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Pierre Alquier, Mohamed Hebiri

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How to relax hypotheses on the LASSO and the Dantzig Selector, and application to the transductive context

Pierre Alquier and Mohamed Hebiri

Abstract

We consider the linear regression problem, where the number p of covariates is possibly larger than the number n of observations $(x_i, y_i)_{i \leq n}$, under sparsity assumptions. On the one hand, several methods have been successfully proposed to perform this task, for example the LASSO in [Tib96] or the Dantzig Selector in [CT07]. On the other hand, consider new values $(x_i)_{n+1 \leq i \leq m}$. If one wants to estimate the corresponding y_i 's, one should think of a specific estimator devoted to this task, referred in [Vap98] as a "transductive" estimator. This estimator may differ from an estimator designed to the more general task "estimate on the whole domain". In this work, we propose a generalized version both of the LASSO and the Dantzig Selector, based on the geometrical remarks about the LASSO in [Alq08, AH08]. The "usual" LASSO and Dantzig Selector, as well as new estimators interpreted as transductive versions of the LASSO, appear as special cases. These estimators are interesting at least from a theoretical point of view: we can give theoretical guarantees for these estimators under hypotheses that are relaxed versions of the hypotheses required in the papers about the "usual" LASSO. These estimators can also be efficiently computed, with results comparable to the ones of the LASSO.

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1 Introduction

In many modern applications, a statistician may have to deal with very large datasets. Regression problems may involve a large number of covariates p , possibly larger than the sample size n . In this situation, a major issue is dimension reduction, which can be performed through the selection of a small amount of relevant covariates - the case where a small amount of covariates is actually relevant being referred as the "sparse" case. For this purpose, numerous regression methods have been proposed in the literature, ranging from the classical information criteria such as AIC [Aka73] and BIC [Sch78] to the more recent regularization-based techniques such as the ℓ_1 penalized least square estimator, known as the LASSO [Tib96], and the Dantzig Selector [CT07]. Regularized regression methods have recently witnessed several developments due to the attractive feature of computational feasibility, even for high dimensional data (i.e., when the number of covariates p is large).

We focus on the usual linear regression model:

$$y_i = x_i \beta^* + \varepsilon_i, \quad i = 1, \dots, n, \tag{1}$$

where the design $x_i = (x_{i,1}, \dots, x_{i,p}) \in \mathbb{R}^p$ is deterministic, $\beta^* = (\beta_1^*, \dots, \beta_p^*)' \in \mathbb{R}^p$ is the unknown parameter vector of interest and $\varepsilon_1, \dots, \varepsilon_n$ are i.i.d. centered Gaussian random variables with known variance σ^2 . Let X denote the matrix with i -th line equal to x_i , and let X_j denote its j -th column, with $i \in \{1, \dots, n\}$ and $j \in \{1, \dots, p\}$. So:

$$X = (x'_1, \dots, x'_n)' = (X_1, \dots, X_p).$$

For the sake of simplicity, we will assume that the observations are normalized in such a way that $X'_j X_j / n = 1$. Let us also put $Y = (y_1, \dots, y_n)'$.

For any $d \in \mathbb{N}$, any vector $v \in \mathbb{R}^d$ and any $\alpha \geq 1$ we will use the usual notation $\|v\|_\alpha = (|v_1|^\alpha + \dots + |v_d|^\alpha)^{1/\alpha}$, in particular $\|\cdot\|_2$ is the euclidean norm. Finally, let us put $\|v\|_0 = \sum_{i=1}^d \mathbf{1}(v_i \neq 0)$.

The LASSO [Tib96] (say $\hat{\beta}^L$), the Dantzig Selector [CT07] (say $\hat{\beta}^{DS}$), the non-negative garrote (in Yuan and Lin [YL07], say $\hat{\beta}^{NNG}$) were proposed to deal with this problem in the case where p is large, even when $p > n$, with very good

practical results (simulations and tests on real data are provided, for example, in [Tib96]). We also refer to [Kol07, Kol09, MVdGB08, vdG08, DT07, CH08] for related work with different estimators: non-quadratic loss, penalties slightly different from ℓ_1 and/or random design.

From a theoretical point of view, Sparsity Inequalities (SI) were proved for these estimators: bounds on $(1/n)\|X\hat{\beta}^L - X\beta^*\|_2^2$ or on $\|\hat{\beta}^L - \beta^*\|_2^2$ which are $\mathcal{O}(\sigma^2\|\beta^*\|_0 \log(p)/n)$ and then involve the number of non-zero coordinates in β^* (multiplied by $\log(p)$), instead of p . Such bounds are given for example in [BTW07]. Some conditions to ensure that $\hat{\beta}^L$ has the same null coordinates than β^* can be found in [Bun08]. SI for $\hat{\beta}^{DS}$ can be found in [CT07], in [BRT07]. As these authors give upper bound on $\|X\hat{\beta}^L - X\beta^*\|_2^2$ and on $\|\hat{\beta}^L - \beta^*\|_2^2$, such results ensure that under some assumption, $X\hat{\beta}^L$ is a good estimator of $X\beta^*$ and, in some cases, that $\hat{\beta}^L$ is a good estimator of β^* . Now, let us assume that we are given additional observations $x_i \in \mathbb{R}^p$ for $n+1 \leq i \leq m$ (with $m > n$), let us introduce the matrix $Z = (x'_1, \dots, x'_m)'$ and let us assume that the objective of the statistician is precisely to estimate $Z\beta^*$: namely, we don't necessarily want a precise estimation of β^* , we just want to predict what would be the labels attached to the additional x_i 's. It is argued in [Vap98] that in such a case, one should think of a specific estimator devoted to this task, referred by Vapnik as a transductive estimator. This estimator may differ from an estimator tailored for the estimation of β^* or $X\beta^*$ like the LASSO. Indeed one usually builds an estimator $\hat{\beta}(X, Y)$ and then computes $Z\hat{\beta}(X, Y)$ to estimate $Z\beta^*$. The approach favored here is to consider estimators $\hat{\beta}(X, Y, Z)$ exploiting the knowledge of Z , and then to compute $Z\hat{\beta}(X, Y, Z)$.

Some methods of supervised classification or regression were successfully extended to the transductive setting, such as the well-known Support Vector Machines (SVM) in [Vap98], the Gibbs estimators in [Cat07]. It is argued in the semi-supervised learning literature (see for example [CSZ06] for a recent survey) that taking into account the information on the design given by the new additional x_i 's have a stabilizing effect on the estimator.

In this paper, we study a family of estimators which generalizes the LASSO and the Dantzig Selector. The considered family depends on a $q \times p$ matrix A , with $q \in \mathbb{N}$, whose choice allows to adapt the estimator to the objective of the statistician. A suitable choice can in particular extend the LASSO and the Dantzig Selector to the transductive setting.

The paper is organized as follows. In the next section, we motivate the use of the studied family of estimators through geometrical considerations stated in [AH08]. In the Sections 3 and 4, we establish Sparsity Inequalities for these estimators. A discussion on the assumption needed to prove the SI is also detailed. In particular, it is shown that the estimators devoted to the transductive setting satisfy these SI with weaker assumption than those needed by the LASSO or the Dantzig Selector, when $m > p > n$. That is, when the number of news points is large enough. The implementation of our estimators and some numerical experiments are the purpose of Section 5. The results clearly show that the use of a transductive version of the LASSO may improve the performance of the

estimation. All proofs of the theoretical results are postponed to Section 7.

2 Preliminary observations

In this section we state geometrical considerations (projections on a confidence region) for the LASSO and the Dantzig Selector. These motivate the introduction of our estimators. Finally we discuss the different objectives considered in this paper.

Let us remind that a definition of the LASSO estimate is given by

$$\arg \min_{\beta \in \mathbb{R}^p} \left\{ \|Y - X\beta\|_2^2 + 2\lambda \|\beta\|_1 \right\} \quad (2)$$

but a dual form (in [OPT00]) of this program is also of interest:

$$\begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|X\beta\|_2^2 \\ s.t. \|X'(Y - X\beta)\|_\infty \leq \lambda; \end{cases} \quad (3)$$

actually it is proved in [Alq08] that any solution of Program 3 is a solution of Program 2 and that the set $\{X\beta\}$ is the same where β is taken among all the solutions of Program 2 or among all the solutions of 3. So both programs are equivalent in terms of estimating $X\beta^*$.

Now, let us remind the definition of the Dantzig Selector:

$$\begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|\beta\|_1 \\ s.t. \|X'(Y - X\beta)\|_\infty \leq \lambda. \end{cases} \quad (4)$$

Alquier [Alq08] observed that both Programs 3 and 4 can be seen as a projection of the null vector $\mathbf{0}_p$ onto the region $\{\beta : \|X'(Y - X\beta)\|_\infty \leq \lambda\}$ that can be interpreted as a confidence region, with confidence $1 - \eta$, for a given λ that depends on η (see Lemma 7.1 here for example). The difference between the two programs is the distance (or semi-distance) used for the projection.

Based on these geometrical considerations, we proposed in [AH08] to study the following transductive estimator:

$$\begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|Z\beta\|_2^2 \\ s.t. \|X'(Y - X\beta)\|_\infty \leq \lambda; \end{cases} \quad (5)$$

that is a projection on the same confidence region, but using a distance adapted to the transductive estimation problem. We proved a sparsity inequality for this estimator exploiting a novel sparsity measure.

In this paper, we propose a generalized version of the LASSO and of the Dantzig Selector, based on the same geometrical remark. More precisely for $q \in \mathbb{N}^*$, let A be a $q \times p$ matrix. We propose two general estimators, $\hat{\beta}_{A,\lambda}$ (extension

of the LASSO, based on a generalization of Program 2) and $\tilde{\beta}_{A,\lambda}$ (transductive Dantzig Selector, generalization of Program 4). These novel estimators depend on two tuning parameters: $\lambda > 0$ is a regularization parameter, it plays the same role as the tuning parameter involved in the LASSO, and the matrix A that will allow to adapt the estimator to the objective of the statistician. More particularly, depending on the choice of the matrix A , this estimator can be adapted to one of the following objectives:

- **denoising objective:** the estimation of $X\beta^*$, that is a denoised version of Y . For this purpose, we consider the estimator $\hat{\beta}_{A,\lambda}$, with $A = X$. In this case, the estimator will actually be equal to the LASSO $\hat{\beta}^L$ and $\tilde{\beta}_{A,\lambda}$, with the same choice $A = X$ will be equal to the Dantzig Selector;
- **transductive objective:** the estimation of $Z\beta^*$, by $\hat{\beta}_{A,\lambda}$ or $\tilde{\beta}_{A,\lambda}$, with $A = \sqrt{n/m}Z$. We will refer the corresponding estimators as the "Transductive LASSO" and "Transductive Dantzig Selector";
- **estimation objective:** the estimation of β^* itself, by $\hat{\beta}_{A,\lambda}$, with $A = \sqrt{n}I$. In this case, it appears that both estimators are well defined only in the case $p < n$ and are equal to a soft-thresholded version of the usual least-square estimator.

For both estimators we prove new SI (Sparsity Inequalities), and we show that these estimators can easily be computed.

3 The "easy case": $\text{Ker}(X) = \text{Ker}(Z)$

In this section, we deal with the "easy case", where $\text{Ker}(A) = \text{Ker}(X)$ (think of $A = X$, $A = \sqrt{n}I$ or $A = \sqrt{n/m}Z$). This setting is natural in the case $p < n$ where both kernels are equal to $\{0\}$ in general. We provide SI (Sparsity Inequality, Theorem 3.3) for the studied estimators, based on the techniques developed in [BTW07].

3.1 Definition of the estimators

Definition 3.1. For a given parameter $\lambda \geq 0$ and any matrix A such that $\text{Ker}(A) = \text{Ker}(X)$, we consider the estimator given by

$$\hat{\beta}_{A,\lambda} \in \arg \min_{\beta \in \mathbb{R}^p} \left\{ -2Y'X(\widetilde{X'X})^{-1}(A'A)\beta + \beta'(A'A)\beta + 2\lambda \|\Xi_A\beta\|_1 \right\},$$

where $(\widetilde{X'X})^{-1}$ is exactly $(X'X)^{-1}$ if $(X'X)$ is invertible, and any pseudo-inverse of this matrix otherwise, and where Ξ_A is a diagonal matrix whose (j, j) -th coefficient is $\xi_j^{\frac{1}{2}}(A)$ where $\xi_j(A) = \frac{1}{n}[(A'A)(\widetilde{X'X})^{-1}(A'A)]_{j,j}$.

Remark 3.1. Equivalently we have

$$\hat{\beta}_{A,\lambda} \in \arg \min_{\beta \in \mathbb{R}^p} \left\{ \left\| \tilde{Y}_A - A\beta \right\|_2^2 + 2\lambda \|\Xi_A\beta\|_1 \right\},$$

where $\tilde{Y}_A = A(\widetilde{X'X})^{-1}X'Y$.

Actually, we are going to consider three particular cases of this estimator in this work, depending on the objective of the statistician:

- **denoising objective:** the LASSO, denoted here by $\hat{\beta}_{X,\lambda}$, given by

$$\begin{aligned}\hat{\beta}_{X,\lambda} &\in \arg \min_{\beta \in \mathbb{R}^p} \left\{ \|Y - X\beta\|_2^2 + 2\lambda \|\beta\|_1 \right\} \\ &= \arg \min_{\beta \in \mathbb{R}^p} \left\{ -2Y'X\beta + \beta'X'X\beta + 2\lambda \|\beta\|_1 \right\}\end{aligned}$$

(note that in this case, $\Xi_X = I$ since X is normalized);

- **transductive objective:** the Transductive LASSO, denoted here by $\hat{\beta}_{\sqrt{n/m}Z,\lambda}$, given by

$$\hat{\beta}_{\sqrt{n/m}Z,\lambda} \in \arg \min_{\beta \in \mathbb{R}^p} \left\{ \frac{n}{m} \left\| \tilde{Y}_Z - Z\beta \right\|_2^2 + 2\lambda \left\| \Xi_{\frac{n}{m}Z} \beta \right\|_1 \right\};$$

- **estimation objective:** $\hat{\beta}_{\sqrt{n}I,\lambda}$, defined by

$$\hat{\beta}_{\sqrt{n}I,\lambda} \in \arg \min_{\beta \in \mathbb{R}^p} \left\{ n \left\| \tilde{Y}_I - \beta \right\|_2^2 + 2\lambda \left\| \Xi_{\sqrt{n}I} \beta \right\|_1 \right\}.$$

Let us give the analogous definition for an extension of the Dantzig Selector.

Definition 3.2. For a given parameter $\lambda > 0$ and any matrix A such that $\text{Ker}(A) = \text{Ker}(X)$, we consider the estimator given by

$$\tilde{\beta}_{A,\lambda} = \begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|\beta\|_1 \\ \text{s.t. } \left\| \Xi_A^{-1} A' A (\widetilde{X'X})^{-1} X'Y - \beta \right\|_\infty \leq \lambda. \end{cases}$$

Here again, we are going to consider three cases, for $A = X$, $A = \sqrt{n/m}Z$ and $A = \sqrt{n}I$, and it is easy to check that for $A = X$ we have exactly the usual definition of the Dantzig Selector (Program 4). Moreover, here again, note that we can rewrite this estimator:

$$\tilde{\beta}_{A,\lambda} = \begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|\beta\|_1 \\ \text{s.t. } \left\| \Xi_A^{-1} A' (\tilde{Y}_A - A\beta) \right\|_\infty \leq \lambda. \end{cases}$$

The following proposition provides an interpretation of our estimators when $A = \sqrt{n}I$.

Proposition 3.1. *Let us assume that $(X'X)$ is invertible. Then $\hat{\beta}_{\sqrt{n}I, \lambda} = \tilde{\beta}_{\sqrt{n}I, \lambda}$ and this is a soft-thresholded least-square estimator: let us put $\hat{\beta}_{LSE} = (X'X)^{-1}X'Y$ then $\hat{\beta}_{\sqrt{n}I, \lambda}$ is the vector obtained by replacing the j -th coordinate $b_j = \left(\hat{\beta}_{LSE}\right)_j$ of $\hat{\beta}_{LSE}$ by $\text{sgn}(b_j) (|b_j| - \lambda \xi_j(nI)/n)_+$, where we use the standard notation $\text{sgn}(x) = +1$ if $x \geq 0$, $\text{sgn}(x) = -1$ if $x < 0$ and $(x)_+ = \max(x, 0)$.*

Proposition 3.2 deals with a dual definition of the estimator $\hat{\beta}_{A, \lambda}$.

Proposition 3.2. *When $\text{Ker}(A) = \text{Ker}(X)$, the solutions β of the following program:*

$$\begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|A\beta\|_2^2 \\ \text{s.t. } \left\| \Xi_A^{-1} A' ((\tilde{Y}_A - A\beta)) \right\|_\infty \leq \lambda \end{cases}$$

all satisfy $X\beta = X\hat{\beta}_{A, \lambda}$ and $A\beta = A\hat{\beta}_{A, \lambda}$.

Proofs can be found in Section 7, page 17.

3.2 Theoretical results

Let us first introduce our main assumption. This assumption is stated with a given $p \times p$ matrix M and a given real number $x > 0$.

Assumption $H(M, x)$: there is a constant $c(M) > 0$ such that, for any $\alpha \in \mathbb{R}^p$ such that $\sum_{j: \beta_j^* = 0} \xi_j(M) |\alpha_j| \leq x \sum_{j: \beta_j^* \neq 0} \xi_j(M) |\alpha_j|$ we have

$$\alpha' M \alpha \geq c(M) n \sum_{j: \beta_j^* \neq 0} \alpha_j^2. \quad (6)$$

First, let us explain briefly the meaning of this hypothesis. In the case, where M is invertible, the condition

$$\alpha' M \alpha \geq c(M) n \sum_{j: \beta_j^* \neq 0} \alpha_j^2$$

is always satisfied for any $\alpha \in \mathbb{R}^p$ with $c(M)$ larger than the smallest eigenvalue of M/n . However, for the LASSO, we have $M = (X'X)$ and M cannot be invertible if $p > n$. Even in this case, Assumption $H(M, x)$ may still be satisfied. Indeed, the assumption requires that Inequality 6 holds only for a small for a small subset of \mathbb{R}^p determined by the condition $\sum_{j: \beta_j^* = 0} \xi_j(M) |\alpha_j| \leq x \sum_{j: \beta_j^* \neq 0} \xi_j(M) |\alpha_j|$.

For $M = (X'X)$, this assumption becomes exactly the one taken in [BTW07]. In that paper, the necessity of such an hypothesis is also discussed.

Theorem 3.3. *Let us assume that Assumption $H(A'A, 3)$ is satisfied. Let us assume that $\text{Ker}(A) = \text{Ker}(X)$. Let us choose $0 < \eta < 1$ and $\lambda = 2\sigma\sqrt{2n \log\left(\frac{p}{\eta}\right)}$. With probability at least $1 - \eta$ on the draw of Y , we have simultaneously*

$$\left\|A\left(\hat{\beta}_{A,\lambda} - \beta^*\right)\right\|_2^2 \leq \frac{128\sigma^2}{c(A'A)} \log\left(\frac{p}{\eta}\right) \sum_{j:\beta_j^* \neq 0} \xi_j(A)$$

and

$$\left\|\Xi_A\left(\hat{\beta}_{A,\lambda} - \beta^*\right)\right\|_1 \leq \frac{64\sigma}{c(A'A)} \left(\frac{\log\left(\frac{p}{\eta}\right)}{2n}\right)^{\frac{1}{2}} \sum_{j:\beta_j^* \neq 0} \xi_j(A).$$

In particular, the first inequality gives

- if assumption $H(X'X, 3)$ is satisfied, with probability at least $1 - \eta$,

$$\frac{1}{n} \left\|X\left(\hat{\beta}_{X,\lambda} - \beta^*\right)\right\|_2^2 \leq \frac{128\sigma^2}{nc(X'X)} \|\beta^*\|_0 \log\left(\frac{p}{\eta}\right);$$

- if assumption $H\left(\frac{n}{m}Z'Z, 3\right)$ is satisfied, and if $\text{Ker}(Z) = \text{Ker}(X)$, with probability at least $1 - \eta$,

$$\frac{1}{m} \left\|Z\left(\hat{\beta}_{Z,\lambda} - \beta^*\right)\right\|_2^2 \leq \frac{128\sigma^2}{nc\left(\frac{n}{m}Z'Z\right)} \sum_{j:\beta_j^* \neq 0} \xi_j\left(\sqrt{n/m}Z\right) \log\left(\frac{p}{\eta}\right);$$

- and if $(X'X)$ is invertible, with probability at least $1 - \eta$,

$$\left\|\hat{\beta}_{\sqrt{n}I,\lambda} - \beta^*\right\|_2^2 \leq \frac{128\sigma^2}{nc(nI)} \sum_{j:\beta_j^* \neq 0} \xi_j(nI) \log\left(\frac{p}{\eta}\right).$$

This result shows that each of these three estimators satisfy at least a SI for the task it is designed for. For example, the LASSO is proved to have "good" performance for the estimation of $X\beta^*$ and the Transductive LASSO is proved to have good performance for the estimation of $Z\beta^*$, but note that we can not be sure that, for example, the LASSO performs better than the Transductive LASSO for the estimation of $Z\beta^*$.

Remark 3.2. *For $A = X$, the particular case of our result applied to the LASSO is quite similar to the result given in [BTW07] on the LASSO. Actually, Theorem 3.3 can be seen as a generalization of the result in [BTW07] and it should be noted that the proof used to prove Theorem 3.3 uses arguments introduced in [BTW07].*

Remark 3.3. As soon as A is better determined than $X'X$, Hypothesis $H(A, x)$ is less restrictive than $H(X'X, x)$. In particular, in the case where $m > n$, Hypothesis $H((n/m)Z'Z, x)$ is expected to be less restrictive than Hypothesis $H(X'X, x)$.

Now we give the analogous result for the estimator $\tilde{\beta}_{A,\lambda}$.

Theorem 3.4. Let us assume that Assumption $H(A'A, 1)$ is satisfied. Let us assume that $\text{Ker}(A) = \text{Ker}(X)$. Let us choose $0 < \eta < 1$ and $\lambda = 2\sigma\sqrt{2n\log\left(\frac{p}{\eta}\right)}$. With probability at least $1 - \eta$ on the draw of Y , we have simultaneously

$$\|A(\tilde{\beta}_{A,\lambda} - \beta^*)\|_2^2 \leq \frac{72\sigma^2}{c(A'A)} \log\left(\frac{p}{\eta}\right) \sum_{j:\beta_j^* \neq 0} \xi_j(A)$$

and

$$\|\Xi_A(\tilde{\beta}_{A,\lambda} - \beta^*)\|_1 \leq \frac{4\sqrt{3}\sigma}{c(A'A)} \left(\frac{\log\left(\frac{p}{\eta}\right)}{n}\right)^{\frac{1}{2}} \sum_{j:\beta_j^* \neq 0} \xi_j(A).$$

4 An extension to the general case

In this section, we only deal with the transductive setting, $A = \sqrt{n/m}Z$. Let us remind that we observe X that contains some observations x_i associated with labels Y_i in Y , for $i \in \{1, \dots, n\}$, and that moreover we have additional observations x_i for $i \in \{n+1, \dots, m\}$ with $m > n$, and we put all the x_i for $i \in \{1, \dots, m\}$ in a matrix Z , and we want to estimate the corresponding labels Y_i (but note that for the moment, we did not precise what is Y_i for $i > n$), let us put $\tilde{Y} = (Y_1, \dots, Y_m)'$.

4.1 General remarks

Let us, for example, look at the definition of $\hat{\beta}_{\sqrt{n/m}Z,\lambda}$, for example as given in Remark 3.1:

$$\hat{\beta}_{\sqrt{n/m}Z,\lambda} \in \arg \min_{\beta \in \mathbb{R}^p} \left\{ \frac{n}{m} \|\tilde{Y}_Z - Z\beta\|_2^2 + 2\lambda \|\Xi_{\frac{n}{m}Z'Z}\beta\|_1 \right\}$$

where actually $\tilde{Y}_Z = Z(\widetilde{X'X})^{-1}XY$ can be interpreted as a preliminary estimator of \tilde{Y} . Hence, in any case, we propose the following procedure.

Let us assume that, depending on the context, the user has a natural (and not necessary efficient) estimator of $\tilde{Y} = (Y_{n+1}, \dots, Y_{n+m})'$. Note this estimator \check{Y} .

Definition 4.1. The Transductive LASSO is given by:

$$\hat{\beta}_{\check{Y},\sqrt{n/m}Z,\lambda} \in \arg \min_{\beta \in \mathbb{R}^p} \left\{ \frac{n}{m} \|\check{Y} - Z\beta\|_2^2 + 2\lambda \|\Xi_{\frac{n}{m}Z'Z}\beta\|_1 \right\},$$

and the Transductive Dantzig Selector is defined as:

$$\tilde{\beta}_{\tilde{Y}, \sqrt{\frac{n}{m}}Z, \lambda} = \begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|\beta\|_1 \\ \text{s.t. } \left\| \frac{n}{m} \Xi^{-1} \frac{1}{\sqrt{n/m}Z} Z'(\tilde{Y} - Z\beta) \right\|_{\infty} \leq \lambda. \end{cases}$$

In the next subsection, we propose a context where we have a natural estimator \tilde{Y} and give a SI on this estimator.

4.2 An example: small labeled dataset, large unlabeled dataset

The idea of this example is to consider the case where the examples x_i for $1 \leq i \leq n$ are "representative" of the large populations x_i for $1 \leq i \leq m$.

Consider, $Z = (x'_1, \dots, x'_m)'$ where the x'_i 's are the points of interest: we want to estimate $\tilde{Y} = Z\beta^*$. However, we just have a very expensive and noisy procedure, that, given a point x_i , returns $Y_i = x_i\beta^* + \varepsilon_i$, where the ε_i 's are $\mathcal{N}(0, \sigma^2)$ and independent. In such a case, the procedure cannot be applied for the whole dataset $Z = (x'_1, \dots, x'_m)'$. We can only make a deal with a "representative" sample of size n . A typical case could be $n < p < m$.

First, let us introduce a slight modification of our main hypothesis. It is also stated with a given $p \times p$ matrix M and a given real number $x > 0$.

Assumption $H'(M, x)$: there is a $c(M) > 0$ such that, for any $\alpha \in \mathbb{R}^p$ such that $\sum_{j: \beta_j^* = 0} |\alpha_j| \leq x \sum_{j: \beta_j^* \neq 0} |\alpha_j|$ we have

$$\alpha' M \alpha \geq c(M)n \sum_{j: \beta_j^* \neq 0} \alpha_j^2.$$

We can now state our main result.

Theorem 4.1. *Let us assume that Assumption $H'((n/m)Z'Z, 1)$ is satisfied. Let us choose $0 < \eta < 1$ and $\lambda_1 = \lambda_2 = 2\sigma\sqrt{2n \log\left(\frac{p}{\eta}\right)}$. Moreover, let us assume that*

$$\forall u \in \mathbb{R}^p \text{ with } \|u\|_1 \leq \|\beta^*\|_1, \quad \left\| \left((X'X) - \frac{n}{m}(Z'Z) \right) u \right\|_{\infty} < \sigma \sqrt{2n \log\left(\frac{p}{\eta}\right)}. \quad (7)$$

Let $\tilde{Y}_{\lambda_1} = Z\tilde{\beta}_{X, \lambda_1/2}$ be a preliminary estimator of \tilde{Y} and then define the Transductive LASSO by

$$\hat{\beta}_{\frac{n}{m}Z, \lambda_2}^* = \begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \frac{n}{m} \|Z\beta\|_2^2 \\ \text{s.t. } \left\| \frac{n}{m} Z'(\tilde{Y}_{\lambda_1} - Z\beta) \right\|_{\infty} \leq 4\lambda_2, \end{cases}$$

and the Transductive Dantzig Selector

$$\tilde{\beta}_{\frac{n}{m}Z, \lambda_2}^* = \begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|\beta\|_1 \\ \text{s.t. } \left\| \frac{n}{m} Z' (\check{Y}_{\lambda_1} - Z\beta) \right\|_\infty \leq \frac{\lambda_2}{2}. \end{cases}$$

With probability at least $1 - \eta$ on the draw of Y , we have simultaneously

$$\frac{1}{m} \left\| Z(\tilde{\beta}_{\frac{n}{m}Z, \lambda_2}^* - \beta^*) \right\|_2^2 \leq \frac{200\sigma^2}{nc((n/m)Z'Z)} \log\left(\frac{p}{\eta}\right) \|\beta^*\|_0,$$

$$\left\| \tilde{\beta}_{\frac{n}{m}Z, \lambda_2}^* - \beta^* \right\|_1 \leq \frac{100\sqrt{2}\sigma}{c((n/m)Z'Z)} \left(\frac{\log\left(\frac{p}{\eta}\right)}{n} \right)^{\frac{1}{2}} \|\beta^*\|_0,$$

and moreover, if $H'((n/m)Z'Z, 3)$ is also satisfied,

$$\frac{1}{m} \left\| Z(\hat{\beta}_{\frac{n}{m}Z, \lambda_2}^* - \beta^*) \right\|_2^2 \leq \frac{256\sigma^2}{nc((n/m)Z'Z)} \log\left(\frac{p}{\eta}\right) \|\beta^*\|_0,$$

$$\left\| \hat{\beta}_{\frac{n}{m}Z, \lambda_2}^* - \beta^* \right\|_1 \leq \frac{128\sigma}{c((n/m)Z'Z)} \left(\frac{\log\left(\frac{p}{\eta}\right)}{n} \right)^{\frac{1}{2}} \|\beta^*\|_0.$$

First, let us remark that the preliminary estimator \check{Y}_{λ_1} is defined using the Dantzig Selector $\tilde{\beta}_{X, \lambda_1/2}$. We could give exactly the same kind of results using the LASSO $\hat{\beta}_{X, \lambda_1/2}$ as a preliminary estimator.

Now, let us give a look at the new hypothesis, Inequality (7). We can interpret this condition as the fact that the x_i 's for $1 \leq i \leq n$ are effectively representative of the wide population: so $X'X/n$ is "not too far" from $Z'Z/m$. We will end this section by a result that proves that this is effectively the case in a typical situation.

Proposition 4.2. *Assume that $m = kn$ for an integer value $k \in \mathbb{N} \setminus \{0, 1\}$. Let us assume that X and Z are build in the following way: we have a population $\chi_1 = (\chi_{1,1}, \dots, \chi_{1,p}) \in \mathbb{R}^p, \dots, \chi_m \in \mathbb{R}^p$ (the points of interest). Then, we draw uniformly without replacement, n of the χ_i 's to be put in X : more formally, but equivalently, we draw uniformly a permutation σ of $\{1, \dots, m\}$ and we put $X = (x'_1, \dots, x'_n)' = (\chi'_{\sigma(1)}, \dots, \chi'_{\sigma(n)})'$ and $Z = (x'_1, \dots, x'_m)' = (\chi'_{\sigma(1)}, \dots, \chi'_{\sigma(m)})'$. Let us assume that for any $(i, j) \in \{1, \dots, n\} \times \{1, \dots, p\}$, $\chi_{i,j}^2 < \kappa$ for some $\kappa > 0$, and that $p \geq 2$. Then, with probability at least $1 - \eta$, for any $u \in \mathbb{R}^p$,*

$$\left\| \left(X'X - \frac{n}{m} Z'Z \right) u \right\|_\infty \leq \|u\|_1 \frac{2\kappa k}{k-1} \sqrt{2 \log \frac{p}{\eta}}.$$

In particular, if we have

$$\|u\|_1 \leq \|\beta^*\|_1 \text{ and } \kappa \leq \frac{k-1}{k} \frac{\sigma}{\|\beta^*\|_1}$$

then we have

$$\left\| \left(X'X - \frac{n}{m} Z'Z \right) u \right\|_{\infty} \leq \sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)}.$$

Let us just mention that the assumption $m = kn$ is not restrictive. It has been introduced for the sake of simplicity.

5 Experimental results

Since the paper of Tibshirani [Tib96], several effective algorithms to compute the LASSO have been proposed and studied (for instance Interior Points methods [KKL⁺07], LARS [EHJT04], Pathwise Coordinate Optimization [FHHT07], Relaxed Greedy Algorithms [HCB08]). For the Dantzig Selector, a linear method was proposed in the first paper [CT07], also note that the LARS method was successfully extended in [JRL09] to compute the Dantzig Selector.

Then there are many algorithms to compute $\hat{\beta}_{A,\lambda}$ and $\tilde{\beta}_{A,\lambda}$, when $A = X$. Thanks to Proposition 3.1, it is also clear that we can easily find an efficient algorithm for the case $A = \sqrt{n}I$.

The general form of the estimators $\hat{\beta}_{A,\lambda}$ and $\tilde{\beta}_{A,\lambda}$ given by Definitions 3.1 and 3.2, allows to use one of the algorithms mentioned previously to compute our estimator in two cases.

For example, from Remark 3.1, we have:

$$\hat{\beta}_{A,\lambda} \in \arg \min_{\beta \in \mathbb{R}^p} \left\{ \left\| \tilde{Y}_A - A\beta \right\|_2^2 + 2\lambda \|\Xi_A \beta\|_1 \right\},$$

then we just have to compute \tilde{Y}_A , to put $B = A\Xi_A^{-1}$, to use any program that computes the LASSO to determine

$$\hat{\gamma} \in \arg \min_{\gamma \in \mathbb{R}^p} \left\{ \left\| \tilde{Y}_A - B\gamma \right\|_2^2 + 2\lambda \|\gamma\|_1 \right\}$$

and then to put $\hat{\beta}_{A,\lambda} = \Xi_A^{-1} \hat{\gamma}$.

In the rest of this section, we compare the LASSO and the transductive LASSO on the classical toy example introduced by Tibshirani [Tib96] and used as a benchmark.

Data description. In the model proposed by Tibshirani, we have

$$Y_i = x_i \beta^* + \varepsilon_i$$

for $i \in \{1, \dots, n\}$, $\beta^* \in \mathbb{R}^p$ and the ε_i are i.i.d. $\mathcal{N}(0, \sigma^2)$. Finally, the $(x_i)_{i \in \{1, \dots, m\}}$ are generated from a probability distribution: they are independent and identi-

cally distributed

$$x_i \sim \mathcal{N} \left(\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho & \dots & \dots & \rho^{p-1} \\ \rho & 1 & \rho & \dots & \rho^{p-2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \rho^{p-2} & \dots & \rho & 1 & \rho \\ \rho^{p-1} & \dots & \dots & \rho & 1 \end{pmatrix} \right)$$

for a given $\rho \in]-1, 1[$.

As in [Tib96], we $p = 8$. In a first experiment, we take $(n, m) = (7, 10)$, $\rho = 0.5$, $\sigma = 1$ and $\beta^* = (3, 1.5, 0, 0, 2, 0, 0, 0)$ ("sparse").

Then, in order to check the robustness of the results, we consider successively $\rho = 0.5$ by $\rho = 0.9$ (correlated variables), $\sigma = 1$ by $\sigma = 3$ (noisy case), $\beta^* = (3, 1.5, 0, 0, 2, 0, 0, 0)$ by $\beta^* = (5, 0, 0, 0, 0, 0, 0, 0)$ ("very sparse" case), $(n, m) = (7, 10)$ by $(n, m) = (7, 20)$ (larger unlabeled set), $(n, m) = (20, 30)$ ($p < n$, note that this is an easier case and that in [Tib96] we always have $n = 20$) and finally $(n, m) = (20, 120)$.

We use the version of the transductive LASSO proposed in Section 4: first we compute a LASSO estimator $\hat{\beta}_{X, \lambda_1}$ for a given λ_1 and then the Transductive LASSO given by

$$\beta_{TL}(\lambda_1, \lambda_2) = \begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \frac{n}{m} \|Z\beta\|_2^2 \\ \text{s.t. } \left\| \frac{n}{m} Z'(Z\hat{\beta}_{X, \lambda_1} - Z\beta) \right\|_\infty \leq \lambda_2 \end{cases}$$

for a given λ_2 . We want to compare this two step procedure with the procedure obtained using the usual LASSO only: $\beta_L(\lambda) = \hat{\beta}_{X, \lambda}$ for a λ that may differ from λ_1 . In both cases, the solutions are computed using PCO algorithm. We compute $\beta_L(\lambda)$ and $\beta_{TL}(\lambda_1, \lambda_2)$ for $(\lambda, \lambda_1, \lambda_2) \in \Lambda^3$ where $\Lambda^3 = \{1.2^k, k = -50, -49, \dots, 30\}$ and in the next subsection, we examine the performance of each estimator according to the value of the regularization parameters.

Results. We illustrate here some of the results obtained in the considered cases.

Case $(n, m) = (7, 10)$, $\rho = 0.5$, $\sigma = 1$ and β^ "sparse"*

We simulated 100 experiments and studied the distribution of

$$PERF(X) = \frac{\min_{(\lambda_1, \lambda_2) \in \Lambda^2} \|X(\beta_{TL}(\lambda_1, \lambda_2) - \beta^*)\|_2^2}{\min_{\lambda \in \Lambda} \|X(\beta_L(\lambda) - \beta^*)\|_2^2},$$

$$PERF(Z) = \frac{\min_{(\lambda_1, \lambda_2) \in \Lambda^2} \|Z(\beta_{TL}(\lambda_1, \lambda_2) - \beta^*)\|_2^2}{\min_{\lambda \in \Lambda} \|Z(\beta_L(\lambda) - \beta^*)\|_2^2}$$

and

$$PERF(I) = \frac{\min_{(\lambda_1, \lambda_2) \in \Lambda^2} \|\beta_{TL}(\lambda_1, \lambda_2) - \beta^*\|_2^2}{\min_{\lambda \in \Lambda} \|\beta_L(\lambda) - \beta^*\|_2^2}$$

over all the experiments.

For example, we plot (Figure 1) the histogram of $PERF(X)$ (actually, the three distributions were quite similar).

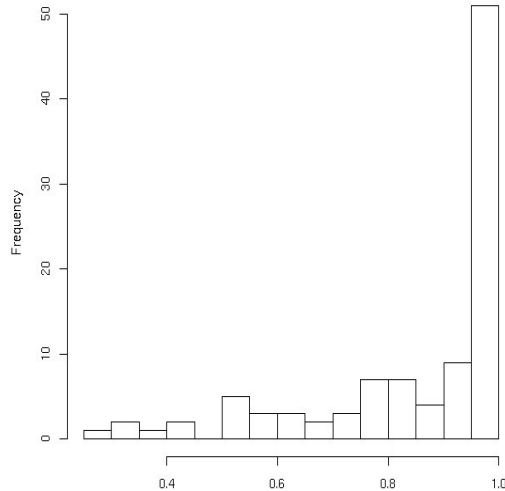


Figure 1: Histogram of $PERF(X)$ with $(n, m) = (7, 10)$, $\rho = 0.5$, $\sigma = 1$ and $\beta^* = (3, 1.5, 0, 0, 2, 0, 0, 0)$.

We observe that in 50% of the simulations, $\min_{(\lambda_1, \lambda_2) \in \Lambda^2} \|X(\beta_{TL}(\lambda_1, \lambda_2) - \beta^*)\|_2^2 = \min_{(\lambda_1, 0) \in \Lambda^2} \|X(\beta_{TL}(\lambda_1, 0) - \beta^*)\|_2^2 = \min_{\lambda \in \Lambda} \|X(\beta_L(\lambda) - \beta^*)\|_2^2$. In these cases, the Transductive LASSO does not improve at all the LASSO. But in the others 50%, the Transductive LASSO can actually improve the LASSO, and the improvement can be really important. We give an overview of the results in Table 1.

The other cases

The following conclusions emerge of the experiments: first, $\beta^* = (5, 0, \dots, 0)$ leads to a more significant improvement of the Transductive LASSO compared to the LASSO (Table 1). On the contrary, $(n, m) = (7, 10)$ and $(n, m) = (7, 20)$ seems to give similar result, while in the case $n > p$, i.e., $(n, m) = (20, 30)$ and $(n, m) = (20, 120)$, the improvement of the Transductive LASSO with respect to the LASSO becomes less significant (Table 1). Finally, ρ and σ have of course a significant influence on the performance of the LASSO, but these parameters does not seem to have any influence on the relative performance of the Transductive LASSO with respect to the LASSO (see for instant the three last rows in Table 1, where we kept $(n, m) = (20, 30)$). Quite surprisingly, the relative performance of both estimators does not strongly depend on the estimation objective β^* , $X\beta^*$ or $Z\beta^*$, but of the particular ex-

Table 1: Evaluation of the mean ME and the quantile Q_3 of order 0.3 of $PERF(I)$, $PERF(X)$ and $PERF(Z)$. In these experiments, σ always equals 1. The case *sparse* corresponds to $\beta^* = (3, 1.5, 0, 0, 2, 0, 0, 0)$ while the case *very sparse* corresponds to $\beta^* = (5, 0, 0, 0, 0, 0, 0, 0)$.

β^*	(n, m)	ρ	σ	$PERF(I)$		$PERF(X)$		$PERF(Z)$	
				ME	Q_3	ME	Q_3	ME	Q_3
VERY SPARSE	(7, 10)	0.5	1	0.74	0.71	0.76	0.71	0.75	0.70
SPARSE	(7, 10)	0.5	1	0.83	0.76	0.86	0.80	0.88	0.88
SPARSE	(7, 20)	0.5	1	0.84	0.79	0.84	0.81	0.88	0.89
SPARSE	(20, 30)	0.5	1	0.91	0.90	0.93	0.93	0.93	0.95
SPARSE	(20, 30)	0.9	1	0.91	0.93	0.94	0.95	0.93	0.96
SPARSE	(20, 30)	0.5	3	0.90	0.89	0.92	0.92	0.92	0.93

periment we deal with. In some cases (about 50%), $\lambda_1 = 0$ is optimal for all the objectives (so the LASSO and the Transductive LASSO are equivalent), in the other cases the Transductive LASSO performs better.

Another surprising fact that is recurrent on the experiments is that when

$$\min_{(\lambda_1, \lambda_2) \in \Lambda^2} \|X(\beta_{TL}(\lambda_1, \lambda_2) - \beta^*)\|_2^2 < \min_{(\lambda_1, 0) \in \Lambda^2} \|X(\beta_{TL}(\lambda_1, 0) - \beta^*)\|_2^2,$$

this minimum *does not significantly depend on* λ_1 for a very large range of values λ_1 . This is quite interesting for a practitioner as it means that when we use the transductive LASSO, there is only one unknown parameter to be chosen by the statistician (λ_2) and not two.

Discussion on the regularization parameter. Finally, we would like to point out the importance of the parameter λ . Let us plot a graph of a typical experiment (Figure 2). There are two curves on this graph, that represent $(1/n)\|X(\beta_L(\lambda) - \beta^*)\|_2^2$ and $(1/m)\|Z(\beta_L(\lambda) - \beta^*)\|_2^2$ vs. λ . We observe that both functions do not reach their minimum value for the same value of λ (the minimum is highlighted on the graph), but their minimum is quite close.

Since we consider variable selection methods, the identification of the true support $\{j : \beta_j^* \neq 0\}$ of the vector β^* is in concern. One expects that the estimator $\hat{\beta}$ and the true vector β^* share the same support at least when n grows to infinity. This is known as the variable selection consistency problem and it has been considered for the LASSO estimator in several works (see [Bun08, MB06, MY09, Wai06, ZY06]). Recently, [Lou08] provided the variable selection consistency of the Dantzig Selector. Other popular selection procedures, based on the LASSO estimator, such as the Adaptive LASSO [Zou06], the SCAD [FL01], the S-LASSO [Heb08] and the Group-LASSO [Bac08], have also been studied under this angle. Following our previous work [AH08], it is possible to provide such results for the Transductive LASSO.

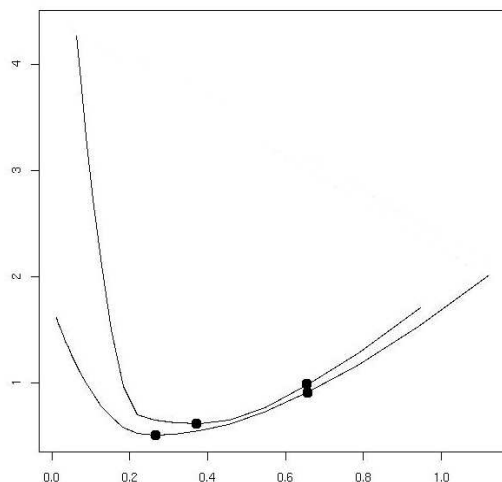


Figure 2: Performance vs. λ .

However, we reported another point on this graph: the minimal value of λ for which the LASSO estimator identifies correctly the non zero components of β^* . This value of λ is quite different from the values that minimizes the prediction losses. This fact is recurrent in almost all the experiments: the estimation $X\beta^*$, $Z\beta^*$ and the support of β^* are three different objectives and have to be treated separately. We cannot expect in general to find a choice for λ which makes the LASSO, for instance, have good performance for all the mentioned objective simultaneously. A more accurate study of the dependence of (a practical choice for) λ to the estimation objective would be needed and will be the topic of a future work.

6 Conclusion

In this paper, we propose variants of the LASSO and the Dantzig Selector, for which we provide theoretical results with less restrictive hypothesis than in previous works. These estimates have a nice interpretation in terms of transductive estimation.

However, the practical pertinence of these estimators is subject to a more accurate investigation of the way to use the additional information given by the new observations. This will be the object of a future work.

7 Proofs

7.1 Proof of Propositions 3.1 and 3.2

Proof of Proposition 3.1. Let us assume that $(X'X)$ is invertible. Then just remark that the criterion minimized by $\hat{\beta}_{\sqrt{n}I, \lambda}$ is just

$$n \left\| \hat{\beta}_{LSE} - \beta \right\|_2^2 + 2\lambda \left\| \Xi_{nI} \beta \right\|_1 = \sum_{j=1}^p \left\{ \left[\left(\hat{\beta}_{LSE} \right)_j - \beta_j \right]^2 + \frac{2\lambda \xi_j(\sqrt{n}I)}{n} |\beta_j| \right\}.$$

So we can optimize with respect to each coordinate β_j individually. It is quite easy to check that the solution is, for β_j ,

$$\text{sgn} \left(\left(\hat{\beta}_{LSE} \right)_j \right) \left(\left| \left(\hat{\beta}_{LSE} \right)_j \right| - \frac{\lambda \xi_j(\sqrt{n}I)}{n} \right)_+.$$

The proof for $\hat{\beta}_{\sqrt{n}I, \lambda}$ is also easy as it solves

$$\begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|\beta\|_1 \\ \text{s.t. } \left\| n \Xi_{nI}^{-1} (\hat{\beta}_{LSE} - \beta) \right\|_\infty \leq \lambda. \end{cases}$$

□

Proof of Proposition 3.2. Let us write the Lagrangian of the program

$$\begin{cases} \arg \min_{\beta \in \mathbb{R}^p} \|A\beta\|_2^2 \\ \text{s.t. } \left\| \Xi_A^{-1}(A'A) \left((\widetilde{X'X})^{-1} X'Y - \beta \right) \right\|_\infty \leq \lambda, \end{cases}$$

$$\begin{aligned} \mathcal{L}(\beta, \gamma, \mu) = & \beta(Z'Z)\beta + \gamma' \left[\Xi_A^{-1}(A'A) \left((\widetilde{X'X})^{-1} X'Y - \beta \right) - \lambda E \right] \\ & + \mu' \left[\Xi_A^{-1}(A'A) (\beta - (\widetilde{X'X})^{-1} X'Y) - \lambda E \right] \end{aligned}$$

with $E = (1, \dots, 1)'$, and for any j , $\gamma_j \geq 0$, $\mu_j \geq 0$ and $\gamma_j \mu_j = 0$. Any solution $\underline{\beta} = \underline{\beta}(\gamma, \mu)$ must satisfy

$$0 = \frac{\partial \mathcal{L}}{\partial \underline{\beta}}(\underline{\beta}, \lambda, \mu) = 2\underline{\beta}(A'A) + (\gamma - \mu) \Xi_A^{-1}(A'A)$$

so

$$(A'A)\underline{\beta} = (A'A) \Xi_A^{-1} \frac{\mu - \gamma}{2}.$$

Note that the conditions $\gamma_j \geq 0$, $\mu_j \geq 0$ and $\gamma_j \mu_j = 0$ means that there is a $\zeta_j \in \mathbb{R}$ such that $\zeta_j = \xi_j^{\frac{1}{2}}(A)(\mu_j - \gamma_j)/2$, $|\zeta_j| = \xi_j^{\frac{1}{2}}(A)(\gamma_j + \mu_j)/2$, and

so $\gamma_j = 2(\zeta_j/\xi_j^{\frac{1}{2}}(A))_-$ and $\mu_j = 2(\zeta_j/\xi_j^{\frac{1}{2}}(A))_+$, where $(a)_+ = \max(a; 0)$ and $(a)_- = \max(-a; 0)$. Let also ζ denote the vector which j -th component is exactly ζ_j , we obtain

$$(A'A)\underline{\beta} = (A'A)\zeta,$$

or, using the condition $\text{Ker}(A) = \text{Ker}(X)$, $X\underline{\beta} = X\zeta$ and $A\underline{\beta} = A\zeta$. This leads to

$$\mathcal{L}(\underline{\beta}, \gamma, \mu) = -2Y'X(\widetilde{X'X})^{-1}(A'A)\zeta + \zeta'(A'A)\zeta + 2\lambda\|\Xi_A\zeta\|_1,$$

and note that the first order condition also implies that γ and μ (and so ζ) maximize \mathcal{L} . This ends the proof. \square

7.2 A useful Lemma

The following lemma will be used in the proofs of Theorems 3.3 and 3.4.

Lemma 7.1. *Let us put $\varepsilon = (\varepsilon_1, \dots, \varepsilon_n)'$. Under the assumption that $\text{Ker}(A) = \text{Ker}(X)$ we have, with probability at least $1 - \eta$,*

$$\forall j \in \{1, \dots, p\}, \left| \left[A'A(\widetilde{X'X})^{-1}X'\varepsilon \right]_j \right| \leq \xi_j(A)\sigma\sqrt{2n\log\frac{p}{\eta}},$$

or, in other words,

$$\|\Xi_A^{-1}(A'A)((\widetilde{X'X})^{-1}X'Y - \beta^*)\|_\infty \leq \sigma\sqrt{2n\log\frac{p}{\eta}}.$$

Proof of the lemma. By definition, $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$ and so

$$(A'A)(\widetilde{X'X})^{-1}X'\varepsilon \sim \mathcal{N}(0, \sigma^2(A'A)(\widetilde{X'X})^{-1}(A'A)).$$

So, for all j , $[(A'A)(\widetilde{X'X})^{-1}X'\varepsilon]_j$ comes from a $\mathcal{N}(0, \sigma^2\xi_j^2(A))$ distribution. This implies the first point, the second one is trivial using $Y = X\beta^* + \varepsilon$. \square

7.3 Proof of Theorems 3.3 and 3.4

Proof of Theorem 3.3. By definition of $\hat{\beta}_{A,\lambda}$ we have

$$\begin{aligned} & -2Y'X(\widetilde{X'X})^{-1}(A'A)\hat{\beta}_{A,\lambda} + \left(\hat{\beta}_{A,\lambda}\right)'(A'A)\hat{\beta}_{A,\lambda} + 2\lambda\|\Xi_{A'A}\hat{\beta}_{A,\lambda}\|_1 \\ & \leq 2Y'X(\widetilde{X'X})^{-1}(A'A)\beta^* + (\beta^*)'(A'A)\beta^* + 2\lambda\|\Xi_A\beta^*\|_1. \end{aligned}$$

Since $Y = X\beta^* + \varepsilon$, we obtain

$$\begin{aligned} & 2(\beta^*)'X'X(\widetilde{X'X})^{-1}(A'A)\left(\beta^* - \hat{\beta}_{A,\lambda}\right) + \left(\hat{\beta}_{A,\lambda}\right)'(A'A)\hat{\beta}_{A,\lambda} - (\beta^*)'(A'A)\beta^* \\ & + 2\varepsilon'X(\widetilde{X'X})^{-1}(A'A)\left(\beta^* - \hat{\beta}_{A,\lambda}\right) \leq 2\lambda\|\Xi_A\beta^*\|_1 - 2\lambda\|\Xi_A\hat{\beta}_{A,\lambda}\|_1. \end{aligned}$$

Now, if $\text{Ker}(X) = \text{Ker}(A)$ then we have $X'X(\widetilde{X'X})^{-1}(A'A) = (A'A)$ and then the previous inequality leads to

$$\begin{aligned} & (\beta^* - \hat{\beta}_{A,\lambda})' (A'A) (\beta^* - \hat{\beta}_{A,\lambda}) \\ & \leq 2\varepsilon' X(\widetilde{X'X})^{-1}(A'A) (\hat{\beta}_{A,\lambda} - \beta^*) + 2\lambda \|\Xi_A \beta^*\|_1 - 2\lambda \|\Xi_A \hat{\beta}_{A,\lambda}\|_1. \end{aligned} \quad (8)$$

Now we have to work on the term $2\varepsilon' X(\widetilde{X'X})^{-1}(A'A) (\hat{\beta}_{A,\lambda} - \beta^*)$. Note that

$$\begin{aligned} 2\varepsilon' X(\widetilde{X'X})^{-1}(A'A) (\hat{\beta}_{A,\lambda} - \beta^*) &= 2 \sum_{j=1}^p (\hat{\beta}_{A,\lambda} - \beta^*)_j \left[(A'A)(\widetilde{X'X})^{-1} X' \varepsilon \right]_j \\ &\leq 2 \sum_{j=1}^p \left| (\hat{\beta}_{A,\lambda} - \beta^*)_j \right| \left| \left[(A'A)(\widetilde{X'X})^{-1} X' \varepsilon \right]_j \right| \\ &\leq 2\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \sum_{j=1}^p \xi_j^{\frac{1}{2}}(A) \left| (\hat{\beta}_{A,\lambda})_j - \beta_j^* \right| \end{aligned}$$

with probability at least $1 - \eta$, by Lemma 7.1. We plug this result into Inequality (8) (and replace λ by its value $2\sigma \sqrt{2n \log(p/\eta)}$) to obtain

$$\begin{aligned} & (\beta^* - \hat{\beta}_{A,\lambda})' (A'A) (\beta^* - \hat{\beta}_{A,\lambda}) \\ & \leq 2\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \sum_{j=1}^p \xi_j^{\frac{1}{2}}(A) \left\{ \left| (\hat{\beta}_{A,\lambda})_j - \beta_j^* \right| + 2 \left(|\beta_j^*| - \left| (\hat{\beta}_{A,\lambda})_j \right| \right) \right\} \end{aligned}$$

and then

$$\begin{aligned} & (\beta^* - \hat{\beta}_{A,\lambda})' (A'A) (\beta^* - \hat{\beta}_{A,\lambda}) \\ & + 2\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \sum_{j=1}^p \xi_j^{\frac{1}{2}}(A) \left| (\hat{\beta}_{A,\lambda})_j - \beta_j^* \right| \\ & \leq 4\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \sum_{j=1}^p \xi_j^{\frac{1}{2}}(A) \left\{ \left| (\hat{\beta}_{A,\lambda})_j - \beta_j^* \right| + |\beta_j^*| - \left| (\hat{\beta}_{A,\lambda})_j \right| \right\} \\ & = 4\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \sum_{j:\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) \left\{ \left| (\hat{\beta}_{A,\lambda})_j - \beta_j^* \right| + |\beta_j^*| - \left| (\hat{\beta}_{A,\lambda})_j \right| \right\} \\ & \leq 8\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \sum_{j:\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) \left| (\hat{\beta}_{A,\lambda})_j - \beta_j^* \right|. \end{aligned} \quad (9)$$

This implies, in particular, that $\beta^* - \hat{\beta}_{A,\lambda}$ is an admissible vector α in Assumption $H(A'A, 3)$ because

$$\sum_{j=1}^p \xi_j^{\frac{1}{2}}(A) \left| \left(\hat{\beta}_{A,\lambda} \right)_j - \beta_j^* \right| \leq 4 \sum_{j:\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) \left| \left(\hat{\beta}_{A,\lambda} \right)_j - \beta_j^* \right|.$$

So, Inequality (9) becomes

$$\begin{aligned} & \left(\beta^* - \hat{\beta}_{A,\lambda} \right)' (A'A) \left(\beta^* - \hat{\beta}_{A,\lambda} \right) + 2\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \left\| \Xi_A \left(\beta^* - \hat{\beta}_{A,\lambda} \right) \right\|_1 \\ & \leq 8\sigma \sqrt{2n \log \left(\frac{p}{\eta} \right)} \sum_{j:\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) \left| \left(\hat{\beta}_{A,\lambda} \right)_j - \beta_j^* \right| \\ & \leq 8\sigma \sqrt{2n \sum_{j:\beta_j^* \neq 0} \left[\left(\hat{\beta}_{A,\lambda} \right)_j - \beta_j^* \right]^2 \sum_{j:\beta_j^* \neq 0} \xi_j(A) \log \left(\frac{p}{\eta} \right)} \\ & \leq 8\sigma \sqrt{\frac{2}{c(A)} \left(\beta^* - \hat{\beta}_{A,\lambda} \right)' (A'A) \left(\beta^* - \hat{\beta}_{A,\lambda} \right) \sum_{j:\beta_j^* \neq 0} \xi_j(M) \log \left(\frac{p}{\eta} \right)}, \end{aligned}$$

by Assumption $H(A'A, 3)$ and then

$$\left(\beta^* - \hat{\beta}_{A,\lambda} \right)' (A'A) \left(\beta^* - \hat{\beta}_{A,\lambda} \right) \leq 128 \frac{\sigma^2}{c(A'A)} \log \left(\frac{p}{\eta} \right) \sum_{j:\beta_j^* \neq 0} \xi_j(A),$$

and

$$\left\| \Xi_A \left(\beta^* - \hat{\beta}_{A,\lambda} \right) \right\|_1 \leq 64 \frac{\sigma}{c(A'A)} \sqrt{\frac{\log \left(\frac{p}{\eta} \right)}{2n}} \sum_{j:\beta_j^* \neq 0} \xi_j(A).$$

□

Proof of Theorem 3.4. We have

$$\begin{aligned} & \left(\tilde{\beta}_{A,\lambda} - \beta^* \right)' (A'A) \left(\tilde{\beta}_{A,\lambda} - \beta^* \right) = \left[\Xi_A \left(\tilde{\beta}_{A,\lambda} - \beta^* \right) \right]' \Xi_A^{-1} (A'A) \left(\tilde{\beta}_{A,\lambda} - \beta^* \right) \\ & \leq \left\| \Xi_A \left(\tilde{\beta}_{A,\lambda} - \beta^* \right) \right\|_1 \left\| \Xi_A^{-1} (A'A) \left(\tilde{\beta}_{A,\lambda} - \beta^* \right) \right\|_\infty \\ & \leq \left\| \Xi_A \left(\tilde{\beta}_{A,\lambda} - \beta^* \right) \right\|_1 \left\{ \left\| \Xi_A^{-1} (A'A) \left((\widetilde{X'X})^{-1} X'Y - \beta^* \right) \right\|_\infty \right. \\ & \quad \left. + \left\| \Xi_A^{-1} (A'A) \left((\widetilde{X'X})^{-1} X'Y - \tilde{\beta}_{A,\lambda} \right) \right\|_\infty \right\}, \quad (10) \end{aligned}$$

by the constraint on the definition on $\tilde{\beta}_{A,\lambda}$ we have

$$\left\| \Xi_A^{-1} (A'A) \left((\widetilde{X'X})^{-1} X'Y - \tilde{\beta}_{A,\lambda} \right) \right\|_\infty \leq \lambda,$$

while Lemma 7.1 implies that for $\lambda = 2\sigma\sqrt{2n\log(p/\eta)}$ we have

$$\|\Xi_A^{-1}(A'A)((\widetilde{X}'\widetilde{X})^{-1}X'Y - \beta^*)\|_\infty \leq \frac{\lambda}{2},$$

with probability at least $1 - \eta$; and so:

$$(\tilde{\beta}_{A,\lambda} - \beta^*)'(A'A)(\tilde{\beta}_{A,\lambda} - \beta^*) \leq \frac{3\lambda}{2} \|\Xi_A(\tilde{\beta}_{A,\lambda} - \beta^*)\|_1.$$

Moreover note that, by definition,

$$\begin{aligned} 0 &\leq \|\Xi_A\beta^*\|_1 - \|\Xi_A\tilde{\beta}_{A,\lambda}\|_1 \\ &= \sum_{\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) |\beta_j^*| - \sum_{\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) |(\tilde{\beta}_{A,\lambda})_j| - \sum_{\beta_j^* = 0} \xi_j^{\frac{1}{2}}(A) |(\tilde{\beta}_{A,\lambda})_j| \\ &\leq \sum_{\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) |\beta_j^* - (\tilde{\beta}_{A,\lambda})_j| - \sum_{\beta_j^* = 0} \xi_j^{\frac{1}{2}}(A) |\beta_j^* - (\tilde{\beta}_{A,\lambda})_j|, \end{aligned}$$

this implies that $\beta^* - (\tilde{\beta}_{A,\lambda})$ is an admissible vector in the relation that defines assumption $H(A'A, 1)$.

Let us combine this result with Inequality (10), we obtain

$$\begin{aligned} (\tilde{\beta}_{A,\lambda} - \beta^*)'(A'A)(\tilde{\beta}_{A,\lambda} - \beta^*) &\leq \frac{3\lambda}{2} \|\Xi_A(\tilde{\beta}_{A,\lambda} - \beta^*)\|_1 \\ &\leq 3\lambda \sum_{\beta_j^* \neq 0} \xi_j^{\frac{1}{2}}(A) |\beta_j^* - (\tilde{\beta}_{A,\lambda})_j| \\ &\leq 3\lambda \sqrt{\left(\sum_{\beta_j^* \neq 0} \xi_j(A) \right) \left(\sum_{\beta_j^* \neq 0} |\beta_j^* - (\tilde{\beta}_{A,\lambda})_j|^2 \right)} \\ &\leq 3\lambda \left(\sum_{\beta_j^* \neq 0} \xi_j(A) \right)^{\frac{1}{2}} \sqrt{\frac{1}{nc(A'A)} (\tilde{\beta}_{A,\lambda} - \beta^*)'(A'A)(\tilde{\beta}_{A,\lambda} - \beta^*)}. \quad (11) \end{aligned}$$

So we have,

$$(\tilde{\beta}_{A,\lambda} - \beta^*)'(A'A)(\tilde{\beta}_{A,\lambda} - \beta^*) \leq 9\lambda^2 \frac{1}{nc(A'A)} \sum_{\beta_j^* \neq 0} \xi_j(A),$$

and as a consequence, Inequality (11) gives the upper bound on $\|\Xi_A(\tilde{\beta}_{A,\lambda} - \beta^*)\|_1$, and this ends the proof. \square

7.4 Proof of Theorem 4.1

Proof of Theorem 4.1. The proof is almost the same as in the previous case. For the sake of simplicity, let us write $\tilde{\beta}^*$ instead of $\tilde{\beta}_{\lambda_2, \sqrt{n/m}Z}^*$ and the same for $\hat{\beta}^*$. We first give a look at the Dantzig Selector:

$$\begin{aligned}
\frac{n}{m} (\tilde{\beta}^* - \beta^*)' Z' Z (\tilde{\beta}^* - \beta^*) &\leq \|\tilde{\beta}^* - \beta^*\|_1 \left\| \frac{n}{m} Z' Z (\tilde{\beta}^* - \beta^*) \right\|_\infty \\
&\leq \|\tilde{\beta}^* - \beta^*\|_1 \left\{ \left\| \frac{n}{m} Z' (Z\tilde{\beta}^* - \check{Y}_{\lambda_1}) \right\|_\infty + \left\| \frac{n}{m} Z' (Z\beta^* - \check{Y}_{\lambda_1}) \right\|_\infty \right\} \\
&\leq \|\tilde{\beta}^* - \beta^*\|_1 \left\{ \left\| \frac{n}{m} Z' (Z\tilde{\beta}^* - \check{Y}_{\lambda_1}) \right\|_\infty + \|X'(X\beta^* - Y)\|_\infty \right. \\
&\quad \left. + \left\| X'(X\tilde{\beta}_{X,\lambda_1/2} - Y) \right\|_\infty + \left\| \left(\frac{n}{m} Z' Z - X'X \right) (\beta^* - \tilde{\beta}_{X,\lambda_1/2}) \right\|_\infty \right\}. \quad (12)
\end{aligned}$$

By Lemma 7.1, for $\lambda_1 = 2\sigma\sqrt{2n\log(p/\eta)}$ we have

$$\|X'Y - X'X\beta^*\|_\infty \leq \frac{\lambda_1}{2},$$

with probability at least $1 - \eta$, while Inequality (7) ensures that

$$\left\| \left(\frac{n}{m} Z' Z - X'X \right) u \right\|_\infty \leq \frac{\lambda_1}{2},$$

for any u such that $\|u\|_1 \leq \|\beta^*\|_1$. Moreover, we have

$$\|\beta^* - \tilde{\beta}_{X,\lambda_1/2}\|_1 \leq \|\beta^*\|_1 + \|\tilde{\beta}_{X,\lambda_1/2}\|_1 \leq 2\|\beta^*\|_1,$$

by definition of the Dantzig Selector. This definition also implies that

$$\left\| X' (X\tilde{\beta}_{X,\lambda_1/2} - Y) \right\|_\infty \leq \frac{\lambda_1}{2},$$

and finally the definition of the estimator leads to

$$\left\| \frac{n}{m} Z' (Z\tilde{\beta}^* - \check{Y}_{\lambda_1}) \right\|_\infty \leq \frac{\lambda_2}{2} = \frac{\lambda_1}{2},$$

and as a consequence Inequality (12) becomes

$$\frac{n}{m} (\tilde{\beta}^* - \beta^*)' Z' Z (\tilde{\beta}^* - \beta^*) \leq \frac{5\lambda_1}{2} \|\tilde{\beta}^* - \beta^*\|_1.$$

Using the fact that $\|\tilde{\beta}^*\|_1 \leq \|\beta^*\|_1$ gives

$$\begin{aligned}
\frac{n}{m} (\tilde{\beta}^* - \beta^*)' Z' Z (\tilde{\beta}^* - \beta^*) &\leq \frac{5\lambda_1}{2} \|\tilde{\beta}^* - \beta^*\|_1 \leq 5\lambda_1 \sum_{\beta_j^* \neq 0} |\beta_j^* - (\tilde{\beta}^*)_j| \\
&\leq 5\lambda_1 \sqrt{|\{j : \beta_j^* \neq 0\}| \left(\sum_{\beta_j^* \neq 0} |\beta_j^* - (\tilde{\beta}^*)_j|^2 \right)} \\
&\leq 5\lambda_1 |\{j : \beta_j^* \neq 0\}|^{\frac{1}{2}} \sqrt{\frac{1}{nc(n/m(Z'Z))} \frac{n}{m} (\tilde{\beta}^* - \beta^*)' Z' Z (\tilde{\beta}^* - \beta^*)}. \quad (13)
\end{aligned}$$

Then we have,

$$\frac{n}{m} \left(\tilde{\beta}^* - \beta^* \right)' Z' Z \left(\tilde{\beta}^* - \beta^* \right) \leq 25\lambda_1^2 |\{j : \beta_j^* \neq 0\}| \frac{1}{nc(n/m(Z'Z))},$$

this ends the proof for the Dantzig Selector.

Now, let us deal with the LASSO case. The dual form of the definition of the estimator leads to

$$\begin{aligned} -2\frac{n}{m}\check{Y}_{\lambda_1} Z\hat{\beta}^* + \frac{n}{m}(\hat{\beta}^*)' Z' Z\hat{\beta}^* + 4\lambda_2\|\hat{\beta}^*\|_1 \\ \leq -2\frac{n}{m}\check{Y}_{\lambda_1} Z\beta^* + \frac{n}{m}(\beta^*)' Z' Z\beta^* + 4\lambda_2\|\beta^*\|_1 \end{aligned}$$

and so

$$\begin{aligned} -2\frac{n}{m}\tilde{\beta}_{X,\lambda_1} Z' Z\hat{\beta}^* + \frac{n}{m}(\hat{\beta}^*)' Z' Z\hat{\beta}^* + 4\lambda_2\|\hat{\beta}^*\|_1 \\ \leq -2\frac{n}{m}\tilde{\beta}_{X,\lambda_1} Z' Z\beta^* + \frac{n}{m}(\beta^*)' Z' Z\beta^* + 4\lambda_2\|\beta^*\|_1. \end{aligned}$$

As a consequence,

$$\begin{aligned} \frac{n}{m} \left(\hat{\beta}^* - \beta^* \right)' Z' Z \left(\hat{\beta}^* - \beta^* \right) \\ \leq 2\frac{n}{m} \left(\hat{\beta}^* - \beta^* \right)' Z' Z \left(\tilde{\beta}_{X,\lambda_1} - \beta^* \right) + 4\lambda_2 \left(\|\beta^*\|_1 - \|\hat{\beta}^*\|_1 \right). \end{aligned}$$

Now, we try to upper bound $\left(\hat{\beta}^* - \beta^* \right)' Z' Z \left(\tilde{\beta}_{X,\lambda_1} - \beta^* \right)$. We remark that

$$\begin{aligned} \frac{n}{m} \left(\hat{\beta}^* - \beta^* \right)' Z' Z \left(\tilde{\beta}_{X,\lambda_1} - \beta^* \right) &\leq \left\| \hat{\beta}^* - \beta^* \right\|_1 \left\| \frac{n}{m} (Z' Z) \left(\tilde{\beta}_{X,\lambda_1} - \beta^* \right) \right\|_\infty \\ &\leq \left\| \hat{\beta}^* - \beta^* \right\|_1 \left[\left\| \left(\frac{n}{m} Z' Z - X' X \right) \left(\tilde{\beta}_{X,\lambda_1} - \beta^* \right) \right\|_\infty \right. \\ &\quad \left. + \left\| \frac{n}{m} (X' X) \left(\tilde{\beta}_{X,\lambda_1} - \beta^* \right) \right\|_\infty \right] \leq \left\| \hat{\beta}^* - \beta^* \right\|_1 \left[\lambda_2 + \frac{\lambda_1}{2} \right], \end{aligned}$$

and then we have

$$\begin{aligned} \frac{n}{m} \left(\hat{\beta}^* - \beta^* \right)' Z' Z \left(\hat{\beta}^* - \beta^* \right) \\ \leq \left\| \hat{\beta}^* - \beta^* \right\|_1 [2\lambda_2 + \lambda_1] + 4\lambda_2 \left(\|\beta^*\|_1 - \|\hat{\beta}^*\|_1 \right) \\ = 3\lambda_1 \left\| \hat{\beta}^* - \beta^* \right\|_1 + 4\lambda_1 \left(\|\beta^*\|_1 - \|\hat{\beta}^*\|_1 \right) \end{aligned}$$

and so

$$\begin{aligned} \frac{n}{m} \left(\hat{\beta}^* - \beta^* \right)' Z' Z \left(\hat{\beta}^* - \beta^* \right) + \lambda_1 \left\| \hat{\beta}^* - \beta^* \right\|_1 \\ \leq 4\lambda_1 \left(\left\| \hat{\beta}^* - \beta^* \right\|_1 + \|\beta^*\|_1 - \|\hat{\beta}^*\|_1 \right) \end{aligned}$$

and the proof of Theorem 4.1 is completed. \square

7.5 Proof of Proposition 4.2

Proof of Proposition 4.2. First, let us remark that

$$\begin{aligned} \left\| \left(X'X - \frac{n}{m} Z'Z \right) u \right\|_{\infty} &= n \sup_{1 \leq i \leq p} \sum_{j=1}^p u_j \left(\frac{X'_i X_j}{n} - \frac{Z'_i Z_j}{m} \right) \\ &\leq n \|u\|_1 \sup_{1 \leq i, j \leq p} \left| \frac{X'_i X_j}{n} - \frac{Z'_i Z_j}{m} \right|. \end{aligned}$$

Now, using the "exchangeable-distribution inequality" in [Cat07] we obtain, for a given pair (i, j) , for any $\lambda > 0$, with probability at least $1 - \eta$,

$$\begin{aligned} \frac{X'_i X_j}{n} - \frac{Z'_i Z_j}{m} &\leq \frac{\lambda k^2}{2n(k+1)^2} \left(\frac{1}{m} \sum_{k=1}^m X_{i,k}^2 X_{j,k}^2 \right) + \frac{\log \frac{1}{\eta}}{\lambda} \\ &\leq \frac{\lambda k^2 \kappa^2}{2n(k+1)^2} + \frac{\log \frac{1}{\eta}}{\lambda} = \frac{\kappa k}{k-1} \sqrt{\frac{2 \log \frac{1}{\eta}}{n}}, \end{aligned}$$

for $\lambda = (\log(1/\eta)(k-1)2n/k\kappa^2)^{1/2}$ and so, by a union bound argument, with probability at least $1 - \eta$, for any pair (i, j) ,

$$\left| \frac{X'_i X_j}{n} - \frac{Z'_i Z_j}{m} \right| \leq \frac{\kappa k}{k-1} \sqrt{\frac{2 \log \frac{2p^2}{\eta}}{n}} \leq \frac{2\kappa k}{k-1} \sqrt{\frac{2 \log \frac{p}{\eta}}{n}},$$

(where we used $p \geq 2$). □

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