.3)).

Theorem 4 below is a direct consequence of Theorem 2 and the bounds (3.2)-(3.3).

**Theorem 4.** Let $n, p$ be positive integers and let $\sigma > 0$. Let $\mu \in \mathbb{R}^n$ and $X$ be any matrix of size $n \times p$. Let $\hat{F}$ be any data-driven subset of $\{1, \ldots, p\}$. Assume that $\mu = X\beta^*$ and let $s := |\beta^*|_0$. Assume that $\xi \sim N(0, \sigma^2 I_{n \times n})$ and that condition $RE(s, 3)$ is satisfied.

Let $\lambda_0 > \ldots > \lambda_K$ be the knots of the Lasso path. Let $\hat{F} = \{\text{supp}(\hat{\beta}^l_{\lambda_j}), j = 0, \ldots, K\}$ be the family of all supports that appear on the Lasso path and let
\( \hat{\mu}_{F,\sigma^2}^{Q} \) be the estimator (2.6) with \( \hat{\sigma}^2 = \sigma^2 \). Then for all \( x > 0 \), the estimator \( \hat{\mu}_{F,\sigma^2}^{Q} \) satisfies with probability greater than \( 1 - 3\exp(-x) \),

\[
\| \hat{\mu}_{F,\sigma^2}^{Q} - X\beta^* \|^2 \leq \frac{(128 + 48\phi_{\text{max}})\sigma^2 s \log p}{\kappa^2(s,3)n} + \frac{24\sigma^2}{n} + \frac{128\sigma^2 s x}{\kappa^2(s,3)n} + \frac{22\sigma^2 x}{n}.
\]

Furthermore,

\[
E\| \hat{\mu}_{F,\sigma^2}^{Q} - X\beta^* \|^2 \leq \frac{(128 + 48\phi_{\text{max}})\sigma^2 s \log p}{\kappa^2(s,3)n} + \frac{384\sigma^2 s}{\kappa^2(s,3)n} + \frac{90\sigma^2}{n}.
\]

Using (2.8), a similar result can be readily obtained for the estimator \( \Pi_{\hat{F},\hat{\sigma}^2}(y) \) with different constants.

Proof of Theorem 4. By Theorem 2 with \( \delta = 0 \), there is an event \( \Omega_{\text{agg}}(x) \) of probability greater than \( 1 - 2\exp(-x) \) such that on \( \Omega_{\text{agg}}(x) \) we have

\[
\| \hat{\mu}_{F,\sigma^2}^{Q} - X\beta^* \|^2 \leq \| X(\hat{\beta}_{\lambda_x}^L - \beta^*) \|^2 + \frac{\sigma^2}{n} \left( 24 + 96|\hat{\beta}_{\lambda_x}^L|_0 \log \left( \frac{ep}{|\hat{\beta}_{\lambda_x}^L|_0 \lor 1} \right) \right) + \frac{22\sigma^2 x}{n}.
\]

Let \( \Omega(x) \) be the event defined in Theorem 3. Using the simple inequality \( \log(p/(|\hat{\beta}_{\lambda_x}^L|_0 \lor 1)) \leq \log p \), and the bounds (3.2)-(3.3), we obtain that (3.4) holds on the event \( \Omega_{\text{agg}}(x) \cap \Omega(x) \). By the union bound, the event \( \Omega_{\text{agg}}(x) \cap \Omega(x) \) has probability greater than \( 1 - 3e^{-x} \). Finally, (3.5) is obtained from (3.4) by integration.

The procedure studied in Theorem 4 aggregates the supports along the Lasso path using the procedure (2.6). A similar result holds for the estimator \( \Pi_{\hat{F},\hat{\sigma}^2}(y) \) with a leading constant equal to 3. Theorem 4 has the following implications.

First, if \( x > 0 \) is fixed, the prediction performance (3.4) of the estimator \( \hat{\mu}_{F,\sigma^2}^{Q} \) is similar to that of the Lasso with the universal tuning parameter \( \lambda_x \), up to a multiplicative factor that only involves numerical constants and the quantity \( \phi_{\text{max}} \). As soon as \( \phi_{\text{max}} \) (the operator norm of \( X^T X/n \)) is bounded from above by a constant, the estimator studied in Theorem 4 enjoys the best known prediction guarantees.

Second, Theorem 4 implies that the estimator \( \hat{\mu}_{F,\sigma^2}^{Q} \) satisfies the prediction bound (3.4) simultaneously for all confidence levels. That is, (3.4) holds for all \( x > 0 \) with probability greater than \( 1 - 3e^{-x} \), in contrast with the Lasso estimator with the universal parameter \( \lambda_{x_0} \) which depends on a fixed confidence level \( 1 - e^{-x_0} \). The Lasso estimator with the universal parameter
\( \lambda_{x_0} \) satisfies the prediction bound (3.3) only for the confidence level \( 1 - e^{-x_0} \), but to our knowledge it is not known whether the Lasso estimator with the universal parameter \( \lambda_{x_0} \) satisfies a similar bound for different confidence levels than \( 1 - e^{-x_0} \). In this regard, the estimator studied in Theorem 4 provides a strict improvement compared to the Lasso with the universal parameter.

Third, the estimator \( \hat{\mu}_{F,\sigma^2}^q \) of Theorem 4 satisfies the bound (3.5), that is, a prediction bound in expectation. Again, to our knowledge, it is not known whether the Lasso estimator with the universal parameter satisfies a similar bound in expectation.

Assuming that the bound (3.3) is tight and putting computational issues aside, the prediction performance of the procedure \( \hat{\mu}_{F,\sigma^2}^q \) of Theorem 4 is substantially better than the performance of the Lasso with the universal parameter, as soon as \( \phi_{max} \) is bounded from above by a constant.

An upper bound similar to (3.2) is given in [Belloni et al., 2014, Theorem 3 and Remark 3]. Namely, Belloni et al. [2014] prove that the square-root Lasso estimator with the universal tuning parameter \( \hat{\beta} \) satisfies \( |\hat{\beta}|_0 \leq C s \) with high probability, where \( s \) is the sparsity of the true parameter and \( C \) is a constant that depends on the sparse eigenvalues of the matrix \( \mathbf{X}^T \mathbf{X}/n \), cf. [Belloni et al., 2014, Condition P]. This upper bound can be used instead of (3.2) to prove results similar to (3.4) where \( \phi_{max} \) is replaced by a smaller constant that depends on the sparse eigenvalues of \( \mathbf{X}^T \mathbf{X}/n \).

4. Computational complexity of the Lasso path and \( \hat{\mu}_{F,\sigma^2}^q \)

Computing the estimator \( \hat{\mu}_{F,\sigma^2}^q \) of Theorem 2 is done in two steps:

1. Compute the full Lasso path and let \( \hat{\mathcal{F}} = \{ \text{supp}(\lambda_0), \ldots, \text{supp}(\lambda_K) \} \) be all the supports that appear on the Lasso path, where \( \lambda_0, \ldots, \lambda_K \) are the knots of the Lasso path.

2. Compute \( \hat{\mu}_{F,\sigma^2}^q \) as a solution of the quadratic program (2.6), where \( \hat{\mathcal{F}} \) is defined by Step 1.

(We assume that the complexity of computing \( \hat{\sigma}^2 \) is negligible compared to the complexity of Step 1 and Step 2 above). The time complexity of Step 2 is the complexity of a convex quadratic program of size \( |\hat{\mathcal{F}}| \leq K \), where \( K \) is the number of knots on the Lasso path. Thus, the global cost of computing the estimator \( \hat{\mu}_{F,\sigma^2}^q \) of Theorem 2 is polynomial in \( K \).

There exist efficient algorithms to compute the entire Lasso path [Efron et al., 2004]. However, Mairal and Yu [2012] proved that for some values of \( \mathbf{X} \) and \( \mathbf{y} \), the regularization path of the Lasso contains more than \( 3^p/2 \) knots. Hence,
for some design matrix \( X \) and some observation \( y \), an exact computation of the full Lasso path is not realizable in polynomial time. In order to fix this computational issue, Mairal and Yu [2012] propose an algorithm that computes an approximate regularization path for the Lasso. For some fixed \( \epsilon > 0 \), this algorithm is guaranteed to terminate with less than \( \mathcal{O}(1/\sqrt{\epsilon}) \) knots and the points on the approximate path have a duality gap smaller than \( \epsilon \). This approximation algorithm can be used instead of computing the exact Lasso path. That is, one may compute the estimator \( \hat{\mu}_{q,\hat{\sigma}^2} \), where \( \hat{\sigma}^2 \) is the collection of supports that appear on the approximate path computed by the algorithm of Mairal and Yu [2012].

Another solution to avoid computational issues is as follows. Let \( M \) be a positive integer. Instead of computing the Lasso path, one may consider a grid of tuning parameters \( \lambda_1, \ldots, \lambda_M > 0 \) and aggregate the supports of corresponding Lasso estimates \( \hat{\beta}_{\lambda_j} \). The advantage of this approach is twofold. First, for all \( j = 1, \ldots, M \) the Lasso estimate \( \hat{\beta}_{\lambda_j} \) can be computed by standard convex optimization solvers. Second, the time complexity of the procedure is guaranteed to be polynomial in \( M \) and \( p \). For any \( x > 0 \), by Corollary 1, this procedure satisfies, with probability greater than \( 1 - 3e^{-x} \)

\[
\| \hat{\mu}_{q,\hat{\sigma}^2} - \mu \|^2 \leq \min_{j=1,\ldots,M} \left( \| X \hat{\beta}_{\lambda_j} - \mu \|^2 + \frac{\hat{\sigma}^2}{n} \left( 24 + 96|\hat{\beta}_{\lambda_j}|_0 \log \left( \frac{e p}{|\hat{\beta}_{\lambda_j}|_0 \vee 1} \right) \right) + \frac{22\sigma^2 x}{n} \right).
\]

This oracle inequality is not as strong as (3.1). However, if at least one of the Lasso estimates \( \{ \hat{\beta}_{\lambda_j}, j = 1, \ldots, M \} \) enjoys a small prediction loss and a small \( \ell_0 \) norm, then the prediction loss of \( \hat{\mu}_{q,\hat{\sigma}^2} \) is also small.

5. A fully data-driven procedure using the Square-Root Lasso

This section proposes a fully data-driven procedure, based on the Square-Root Lasso. The choice of grid comes from the empirical and theoretical observations that for a correlated design matrix, there exists a tuning parameter smaller than the universal parameter which enjoys better prediction performance than the universal parameter [van de Geer and Lederer, 2013, Hebiri and Lederer, 2013, Dalalyan et al., 2014].

1. Let \( \lambda_{\max} = 2\sqrt{\log(p/0.01)/n} \) be the universal parameter of the Square-Root Lasso [Belloni et al., 2014] with confidence level 0.01.
2. Let \( \lambda_{\min} \) be a conservatively small value of the tuning parameter.
3. Let \( M \) be an integer.
4. Consider the geometric grid \( \{ \lambda_1, \ldots, \lambda_M \} \) such that
\[
\lambda_j = \lambda_{\min} \left( \frac{\lambda_{\max}}{\lambda_{\min}} \right)^{\left( (j-1)/M - 1 \right)}, \quad j = 1, \ldots, M.
\]

5. Compute the Square-Root Lasso estimators \( \hat{\beta}_{\lambda_1}^{\text{SQ}}, \ldots, \hat{\beta}_{\lambda_M}^{\text{SQ}} \) with parameters \( \lambda_1, \ldots, \lambda_M \) (it is possible to perform this computation simultaneously for all \( \lambda_1, \ldots, \lambda_M \), cf. Pham et al. [2014] and the references therein).

6. Let \( \hat{F} = \{ \text{supp}(\hat{\beta}_{\lambda_j}^{\text{SQ}}), j = 1, \ldots, M \} \) be the supports of the computed Square-Root Lasso estimators.

7. Let \( \hat{\sigma}^2 \) be the variance estimated by the Square-Root Lasso with the universal parameter \( \lambda_{\max} \).

8. For this choice of \( \hat{\sigma}^2 \) and \( \hat{F} \), return the estimator \( \hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2} \) or the estimator \( \Pi_{\hat{F}_q, \hat{\sigma}^2} (y) \).

This estimator \( \hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2} \) returned by this procedure enjoys the theoretical guarantee
\[
\| \hat{\mu}^Q_{\hat{F}, \hat{\sigma}^2} - \mu \|^2 \leq \min_{j=1,\ldots,M} \left( \| \hat{X} \hat{\beta}_{\lambda_j}^{\text{SQ}} - \mu \|^2 + \frac{\hat{\sigma}^2}{n} \left( 24 + 96 |\hat{\beta}_{\lambda_j}^{\text{SQ}}|_0 \log \left( \frac{ep}{|\hat{\beta}_{\lambda_j}^{\text{SQ}}|_0 \lor 1} \right) \right) \right) + \frac{22 \sigma^2 x}{n}
\]
with probability greater than \( 1 - 3e^{-x} \). A similar guarantee with leading constant 3 can be obtained for the estimator \( \Pi_{\hat{F}_q, \hat{\sigma}^2} (y) \) using (2.8).

6. Concluding remarks

We have presented two procedures (2.3) and (2.6) that aggregates a data-driven collection of supports \( \hat{F} \). These procedures satisfy the oracle inequalities given in Theorem 1 above, which is the main result of the paper. Sections 3 and 4 study the situation where \( \hat{F} \) is the collection of supports that appear along the Lasso path. These procedures may be used for other data-driven collections \( \hat{F} \) as well.

These procedures allow one to perform a trade-off between prediction performance and computational cost. If \( \hat{F} \) contains all the \( 2^p \) supports, these procedures achieve optimal prediction guarantees with no assumption on the design matrix \( X \), but can not be realized in polynomial time. On the other hand, if the cardinality of \( \hat{F} \) is small (say, polynomial in \( n \) and \( p \)), then it is possible to compute the estimators (2.3) and (2.6) in polynomial time. In view of (1.3), one should look for a data-driven set \( \hat{F} \) with the following properties.
1. The set $\hat{F}$ is small so that the estimators (2.6) and (2.3) can be computed rapidly,
2. The set $\hat{F}$ contains a support $T$ such that $|T|$ and $\|\pi_T\mu - \mu\|^2$ are simultaneously small, so that the procedures (2.6) and (2.3) enjoy good prediction performance.

A natural choice for $\hat{F}$ is the collection of supports that appear along the Lasso path. This choice of $\hat{F}$ was studied in Sections 3 and 4. Another natural choice is to aggregate the supports of several hard-thresholded Lasso estimators, since the hard-thresholded Lasso is sign-consistent under weak conditions on the design [Meinshausen and Yu, 2009, Definition 5 and Corollary 2]. Further research will investigate other means to construct a data-driven collection $\hat{F}$ such that the above two properties are satisfied.

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Appendix A: Proof of Theorem 1

For any matrix $A \in \mathbb{R}^{n \times n}$, define the operator norm of $A$ and the Frobenius norm of $A$ by

$$
\|A\|_2 := \sup_{|u|^2 = 1} |Au|_2, \quad \|A\|_F = \sqrt{\text{Tr}(A^T A)},
$$

respectively.

Proof of (2.7). For all $S, T \subset \{1, \ldots, p\}$, define the event

$$\Omega_{S,T} = \left\{ Z(S, T) \leq 4\sigma^2|S| + 22\sigma^2 \left( \log \frac{1}{\pi_S \pi_T} + x \right) \right\},$$

where

$$Z(S, T) = 2\xi^T (\Pi_S y - \Pi_T \mu) - \frac{1}{2} |\Pi_S y - \Pi_T y|^2. \quad (A.1)$$

Define the event $\mathcal{V} := \{\sigma^2 \geq \sigma^2\}$. On the event $\mathcal{A} := \mathcal{V} \cap (\cap_{S,T \subset \{1,\ldots,p\}} \Omega_{S,T})$, we have simultaneously for all supports $S, T$

$$Z(S, T) - 26\sigma^2 \log \frac{1}{\pi_S} - 42\sigma^2 \log \frac{1}{\pi_T} \leq 22\sigma^2 x + 4\sigma^2 |S| - 4\sigma^2 \log \frac{1}{\pi_S} \leq 22\sigma^2 x$$
where we have used that $\log \frac{1}{\pi_S} \geq |S|$, cf. (2.2). By Lemma 1, on the event $A$ we have

$$|\hat{\Sigma}_F^\alpha - \mu|_2^2 \leq \min_{T \in \hat{F}} \left( |\Pi_T \mu - \mu|_2^2 + (26\hat{\sigma}^2 + 22\sigma^2) \log \frac{1}{\pi_T} \right) + 22\sigma^2 x.$$ 

To obtain (2.7), we use (2.2) and the fact that on the event $V$, $26\hat{\sigma}^2 + 22\sigma^2 \leq 48\hat{\sigma}^2$.

It remains to bound from below the probability of the event $A$. Denote by $B$ the complement of any event $A$. We proceed with the union bound as follows,

$$\mathbb{P}(A^c) \leq \mathbb{P}(V^c) + \sum_{S,T \subset \{1,\ldots,p\}} \mathbb{P}(\Omega_{S,T}^c).$$

By definition, $\delta = \mathbb{P}(V^c)$ and for any $S, T \subset \{1,\ldots,p\}$, Lemma 2 with $t = x + \log \frac{1}{\pi_S \pi_T}$ yields that $\mathbb{P}(\Omega_{S,T}^c) \leq \pi_S \pi_T \exp(-x)$. As $\sum_{S,T \subset \{1,\ldots,p\}} \pi_S \pi_T = (\sum_{S \subset \{1,\ldots,p\}} \pi_S)^2 = 1$, we have established that

$$\mathbb{P}(A^c) \leq \delta + 2 \exp(-x).$$

The proof of (2.8) is close to the argument used in Birgé and Massart [2001], cf. [Giraud, 2015, Section 2.3] for a recent reference on model selection. The novelty of the present paper is to consider a data-driven collection of estimators.

**Proof of (2.8).** Let $\hat{\Lambda} = 18\hat{\sigma}^2$ and let $\hat{T} = \hat{T}_{\hat{F},\hat{\sigma}^2}$ for notational simplicity. By definition of $\Pi_{\hat{T}_{\hat{F},\hat{\sigma}^2}}(y) = \Pi_T y$, for all $T \in \hat{F}$ we have $\text{Crit}_{\hat{\sigma}^2}(\hat{T}) \leq \text{Crit}_{\sigma^2}(T)$ which can be rewritten as

$$|\Pi_{\hat{T}_{\hat{F},\hat{\sigma}^2}}(y) - \mu|_2^2 + \hat{\Lambda} \log \frac{1}{\pi_T} \leq |\Pi_T y - \mu|_2^2 + \hat{\Lambda} \log \frac{1}{\pi_T} + 2\xi^T(\Pi_T y - \Pi_T y),$$

$$\leq |\Pi_T \mu - \mu|_2^2 + \hat{\Lambda} \log \frac{1}{\pi_T} + 2\xi^T \Pi_T \xi + 2\xi^T (\Pi_T \mu - \Pi_T \mu) - |\Pi_T \xi|_2^2.$$  

Define the event $V := \{\hat{\sigma}^2 \geq \sigma^2\}$. For all $S, T \subset \{1,\ldots,p\}$, define

$$W(S) = 2\xi^T \Pi_S \xi - 10\sigma^2 \log \frac{1}{\pi_S},$$

$$W'(S, T) = 2\xi^T (\Pi_S \mu - \Pi_T \mu) - 8\sigma^2 \log \frac{1}{\pi_S \pi_T} - \frac{1}{4} |\Pi_S \mu - \Pi_T \mu|_2^2.$$
With this notation, using the simple inequality $-|\Pi_T \xi|^2 \leq 0$, (A.2) implies that on the event $\mathcal{V}$,

$$|\Pi_{F,\sigma^2}(y) - \mu|^2 \leq |\Pi_T \mu - \mu|^2 + \Lambda \log \frac{1}{\pi_T} + 8\sigma^2 \log \frac{1}{\pi_T} + W(\hat{T}) + W'(\hat{T}, T) + \frac{1}{4}|\Pi_T \mu - \Pi_T \mu|^2,$$

Using that $|\Pi_T \mu - \Pi_T \mu|^2 \leq 2|\Pi_T \mu - \mu|^2 + 2|\mu - \Pi_T \mu|^2$ and that $|\Pi_T \mu - \mu|^2 \leq |\Pi_T y - \mu|^2$, we obtain

$$\frac{1}{2}|\Pi_{F,\sigma^2}(y) - \mu|^2 \leq \frac{3}{2}|\Pi_T \mu - \mu|^2 + \Lambda \log \frac{1}{\pi_T} + 8\sigma^2 \log \frac{1}{\pi_T} + W(\hat{T}) + W'(\hat{T}, T).$$

For all $S, T \subset \{1, \ldots, p\}$, define the events

$$\Omega_S := \{W(S) \leq 6\sigma^2 x\}, \quad \Omega_{S,T} := \{W'(S, T) \leq 8\sigma^2 x\}.$$

On the event $\mathcal{V} \cap (\cap_{S \subset \{1, \ldots, p\}} \Omega_S) \cap (\cap_{S, T \subset \{1, \ldots, p\}} \Omega_{S,T})$, (2.8) holds. It remains to bound from below the probability of this event.

For any fixed $S \subset \{1, \ldots, p\}$, using (2.2) and (B.4) with $t = x + \log \frac{1}{\pi_S}$ we have $P(\Omega_S^c) \leq \pi_S e^{-x}$.

Let $S, T \subset \{1, \ldots, p\}$ be fixed. By using (B.3) with $v = 2(\Pi_S \mu - \Pi_T \mu)$ and $t = x + \log \frac{1}{\sigma_S \pi_T}$, we have that on an event of probability greater than $1 - \pi_S \pi_T e^{-x}$,

$$2\xi^T (\Pi_S \mu - \Pi_T \mu) \leq 2\sigma \sqrt{2(x + \log(1/\pi_S \pi_T))}\Pi_S \mu - \Pi_T \mu \leq 8\sigma^2 \left(x + \log \frac{1}{\pi_S \pi_T}\right) + \frac{1}{4}|\Pi_S \mu - \Pi_T \mu|^2.$$

Thus, $P(\Omega_{S,T}^c) \leq \pi_S \pi_T e^{-x}$.

As in the proof of (2.7), the union bound completes the proof. \(\square\)

**Appendix B: Technical Lemmas**

**Lemma 1.** For any estimator $\hat{\sigma}^2$, let $\hat{\theta}$ be a minimizer of (2.4). Then, almost surely,

$$|\hat{\mu}_\theta - \mu|^2 \leq \min_{k=1,\ldots,M} \left(|\Pi_{T_k} \mu - \mu|^2 + (26\sigma^2 + 22\sigma^2) \log \frac{1}{\pi_{T_k}}\right) + W, \quad (B.1)$$

where

$$W := \max_{S,T \in F} \left(Z(S, T) - 26\sigma^2 \log \frac{1}{\pi_S} - 22\sigma^2 \log \frac{1}{\pi_T}\right)$$

and $Z(\cdot, \cdot)$ is defined in (A.1).
Proof of Lemma 1. Let $\hat{\Lambda} = 26\hat{\sigma}^2$. The function $H_{F,\hat{\sigma}^2}$ is convex and differentiable, it can be rewritten as

$$\forall \theta \in \Lambda^M, \ H_{F,\hat{\sigma}^2}(\theta) = \frac{1}{2} \|\hat{\mu}_\theta\|_2^2 + |y|^2 + \sum_{j=1}^M \theta_j \left(-2y^T \hat{\mu}_j + \frac{1}{2} |\hat{\mu}_j|^2 + \hat{\Lambda} \log \frac{1}{\pi \hat{T}_j}\right).$$

By simple algebra, for any $\theta' \in \mathbb{R}^M$,

$$\nabla H_{F,\hat{\sigma}^2}(\hat{\theta})^T \theta' = \hat{\mu}^T \mu' + \sum_{j=1}^M \theta_j \left(-2y^T \hat{\mu}_j + \frac{1}{2} |\hat{\mu}_j|^2 + \hat{\Lambda} \log \frac{1}{\pi \hat{T}_j}\right), \quad (B.2)$$

$$\nabla H_{F,\hat{\sigma}^2}(\hat{\theta})^T (-\hat{\theta}) = -|\hat{\mu}_\theta - \mu|^2_2 + |\mu|^2_2 + \sum_{j=1}^M \hat{\theta}_j \left(2\xi^T \hat{\mu}_j - \frac{1}{2} |\hat{\mu}_j|^2 - \hat{\Lambda} \log \frac{1}{\pi \hat{T}_j}\right),$$

By summing the last display and equality (B.2) applied to $\theta' = e_k$, we get

$$\nabla H_{F,\hat{\sigma}^2}(\hat{\theta})^T (e_k - \hat{\theta}) = -|\hat{\mu}_\theta - \mu|^2_2 + |\mu|^2_2 + \hat{\Lambda} \log \frac{1}{\pi \hat{T}_k} + \sum_{j=1}^M \hat{\theta}_j \left[2\xi^T (\hat{\mu}_j - \hat{\mu}_k) - \frac{1}{2} |\hat{\mu}_j - \hat{\mu}_k|^2 - \hat{\Lambda} \log \frac{1}{\pi \hat{T}_j}\right].$$

Since $\hat{\mu}_k = \Pi_{\hat{T}_k} y$ is a Least Squares estimator over the linear span of the covariates in $\hat{T}_k$, we have $|\hat{\mu}_k - y|^2_2 \leq |\Pi_{\hat{T}_k} \mu - y|^2_2$ which can be rewritten as

$$|\hat{\mu}_k - \mu|^2_2 \leq |\Pi_{\hat{T}_k} \mu - \mu|^2_2 + 2\xi^T (\hat{\mu}_k - \Pi_{\hat{T}_k} \mu).$$

We thus have

$$\nabla H_{F,\hat{\sigma}^2}(\hat{\theta})^T (e_k - \hat{\theta}) \leq -|\hat{\mu}_\theta - \mu|^2_2 + |\Pi_{\hat{T}_k} \mu - \mu|^2_2 + (\hat{\Lambda} + 22\hat{\sigma}^2) \log \frac{1}{\pi \hat{T}_k} + \sum_{j=1}^M \hat{\theta}_j \left[2\xi^T (\hat{\mu}_j - \Pi_{\hat{T}_k} \mu) - \frac{1}{2} |\hat{\mu}_j - \hat{\mu}_k|^2 - \hat{\Lambda} \log \frac{1}{\pi \hat{T}_j} - 22\hat{\sigma}^2 \log \frac{1}{\pi \hat{T}_k}\right].$$

For all $k = 1, \ldots, \hat{M}$, [Boyd and Vandenberghe, 2009, Section 4.2.3] yields $\nabla H_{F,\hat{\sigma}^2}(\hat{\theta})^T (e_k - \hat{\theta}) \geq 0$. Furthermore, a linear function over the simplex is maximized at a vertex, so almost surely we obtain (B.1).
Lemma 2. Let $t > 0$. For any supports $S, T \subset \{1, \ldots, p\}$, the quantity $Z(S, T)$ defined in (A.1) satisfies with probability greater than $1 - 2 \exp(-t)$,

$$Z(S, T) \leq 4\sigma^2|S| + 22\sigma^2 t.$$

Proof of Lemma 2. Let $D = \Pi_S - \Pi_T$. Then almost surely,

$$Z(S, T) = 2\xi^T \Pi_S \xi + \xi^T (2D\mu - D^2\mu) - \frac{1}{2} D\mu^2 - \frac{1}{2} |D\xi|^2.$$

It is clear that $-|D\xi|^2 \leq 0$. As $\xi$ satisfies (1.1), a Chernoff bound yields that for all $v \in \mathbb{R}^n$,

$$P\left(\xi^Tv > \sigma|v|_2\sqrt{2t}\right) \leq \exp(-t). \quad (B.3)$$

It is clear that $\|D\|_2 \leq 2$. We apply this concentration inequality to $v = 2D\mu - D^2\mu$ to get that with probability greater than $1 - \exp(-t)$,

$$\xi^T (2D\mu - D^2\mu) \leq \sigma |2D\mu - D^2\mu|_2\sqrt{2t} \leq \sigma \|2I_n - D\|_2 |D\mu|_2 \sqrt{2t},$$

$$\leq \sigma 4|D\mu|_2 \sqrt{2t} \leq 16\sigma^2 t + \frac{1}{2} |D\mu|_2^2.$$  

Finally, let $r \leq |S|$ be the rank of $\Pi_S$. The matrix $\Pi_S$ is an orthogonal projector. Hence $\|\Pi_S\|_F^2 = r$ and $\|\Pi_S\|_2 \leq 1$, so that applying the concentration inequality from Hsu et al. [2012] yields that with probability greater than $1 - \exp(-t)$,

$$2\xi^T \Pi_S \xi \leq 2\sigma^2 (r + 2\sqrt{rt} + 2t) \leq 4\sigma^2 r + 6\sigma^2 t \leq 4\sigma^2 |S| + 6\sigma^2 t. \quad (B.4)$$

A union bound completes the proof. \qed

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