Asymptotic Confidence Regions for Highdimensional Structured Sparsity.

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Abstract

In the setting of high-dimensional linear regression models, we propose two frameworks for constructing pointwise and group confidence sets for penalized estimators which incorporate prior knowledge about the organization of the non-zero coefficients. This is done by desparsifying the estimator as in van de Geer et al. [18] and van de Geer and Stucky [17], then using an appropriate estimator for the precision matrix Θ . In order to estimate the precision matrix a corresponding structured matrix norm penalty has to be introduced. After normalization the result is an asymptotic pivot. The asymptotic behavior is studied and simulations are added to study the differences between the two schemes.

Keywords— Asymptotic confidence regions, structured sparsity, high-dimensional linear regression, penalization.

1 Introduction

We focus on the basic high dimensional linear regression model, which is at the core of understanding more complex models:

$$Y = X\beta^0 + \epsilon. \tag{1.1}$$

Here $Y \in \mathbb{R}^n$ is an observable response variable, X is a given $n \times p$ design matrix with p >> n, $\beta^0 \in \mathbb{R}^p$ is a parameter vector of unknown coefficients and $\epsilon \in \mathbb{R}^n$ is unobservable noise. Due to the high-dimensionality of the design the question arises as to find the solution to an underdetermined system. The idea to restrict ourselves to sparse solutions has become the new paradigm to solve this problem for high-dimensional data. In such a setting, the LASSO estimator (introduced by Tibshirani [15]) is the most widely used method in pursuance of estimating the unknown parameter vector β^0 , while avoiding the high-dimensional problem of overfitting:

$$\hat{\beta}_{\ell_1} := \operatorname*{arg\,min}_{\beta \in \mathbb{R}^p} \left\{ \|Y - X\beta\|_n^2 + 2\lambda_L \|\beta\|_1 \right\}.$$

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The loss function is defined as $||Y - X\beta||_n^2 := \sum_{j=1}^n (Y - X\beta)_j^2/n$, and $||\beta||_1$ denotes the ℓ_1 -norm. The main purpose of the added ℓ_1 -norm penalty is to achieve an entry-wise sparse $\hat{\beta}_{\ell_1}$ solution, while at the same time the least squares loss ensures good prediction properties. Furthermore the constant $\lambda_L > 0$ is the penalty level, regulating the amount of sparsity introduced to the solution.

The ℓ_1 -norm penalty is a simple convex relaxation of the non-convex ℓ_0 penalty ($\|\beta\|_{\ell_0} := \#\{i: \beta_i \neq 0\}$). Let us recall that the ℓ_1 -norm penalty does not promote any specific sparsity structure. In other words the LASSO estimator does not assume anything about the organization of the non-zero coefficients. In this sense the LASSO estimator does not incorporate any prior knowledge of the structure of the true unknown active set $S_0 := \{i: \beta_{0,i} \neq 0\}$. In practice however, prior knowledge is often available. Prior knowledge may emerge from physical systems or known biological processes. For the purpose of integrating the available prior information, the ℓ_1 -norm penalty needs to be replaced in such a way, that the new penalty reflects this knowledge. One can find many examples of such penalties and their properties in the recently emerging literature on the sparsity structure of the unknown parameter vector, see for example Bach [2], Bach et al. [1], Micchelli et al. [10], Micchelli et al. [9], Maurer and Pontil [6]. A more comprehensive overview can be found in Obozinski and Bach [12].

We will focus on norm penalties and therefore generalize the LASSO estimator to a large family of penalized estimators (see van de Geer [16] and Stucky and van de Geer [14]), each with distinct properties to promote sparsity structures in the parameter vector:

$$\hat{\beta}_{\Omega} := \underset{\beta \in \mathbb{R}^p}{\arg \min} \left\{ \|Y - X\beta\|_n^2 + \lambda \Omega(\beta) \right\}. \tag{1.2}$$

Here Ω is any norm on \mathbb{R}^p that reflects some aspects of the pattern of sparsity for the parameter vector β^0 . Again for readability we let $\hat{\beta} = \hat{\beta}_{\Omega}$. We characterize the Ω -norm in terms of its weakly decomposable subsets of \mathbb{R}^p . A weakly decomposable norm is in some sense able to split up into two norms, one norm measuring the size of the vector on the active set and the other norm the size on its complement. The weakly decomposable norm itself reflects the prior information of the underlying sparsity.

Notation: Depending on the context, for a set $J \subset \{1, ..., p\}$ and a vector $\beta \in \mathbb{R}^p$ the vector β_J is either the |J|-dimensional vector $\{\beta_j: j \in J\}$ or the p-dimensional vector $\{\beta_j | \{j \in J\}: j = 1, ..., p\}$. More generally, for a vector $w_J := \{w_j: j \in J\}$, we use the same notation for its extended version $w_J \in \mathbb{R}^p$ where $w_{j,J} = 0$ for all $j \notin J$. For a set \mathcal{B} we let $\mathcal{B}_J = \{\beta_J: \beta \in \mathcal{B}\}$.

The definition of a weakly decomposable norm is crucial to the following sections, so we introduce it as in van de Geer [16] or Stucky and van de Geer [14]. This idea goes back to Bach et al. [1].

Definition 1 (Weak decomposability). A norm Ω in \mathbb{R}^p is called weakly decomposable for an index set $S \subset \{1,...,p\}$, if there exists another norm Ω^{S^c} on $\mathbb{R}^{|S^c|}$ such that

$$\forall \beta \in \mathbb{R}^p: \quad \Omega(\beta_S) + \Omega^{S^c}(\beta_{S^c}) \le \Omega(\beta). \tag{1.3}$$

A set S is called allowed if Ω is a weakly decomposable norm for this set. From now on we use the notation $\Upsilon_S(\beta) := \Omega(\beta_S) + \Omega^{S^c}(\beta_{S^c})$ the lower bounding norm from the weak decomposability definition and $\Lambda_S(\beta) := \Omega(\beta_S) + \Omega(\beta_{S^c})$ the upper bounding norm from the triangle inequality. The weak decomposability now reads

$$\Upsilon_S(\beta) \leq \Omega(\beta) \leq \Lambda_S(\beta)$$
.

Therefore the Υ_S -norm mimics the decomposability property of the ℓ_1 -norm $(\|\beta\|_1 = \|\beta_S\|_1 + \|\beta_{S^c}\|_1)$ for the set S.

For the LASSO estimator, most work up until recently has been focusing on point estimation among other topics, with not much focus on establishing uncertainty in high dimensional models. Interest has been growing rapidly on the very important topic of constructing confidence regions for the LASSO estimator, see for example van de Geer et al. [18], van de Geer and Stucky [17], Zhang and Zhang [21], Javanmard and Montanari [5] and Meinshausen [7]. When it comes to confidence regions for structured sparsity estimators there has not yet been done much work to our knowledge. The paper van de Geer and Stucky [17] mentions one approach for group confidence regions for structured sparsity briefly, which we will develop further.

The main goal of this paper is therefore to construct asymptotic group confidence regions for structured sparsity estimators in two possible ways. In order to do this, we introduce a de-sparsified version of the estimators in (1.2), following the idea of van de Geer et al. [18]. An appropriate estimation of the precision matrix will be needed for the definition of a de-sparsified estimator. The estimation of the precision matrix can be done in two ways which are beneficial for the construction of asymptotic confidence regions. These two frameworks differ in the structure of the penalty function. The theoretical behavior and the assumptions on the sparsity is studied. Furthermore, a simulation compares these two frameworks in the high dimensional case and outlines potential applications.

2 De-sparsified Ω structured estimator

For a given norm $\Omega(\cdot)$ on \mathbb{R}^p we can determine its sparsity structure by listing all the subsets $\mathfrak{S} := \{S_1, ..., S_k\}$ for which the norm is weakly decomposable. The estimator $\hat{\beta}_{\Omega}$ (1.2) prefers to set the complement of any of the sets $S_1^c, ..., S_k^c$ to zero. Unfortunately the joint distribution of estimator (1.2) is not easy to access. But it is possible to de-sparsify (1.2) and asymptotically describe the distribution of this new estimator. The essential idea for the de-sparsified estimator comes from the following lemma, which establishes a variation to the KKT conditions of $\hat{\beta}_{\Omega}$, following directly from Stucky and van de Geer [14].

Lemma 1. For the estimator defined in (1.2) with $\hat{\epsilon} := Y - X\hat{\beta}$ the KKT conditions are $X^T\hat{\epsilon}/n = \lambda \hat{Z}$, where $\Omega^*(\hat{Z}) \leq 1$ and $\hat{Z}^T\hat{\beta} = \Omega(\hat{\beta})$.

Here $\Omega^*(\cdot)$ is another norm on \mathbb{R}^p called the dual norm.

$$\Omega^*(\alpha) := \sup_{\beta \in \mathbb{R}^p, \Omega(\beta) = 1} \beta^T \alpha.$$

Since $Y = X\beta^0 + \epsilon$ and using the notation $\hat{\Sigma} := X^T X/n$ we can write the KKT conditions as

$$\hat{\Sigma}(\hat{\beta} - \beta^0) + \lambda \hat{Z} = X^T \epsilon / n.$$

Suppose we have an appropriate surrogate for the precision matrix $\hat{\Theta}$, we get

$$\hat{\Theta}\hat{\Sigma}(\hat{\beta}-\beta^0) + \lambda\hat{\Theta}\hat{Z} = \hat{\Theta}X^T\epsilon/n$$
, and

$$\hat{\beta} + \lambda \hat{\Theta} \hat{Z} - \beta^0 = \hat{\Theta} X^T \epsilon / n + \Delta / \sqrt{n}$$

Here $\Delta := \sqrt{n}(\hat{\Theta}\hat{\Sigma} - I)(\hat{\beta} - \beta^0)$ is the error term. We define the de-sparsified Ω structured estimator as follows.

Definition 2. The de-sparsified Ω structured estimator is

$$\hat{b}_{\Omega} := \hat{\beta} + \lambda \hat{\Theta} \hat{Z}.$$

When $\Omega(\cdot) = \|\cdot\|_1$ is the ℓ_1 -norm, and if we have a β_{ℓ_1} sparsity assumption of order $o(\sqrt{n}/\log(p))$, a reasonable sparsity assumption on the precision matrix and if we assume the errors to follow i.i.d. Gaussian distributions, then van de Geer et al. [18] have shown that the de-sparsified ℓ_1 structured estimator follows an asymptotic Gaussian distribution with an asymptotically negligible error term.

In order to get similar results for the Ω penalization, we need to discuss how to estimate the precision matrix $\hat{\Theta}$. The main problem that arises is, that good estimation error bounds are only available expressed in the $\Upsilon_{S_{\star}}$ -norm, where S_{\star} is the unknown oracle set from the main theorem in Stucky and van de Geer [14]. The next two sections give two different ways to estimate $\hat{\Theta}$ in such a way that Δ is asymptotically negligible.

3 First framework: gauge confidence regions

A way to construct an estimate for the precision matrix is to do |J|-wise regression with any fixed set $J \subset \{1,...,p\}$. |J|-wise regression is a very similar method as node-wise regression (introduced by Meinshausen and Bühlmann [8]), but instead of one node, we have simultaneously |J| nodes. With this |J|-wise regression we try to capture the group interdependencies stored in the precision matrix. This is why we require a multivariate model of the form

$$\hat{B}_{J} := \underset{B_{J} \in \mathbb{R}^{|J^{c}| \times |J|}}{\arg \min} \left(\|X_{J} - X_{J^{c}} B_{J}\|_{nuc} + \lambda_{J} \Psi(B_{J}) \right). \tag{3.1}$$

The nuclear norm is defined as

$$||A||_{nuc} := \operatorname{tr}\left(\sqrt{A^T A}\right) = \sum_{i=1}^{\min(n,|J|)} \sigma_i(A),$$

where $\sigma_i(A)$ are the singular values of a $n \times |J|$ matrix A and for a square $m \times m$ matrix B the trace function is defined as $\operatorname{tr}(B) := \sum_{i=1}^m B_{i,i}$. Furthermore the penalty is defined as

$$\Psi(A) := \sum_{j=1}^{|J|} g(A_j). \tag{3.2}$$

It is a matrix norm on $\mathbb{R}^{|J^c| \times |J|}$ (it is the dual matrix norm of an operator norm), that uses the computational cost effective ℓ_1 -norm on the columns together with another norm g on \mathbb{R}^p . Here $A_j \in \mathbb{R}^p$ is equal to the j-th column of the matrix A on the set J^c , and 0 on the set J. The norm g is defined so that it lower bounds all Υ_S -norms where $S \in \mathfrak{S}$ is any non trivial allowed set of the Ω -norm. Furthermore the norm g should satisfy the following reflection property

$$g(\beta_{f(J)}) = g(\beta)$$
, where $\beta_{f(J)} := \beta_J - \beta_{J^c}$.

This is a natural condition on g, because for each allowed set S we have

$$\Upsilon_S(\beta_{f(S)}) = \Upsilon_S(\beta).$$

Where Υ_S is defined as $\Upsilon_S(\beta) := \Omega(\beta_S) + \Omega^{S^c}(\beta_{S^c})$. In order to construct the norm g we construct a convex set where we will take the gauge function. Remark that $\min_{S \in \mathfrak{S}} \Upsilon_S(\cdot)$ is in general not a norm, therefore we need to take the convex hull. The convex set is defined through

$$\overline{B} := \bigcup_{S \text{ allowed}} B_{\Upsilon_S}, \text{ with } B_{\Upsilon_S} \text{ the unit ball of } \Upsilon_S - \text{norm},$$

$$B_g:=\operatorname{Conv}\left(\overline{B}\cup\operatorname{flip}_J(\overline{B})\right).$$

The function $\operatorname{flip}_J(\cdot)$ reflects a set along the hyperplane defined by the subset J. To be more precise for a subset $B \subset \mathbb{R}^p$ we have

$$\text{flip}_J(B) := \{ \gamma : \gamma_J = \beta_J \text{ and } \gamma_{J^c} = -\beta_{J^c}, \forall \beta \in B \}.$$

Then we can define its gauge function (also known as Minkowski functional) as follows:

$$q(x) := \inf (\lambda > 0; x \in \lambda B_a).$$

See Figure 1 for a graphical representation of the gauge function. From this definition of the g we can see that the following Lemma holds.

Lemma 2. For the gauge function g the following properties hold

- (1): q defines a norm on \mathbb{R}^p .
- (2): $g(\beta) \leq \Upsilon_S(\beta) \leq \Omega(\beta)$ and $g(\beta) \leq \Upsilon_S(\beta_{f(J)})$, $\forall S$ allowed sets.

(3):
$$g(\beta) = \left(\max_{S \text{ allowed}} \max \left(\Upsilon_S^*(\beta), \Upsilon_S^*(\beta_{f(J)})\right)\right)^*.$$
Furthermore $\Upsilon_S^*(z) = \max \left(\Omega^*(\beta_S), \Omega^{S^{c,*}}(\beta_{S^c})\right) \ \forall \beta \in \mathbb{R}^p.$

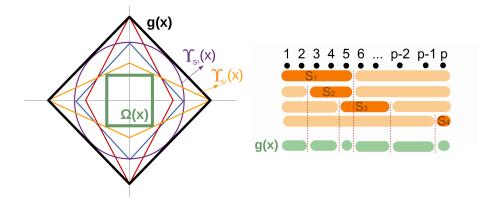


Figure 1: Intuition about the gauge function. Left: lower bounding nature, right: additive nature.

(4):
$$q(\beta_{J^c}) < q(\beta)$$
 for all $\beta \in \mathbb{R}^p$.

Lemma 2 covers the main properties of the gauge function. Result (1) shows that Ψ is in fact a matrix norm. Result (3) gives a characterization of what the gauge function is in our case. Results (2) and (4) are the main properties of the function g, which will be needed to let the error term for the de-sparsified estimator go to 0. Why we chose to construct the Ψ -norm for the |J|-wise regression as a column sum of this gauge function g will become more evident later in this paper. Regarding the construction of confidence sets by means of estimating the precision matrix through the |J|-wise multivariate regression, we will need to specify the Karush-Kuhn-Tucker (KKT) conditions for the multivariate regression estimator \hat{B}_J . The first thing we will need is the subdifferential of a matrix norm. In the paper of Watson [19] one can find the formulation of the subdifferential for a norm of a $m \times n$ matrix A

$$\partial ||A|| = \left\{ G \in \mathbb{R}^{m \times n} : ||B|| \ge ||A|| + \operatorname{tr}\left((B - A)^T G \right), \ \forall \ B \in \mathbb{R}^{m \times n} \right\}.$$

Furthermore we have the following characterization of the subdifferential

$$G \in \partial ||A|| \iff \begin{cases} i) \ ||A|| = \operatorname{tr} \left(G^T A \right) \\ ii) \ ||G||^* \le 1 \end{cases}$$
 (3.3)

Here the dual matrix norm is defined as $||A||^* = \sup_{B: ||B|| \le 1} \operatorname{tr}(B^T A)$. Let us

briefly note that, by definition of the dual matrix norm, a generalized version of the Cauchy Schwartz Inequality holds true for matrices

$$\operatorname{tr}(AB^T) \le ||A|| \cdot ||B||^*.$$

Therefore the dual of the Ψ -matrix norm is defined as

$$\Psi^*(A) := \sup_{B: \ \Psi(B) \le 1} \operatorname{tr} \left(B^T A \right).$$

Applying equation (3.3) to the optimal solution of equation (3.1) leads to the KKT conditions (in the case of $||X_J - X_{J^c} \hat{B}_J||_{nuc} \neq 0$):

$$\hat{B}_{J} \text{ is optimal } \iff \frac{1}{\lambda_{J}} X_{J^{c}}^{T} (X_{J} - X_{J^{c}} \hat{B}_{J}) \hat{\Sigma}_{J}^{-1/2} / n \in \partial \Psi(\hat{B}_{J})$$

$$\iff \begin{cases} i) \quad \lambda_{J} \Psi(\hat{B}_{J}) = \operatorname{tr} \left(\left\{ X_{J^{c}}^{T} (X_{J} - X_{J^{c}} \hat{B}_{J}) \hat{\Sigma}_{J}^{-1/2} / n \right\}^{T} \hat{B}_{J} \right) \\ ii) \quad \lambda_{J} \geq \Psi^{*} \left(X_{J^{c}}^{T} (X_{J} - X_{J^{c}} \hat{B}_{J}) \hat{\Sigma}_{J}^{-1/2} / n \right). \end{cases}$$

$$(3.4)$$

Here we denote $\hat{\Sigma}_J := (X_J - X_{J^c} \hat{B}_J)^T (X_J - X_{J^c} \hat{B}_J)/n$ (assumed to be non-singular). Let us additionally define the |J| de-sparsified Ω structured estimator with the help of the following notations.

$$T_J := (X_J - X_{J^c} \hat{B}_J) X_J / n.$$

The normalizing matrix can then be written as

$$M := \sqrt{n} \hat{\Sigma}_J^{-1/2} T_J$$

This leads to the definition of the |J| de-sparsified Ω structured estimator. Defining a de-sparsified estimator in this way lets us deal with group-wise confidence sets.

Definition 3. The |J| de-sparsified Ω structured estimator is

$$\hat{b}_J := \hat{\beta}_J + T_J^{-1} (X_J - X_{J^c} \hat{B}_J)^T (Y - X \hat{\beta}) / n.$$
(3.5)

With these definitions we are now ready to describe the asymptotic behavior of the estimator (3.5) in the following Theorem.

Theorem 1. Assume that the error in the model (1.1) is i.i.d. Gaussian distributed $\epsilon \sim \mathcal{N}_n(0, \sigma_0^2 I)$. Then with the definition \hat{b}_J from (3.5) together with \hat{B}_J as an estimator of the precision matrix and its normalized version $M\hat{b}_J$ we have

$$M(\hat{b}_J - \beta_J^0)/\sigma_0 = \mathcal{N}_{|J|}(0, I) + rem,$$

where the ℓ_{∞} norm of the reminder term rem can be upper bounded by

$$||rem||_{\infty} \leq \sqrt{n} \lambda g(\hat{\beta}_{J^c} - \beta_{J^c}^0) / \sigma_0$$

$$\leq \sqrt{n} \lambda \Upsilon_{S_{\star}}(\hat{\beta} - \beta^0) / \sigma_0.$$
 (3.6)

As we can see from Lemma 2 (4) we can upper bound part of the reminder term from Theorem 1 as $g(\hat{\beta}_{J^c} - \beta_{J^c}^0) \leq g(\hat{\beta} - \beta^0)$. By the definition of the gauge function g, from Lemma 2 (2) we get that

$$g(\hat{\beta}_{J^c} - \beta_{J^c}^0) \leq \Upsilon_S(\hat{\beta} - \beta^0), \ \forall \ S \text{ allowed sets of } \Omega.$$

But how can we bound $\Upsilon_{S_{\star}}(\hat{\beta}-\beta^0)$? From van de Geer [16] and Stucky and van de Geer [14] we can get sharp oracle results for an estimation error expressed in a measure very close to the $\Upsilon_{S_{\star}}$ -norm, where S_{\star} is the active set of the oracle, but the used measure is not quite the $\Upsilon_{S_{\star}}$ -norm. A refined version of the theorem in van de Geer [16] leads to sharp oracle result, which we will use to upper bound $\|rem\|_{\infty}$. The Lemma 16 can be found in the Appendix. In conclusion Theorem 1 together with Lemma 16 leads to the asymptotic normality of the normalized de-sparsified Ω estimator on the set J. A studentized version leads to an asymptotic pivot. To get the studentized version one could for example use Stucky and van de Geer [14] or generalize the more optimal bounds from the paper van de Geer and Stucky [17]. The results are summarized in the following corollary.

Corollary 1. Assume that the error in the model (1.1) is i.i.d. Gaussian distributed $\epsilon \sim \mathcal{N}_n(0, \sigma_0^2 I)$. The de-sparsified estimator \hat{b}_J is as in (3.5) and the normalized version $M\hat{b}_{J^c}$, together with the multivariate estimator \hat{B}_J from (3.2), as an estimator of the precision matrix. Assume that $0 \leq \delta < 1$, and also that $\lambda^m < c\lambda_J$, with λ^m as in Lemma 16. Furthermore assume $\sqrt{n}\lambda_J\zeta \longrightarrow 0$ as $n \to \infty$. We invoke weak decomposability for S and Ω . Assume we have a consistent estimator of σ_0 . Then we have

$$||M(\hat{b}_J - \beta_J^0)||_{\ell_2}^2/\hat{\sigma} = \chi_{|J|}^2(1 + o_{\mathbb{P}}(1)).$$

With Corollary 1 asymptotic confidence sets can be constructed. But the size of the set J is not controlled. One can find an approach with the group LASSO and the nuclear norm as a penalty in Mitra and Zhang [11], but they need more assumptions. We only need to assume the usual sparsity assumptions on β^0 , we do not assume sparsity on X. It just happens, due to the KKT conditions, that a sparse surrogate of the precision matrix bounds the remainder term

4 Second framework: Ω confidence sets

The first framework made use of the gauge function g, which is able to lower bound all the Υ_S -norms associated with the Ω -norm, therefore the remainder term was asymptotically negligible. But here we will discuss a more direct approach in order to estimate the precision matrix with the Ω -norm itself. But there might be a price to pay. This approach was discussed briefly in van de Geer and Stucky [17] but without mentioning the full consequences of this approach. In contrast to the first framework, J needs to be a non trivial allowed set of Ω (complements of allowed sets would also work). It is quite natural to be interested in allowed sets (or complements of it). We define another multivariate optimization procedure to get an approximation of the precision matrix as

$$\hat{C}_{J} := \underset{C_{J} \in \mathbb{R}^{|J^{c}| \times |J|}}{\arg \min} \left(\|X_{J} - X_{J^{c}} C_{J}\|_{nuc} + \lambda_{J} \Xi(C_{J}) \right). \tag{4.1}$$

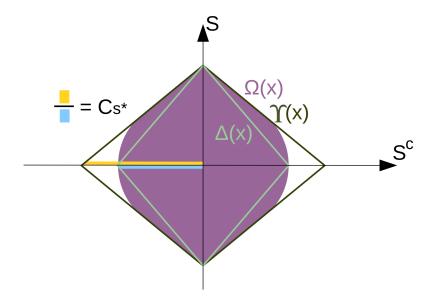


Figure 2: Intuition about the constant $C_{S_{\star}}$.

Here we again use the nuclear norm for its nice KKT properties together with the following norm

$$\Xi(A) := \sum_{j=1}^{|J|} \Omega(A_j). \tag{4.2}$$

In fact we use the Ω -norm as a measure of the columns of a $|J^c| \times |J|$ matrix A, where A_j denotes again the j-th column of the matrix A on the set J^c , and 0 on the set J. One new problem arises in this setting, namely that for all allowed sets S

$$\Upsilon_S(\beta) < \Omega(\beta), \ \forall \ \beta \in \mathbb{R}^p.$$

Therefore some work has to be done in order to get good bounds for the estimation error expressed in the Ω -norm. And this is why we will need to modify the sparsity assumption in order for the reminder term of a de-sparsified version of $\hat{\beta}_J$ to be asymptotically negligible.

Lemma 3. For any weakly decomposable norm Ω there exists a constant $C_{S_{\star}}$ which may depend on the support S_{\star} of the true underlying parameter β^0 such that

$$\Omega(\beta_{S_{\downarrow}^c}) \le C_{S_{\star}} \Omega^{S_{\star}^c}(\beta_{S_{\downarrow}^c}), \forall \beta \in \mathbb{R}^p.$$

Here S_{\star} denotes again the optimal allowed oracle set from Lemma 16.

This means that we need to quantify how far off the $\Upsilon_{S_{\star}}$ -norm on S_{\star}^{c} is compared to the Ω norm, see Figure 2.

For the estimation error expressed in the Ω -norm one can already find oracle results in the literature. One can see for example the consistency result Proposition 6 in Obozinski and Bach [12]. But the result from Lemma 3 together with Lemma 16 provides more optimal results for our case. This is due to the fact, that the sub optimal constant $1/\rho$ from Obozinski and Bach [12] appears squared in the bound. Therefore our constant is better suited for our problem. In the Section 5 we will further discuss this for some widely used examples and show how to choose the constant $C_{S_{\star}}$ for those examples.

Again, as in Section 3 we need to define a de-sparsified version of the estimator $\hat{\beta}$. This will be a different de-sparsified estimator due to a different estimation of the precision matrix. In a similar fashion to Section 3 we have the following definitions

$$T_J := (X_J - X_{J^c} \hat{C}_J)^T X_J / n$$
$$\hat{\Sigma}_J := (X_J - X_{J^c} \hat{C}_J)^T (X_J - X_{J^c} \hat{C}_J) / n.$$

For the sake of simplicity and readability we keep the same notations as in Section 3 for all these definitions, even though they are defined through \hat{C}_J and not \hat{B}_J .

Definition 4. The |J| de-sparsified Ω estimator is again defined as

$$\hat{b}_J := \hat{\beta}_J + T_J^{-1} (X_J - X_{J^c} \hat{C}_J)^T (Y - X \hat{\beta}) / n. \tag{4.3}$$

Here $M := \sqrt{n}\hat{\Sigma}^{-1/2}T_J$ and the normalized version of \hat{b}_J is $M\hat{b}_J$.

Now with the help of Lemma 3 we can formulate the following theorem.

Theorem 2. Assume that the error in the model (1.1) is i.i.d. Gaussian distributed $\epsilon \sim \mathcal{N}_n(0, \sigma_0^2 I)$. Then with the definition \hat{b}_J from (4.3) together with \hat{B}_J as an estimator of the precision matrix and its normalized version $M\hat{b}_J$ we have

$$M(\hat{b}_J - \beta_J^0) = \mathcal{N}_{|J|}(0, I) + rem.$$

Where the ℓ_{∞} norm of the reminder term rem can be upper bounded by

$$||rem||_{\infty} < 2\sqrt{n}\lambda C_{S_*} \Upsilon_{S_*}(\hat{\beta} - \beta^0).$$

Again a similar corollary to Corollary 1 holds for this construction of confidence regions, but with an additional sparsity assumption. This sparsity assumption needs to be specified case by case. It depends on the Ω -norm.

5 Examples of penalties and their behavior in the two frameworks

In this section we try to give the gauge functions g and the constant C^* for some of the common norm penalties used in the literature and for some interesting

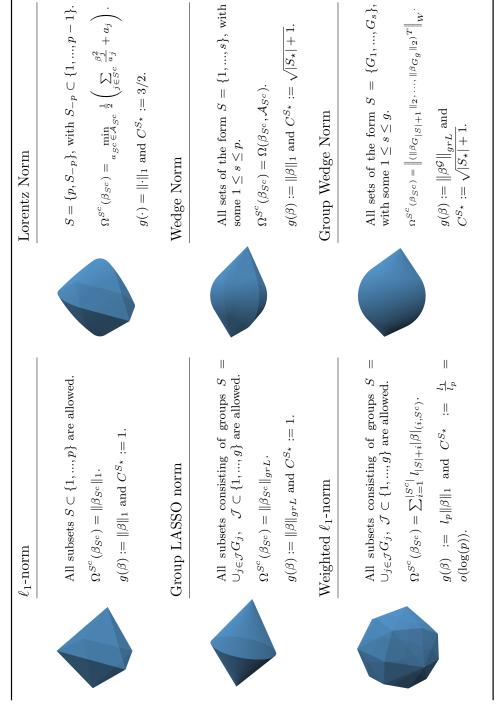


Table 1: Summary of norm properties.

new norm penalties. Furthermore Table ${1\over 2}$ gives an overview of the properties of each example.

5.1 LASSO: the ℓ_1 Penalty

As already mentioned the weak decomposable norms all collapse into the ℓ_1 norm due its decomposability. Therefore the gauge function is $g(\beta) = \|\beta\|_1$.
This means that both of the frameworks for constructing asymptotic confidence
sets are in fact the same. Indeed ℓ_1 has a constant of $C_{S_*} = 1$.

5.2 Group LASSO

The Group LASSO norm is defined by $\|\beta\|_{grL} := \sum_{i=1}^g \|\beta_{G_i}\|_{\ell_2}$, where $\{G_1, ..., G_g\}$ is a partition of $\{1, ..., p\}$. We know that the active sets for this norm are the groups themselves $S = \bigcup_{i \in S_g} G_i$ where S_g is any subset of $\{1, ..., g\}$. The gauge function is the group LASSO itself $g(\beta) = \sum_{i=1}^g \|\beta_{G_i}\|_{\ell_2}$.

Due to the nested ℓ_1 -nature of the group LASSO penalty, we have similar decomposable properties as the ℓ_1 -norm and get $C_{S_{\star}} = 1$.

5.3 SLOPE

The sorted ℓ_1 norm together with some decreasing sequence $1 \ge l_1 \ge l_2 \ge ... \ge l_p > 0$ is defined as

$$J_l(\beta) := l_1 |\beta|_{(1)} + \dots + l_p |\beta|_{(p)}.$$

This was shown to be a norm by Zeng and Figueiredo [20]. The SLOPE was introduced by Bogdan et al. [3] in order to control the false discovery rate:

$$\hat{\beta}_{SLOPE} := \arg\min_{\beta \in \mathbb{R}^p} \left\{ \|Y - X\beta\|_n^2 + \lambda J_l(\beta) \right\}.$$

For the SLOPE we have the following two lemmas.

Lemma 4. For the SLOPE $q(\beta) = l_n ||\beta||_1$.

Lemma 5. The SLOPE has $C_{S_{\star}} = l_1/l_p$.

5.4 Wedge

The wedge norm was introduced in Micchelli et al. [9], and fits in a more broader structured sparsity concept. This concept is nicely compatible from the view-point of weakly decomposable norms, as discussed at length in van de Geer [16]. Let us define the convex cone $\mathcal{A} := \{a : a \in \mathbb{R}^p_{++}, a_j \geq a_{j+1}, j \in \mathbb{N}_{n-1}\}$, where \mathbb{R}^p_{++} denotes the positive orthant. Then the wedge norm is defined as

$$\|\beta\|_W = \Omega(\beta; \mathcal{A}) := \min_{a \in \mathcal{A}} \frac{1}{2} \sum_{j=1}^p \left(\frac{\beta_j^2}{a_j} + a_j \right),$$

with the notation 0/0 = 0. Define

$$\mathcal{A}_S := \{a_S : a \in \mathcal{A}\}.$$

Moreover, van de Geer [16] showed that any S satisfying $A_S \subset A$ is an allowed set for the wedge norm with $\Omega^{S^c}(\beta_{S^c}) := \Omega(\beta_{S^c}, A_{S^c})$. This leads to $S := \{1, ..., s\}$ for any $s \in \{1, ..., p-1\}$ being an allowed set. Hence the wedge estimator can be defined as

$$\hat{\beta}_{Wedge} = \operatorname*{arg\,min}_{\beta \in \mathbb{R}^p} \left\{ \|Y - X\beta\|_n^2 + \lambda \|\beta\|_W \right\}.$$

Lemma 6. For the wedge norm the gauge function is the ℓ_1 -norm $g(\beta) = ||\beta||_1$, for all $\beta \in \mathbb{R}^p$.

The next lemma shows that the wedge estimator has an influence on the amount of sparsity needed for confidence sets. But as the simulations will suggest this might be improvable.

Lemma 7. For the wedge penalty we have $C_{S_{\star}} = \sqrt{|S_{\star}| + 1}$.

5.5 Group Wedge

This is a new idea for a more general wedge norm. It is based on the concept of grouping variables together. Assume that we have g disjoint groups $\{G_1,...,G_g\}=\mathcal{G}$ with $\bigcup_{i=1}^g G_i=\{1,...,p\}$. Let us denote for a vector $\beta\in\mathbb{R}^p$ the ℓ_2 -norm on a given group G_j as $\|\beta_{G_j}\|_{\ell_2}:=\sqrt{|G_j|}\sqrt{\sum_{i\in G_j}\beta_i^2}$. Then for a vector β we define the following g-dimensional vector

$$\beta^{\mathcal{G}} := (\|\beta_{G_1}\|_{\ell_2}, \|\beta_{G_2}\|_{\ell_2}, ..., \|\beta_{G_g}\|_{\ell_2})^T.$$

Now we are able to define the group wedge in terms of the previously defined g-dimensional wedge norm on \mathbb{R}^g as

$$\|\beta\|_{GWedge} := \|\beta^{\mathcal{G}}\|_{W}.$$

We recover the wedge penalty again if we set the groups to be $G_i := \{i\}$ for any $i \in \{1, ..., p\}$. The first lemma shows that we have a norm again, the proof can be found in Section 8.

Lemma 8. The group Wedge is in fact a norm.

Lemma 9. The active sets are of the form $S = \bigcup_{i \in S_g} G_i$ for some subset of group indices $S_g \subset \{1, ..., g\}$, and we have

$$\Omega^{S^c}(\beta_{S^c}) = \|(\|\beta_{G_{s+1}}\|_{\ell_2}, ..., \|\beta_{G_g}\|_{\ell_2})^T\|_W.$$

Moreover, the lower bounding gauge norm is the the Group LASSO norm with wedge groups $g(\beta) = \sum_{i=1}^g \|\beta_{G_g}\|_{\ell_2}$.

Lemma 10. For the group wedge penalty we have $C_{S_{\star}} = \sqrt{|S_{\star}| + 1}$, where S_{\star} denotes the oracle set.

5.6 Lorentz norm

Let us first define the Lorentz Cone (also known as the Ice Cream Cone):

$$\mathcal{A} := \left\{ \begin{pmatrix} a_1 \\ \vdots \\ a_{p-1} \\ a_p \end{pmatrix} \in \mathbb{R}_{++}^p \middle| a_p \ge \left\| \begin{pmatrix} a_1 \\ \vdots \\ a_{p-1} \end{pmatrix} \right\|_{\ell_2} \right\}$$

In a similar fashion to the definition of the wedge norm, the Lorentz norm is $\|\beta\|_{Lo} := \frac{1}{2} \min_{a \in \mathcal{A}} \sum_{i=1}^{p} \left(\frac{\beta_i^2}{a_i} + a_i \right)$. This next lemma shows, that the Lorentz norm lets the index p always be part of the preferred active sets.

Lemma 11. For the Lorentz norm it holds true that all the allowed sets contain p and are of the form

$$S = \{p, \dots \text{ any combination of other variables}\}.$$

And we get the next lemma.

Lemma 12. For the Lorentz norm $g(\cdot) = ||\cdot||_1$.

Lemma 13. For the Lorentz norm $C_{S_{\star}} = 3/2$.

The Lorentz norm can be generalized to include any set $P \subset \{1,..,p\}$ in the allowed sets. The generalized convex cone is

$$\mathcal{B} := \left\{ b \in \mathbb{R}^p_{++} \middle| b_j \ge ||b_{P^c}||_{\ell_2} \, \forall j \in P \right\},\,$$

and the generalized Lorentz norm can be defined as

$$\|\beta\|_{genLo} := \frac{1}{2} \min_{b \in \mathcal{B}} \sum_{i=1}^{p} \left(\frac{\beta_i^2}{b_i} + b_i \right).$$

Now by an analogous proof to the proof of Lemma 11, we can see that the allowed sets of the generalized Lorentz norm always contain the set P. In particular an allowed set S is of the form $S = P \cup B$, with $B \subset P^c$ being any subset of the complement of P. The gauge function does not change, it is the ℓ_1 -norm and we still get a constant of $C_{S_*} = (|P| + 2)/2$.

6 Simulations

We look at the following linear model: $Y = X\beta^0 + \epsilon$, where we have n = 100 observations and p = 150 variables with $\epsilon \sim \mathcal{N}(0, I)$. The design X is randomly chosen, such that the covariance matrix has the following Toeplitz structure $\Sigma_{i,j} = 0.9^{|i-j|}$. The underlying parameter vector β^0 is chosen to be the regularly decreasing sequence

$$\beta_{\{1,...,s_0\}} := \left(4, 4 - \frac{2}{s_0 - 1}, 4 - 2 \cdot \frac{2}{s_0 - 1}, ..., 4 - (s_0 - 2) \cdot \frac{2}{s_0 - 1}, 2\right)^T,$$

where $s_0 = |S_0|$ will be different values. This structure of active set fits nicely in the wedge framework. Therefore to find a solution for the unknown β^0 we use the wedge

$$\hat{\beta}_{Wedge} = \operatorname*{arg\,min}_{\beta \in \mathbb{R}^p} \left\{ \|Y - X\beta\|_n^2 + \lambda \min_{a \in \mathcal{A}} \frac{1}{2} \sum_{j=1}^p \left(\frac{\beta_j^2}{a_j} + a_j \right) \right\}.$$

Now we will construct confidence sets based on the two frameworks for the point-wise sets $\{1\},\{2\},...,\{p\}$. For each of these p sets we compute r=100 repetitions. To find the solution of the LASSO (ℓ_1 is the gauge function in this case), the glmnet R package Simon et al. [13] has been used. To solve the wedge the same code as in Micchelli et al. [9] has been used. The following two cases have been considered: $s_0 = 5$ and $s_0 = 18$. Let us remark that $n/\log(p) \approx 20$ and $(n/\log(p))^{2/3} \approx 7$. For each case the average coverage out of these 100 replications has been computed together with the average confidence set length. The penalty level for the node-wise LASSO and node-wise Wedge have been chosen such that the average coverage are about the same, in order to compare their average set lengths. Of course a reasonable penalty level for practical applications is up for debate.

Sparsity $s_0 = 5$: For a very sparse setting the simulations, as seen in Figure 3, show that there is no essential difference between using the node-wise LASSO or the node-wise Wedge in order to construct the estimate of the precision matrix.

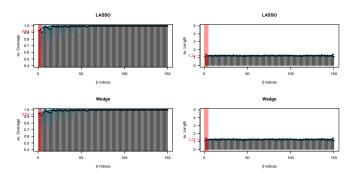


Figure 3: Left: Average coverage, Right: Average length, $s_0 = 5$, $\lambda_{LASSO} = 15.5$, $\lambda_{Wedge} = 15$ and in red are the mean values over all point-wise sets of the active set S_0 .

Sparsity $s_0 = 18$: Surprisingly for a less sparse setting the simulations, see Figure 4, still show no noticeable difference between the node-wise LASSO or the node-wise Wedge. This might indicate that there could be a more direct way bound the estimation error expressed in the Ω norm, and that the bound of the remainder term $\sqrt{n}\lambda C_{S_{\star}}\Upsilon_{S_{\star}}(\hat{\beta}_J - \beta_J^0)$ might not be optimal for the wedge.

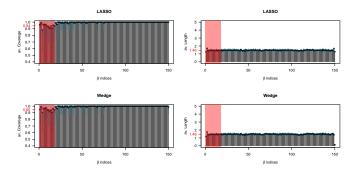


Figure 4: Left: Average coverage, Right: Average Length, $s_0 = 18$, $\lambda_{LASSO} = 12$, $\lambda_{Wedge} = 10$, and in red are the mean values over all point-wise sets of the active set S_0 .

7 Conclusion

Two frameworks for penalized estimators which incorporate structured sparsity patterns have been proposed. The first framework makes use of the gauge function, which is in most cases an ℓ_1 type norm due to the additivity of the lower bounding weak decomposable norms. The second framework is penalized by the structured sparse norm itself. They are both quite general in the sense that they can be used in case of any weakly decomposable norm penalty, but they have their own properties regarding sparsity assumptions. Interestingly the simulations suggest that at least for the presented Toeplitz case both frameworks seem to perform nearly indistinguishable, even for less strict sparsity assumptions. Therefore it would be very interesting for future research to further understand if oracle results for the estimation error expressed in the weakly decomposable norms can be achieved.

8 Proofs

In the dual world inequalities for norms change the direction.

Lemma 14. Let $\Omega(\cdot)$ and $\Upsilon(\cdot)$ be any two norms on \mathbb{R}^p satisfying $\Upsilon(\beta) \leq \Omega(\beta), \forall \beta \in \mathbb{R}^p$. Then for the corresponding dual norms we have the following inequality:

$$\Upsilon^*(\omega) \ge \Omega^*(\omega), \forall \omega \in \mathbb{R}^p.$$

Proof. First, let us remark that the unit balls $B_{\Upsilon} := \{\beta : \Upsilon(\beta) \leq 1\}$ and $B_{\Omega} := \{\beta : \Omega(\beta) \leq 1\}$ fulfill the following

$$B_{\Upsilon} \supset B_{\Omega}$$
.

This is due to the fact that for all $\beta \in B_{\Omega}$ we have

$$\Upsilon(\beta) \le \Omega(\beta) \le 1$$
,

which means that such β are also element of the B_{Υ} -Ball. Now if we look at the definition of the dual norm together with the fact that the supremum over the set B_{Υ} can only be bigger than over the set B_{Ω} , we get

$$\Upsilon^*(\omega) = \sup_{\beta \in B_{\Upsilon}} \omega^T \beta \ge \sup_{\beta \in B_{\Omega}} \omega^T \beta = \Omega^*(\omega), \forall \omega \in \mathbb{R}^p.$$

Due to the disjoint nature of the definition of Υ_S as a sum of two norms on the set S and set S^c we can get an explicit formula for the dual norm.

Lemma 15. For the weakly decomposable norm it holds true that

$$\Upsilon_S^*(\beta) = \max(\Omega^*(\beta_S), \Omega_{S^c}^*(\beta_{S^c})), \forall \beta \in \mathbb{R}^p.$$

Proof. Let us show how to lower and upper bound it. Inequality 1: To show " \geq ":

$$\Upsilon_S^*(\omega) := \sup_{\Upsilon_S(\beta)=1} \beta^T \omega \ge \sup_{\substack{\Upsilon_S(\beta)=1, \\ \beta=\beta_S}} \beta^T \omega$$
$$= \sup_{\Omega(\beta_S)=1} \beta^T \omega \ge \Omega^*(\omega_S)$$

A similar result holds true if we restrict β to β_{S^c} . Therefore the maximum lower bounds the dual of the Υ_S -norm.

Inequality 2: To show " \leq ":

$$\begin{split} \Upsilon_S^*(\omega) &= \sup_{\Upsilon_S(\beta)=1} \beta^T \omega = \sup_{\Upsilon_S(\beta)=1} \left\{ \beta_S^T \omega_S + \beta_{S^c}^T \omega_{S^c} \right\} \\ &= \sup_{\Upsilon_S(\beta)=1} \left\{ \frac{\beta_S^T \omega_S \Omega(\beta_S)}{\Omega(\beta_S)} + \frac{\beta_{S^c}^T \omega_{S^c} \Omega^{S^c}(\beta_{S^c})}{\Omega^{S^c}(\beta_{S^c})} \right\} \\ &\leq \sup_{\Upsilon_S(\beta)=1} \left\{ \Omega^*(\omega_S) \Omega(\beta_S) + \Omega_*^{S^c}(\omega_{S^c}) \Omega^{S^c}(\beta_{S^c}) \right\} \\ &= \sup_{a+b=1} \left\{ \Omega^*(\omega_S) a + \Omega_*^{S^c}(\omega_{S^c}) b \right\} \\ &= \max \left(\Omega^*(\omega_S), \Omega_*^{S^c}(\omega_{S^c}) \right) \end{split}$$

Proof of Lemma 2.

- (1): The gauge function is again a norm on \mathbb{R}^p , because 0 is in the convex set, see for example Clarke [4] Theorem 2.36.
- (2): First of all, the unit ball B_g of norm g contains all the unit balls B_{Υ_S} and $\mathrm{flip}_J(B_{\Upsilon_S})$, therefore

$$g(\beta) \le \Upsilon_S(\beta) \ \forall S$$
 allowed and $g(\beta) \le \Upsilon_S(\beta_{f(J)}) \ \forall S$ allowed.

(3): To prove that the dual norm of g is the maximum we need to make the following observations. First, from Lemma 14 together with Lemma 2 (2) we have

$$\Upsilon_S^*(\beta) \leq g^*(\beta) \ \forall \ S \text{ allowed.}$$

Due to the fact that this holds for all allowed sets S we get

$$\max\left(\max_{S \text{ all.}} \Upsilon_S^*(\beta), \ \max_{S \text{ all.}} \Upsilon_S^*(\beta_{f(J)})\right) \leq g^*(\beta).$$

To prove the other inequality we need to look at the definition of the dual norm g^* :

$$g^*(z) = \max_{g(x) \le 1} z^T x.$$

Because the convex hull in the definition of g is the set of all convex combinations of points in $\overline{B} \cup \text{flip}_I(\overline{B})$ we have that

$$x \in \{y : g(y) \le 1\} \Leftrightarrow x \in B_g$$

 \Leftrightarrow There exists some $n \in \mathbb{R}^p$ and $\sum_{i=1}^n \alpha_i = 1, \alpha_i \ge 0$,
with a sequence of $b_i \in \overline{B} \cup \text{flip}_J(\overline{B})$,
such that we can write $x = \sum_{i=1}^n \alpha_i b_i$.

That is why we can write

$$g^{*}(z) = \max_{\substack{n \in \mathbb{N}, \sum_{i}^{n} \alpha_{i} = 1, \\ b_{i} \in \overline{B} \cup \text{flip}_{J}(\overline{B})}} \sum_{i=1}^{n} \left(\alpha_{i} z^{T} b_{i}\right)$$

$$\leq \max_{\substack{n \in \mathbb{N}, \sum_{i}^{n} \alpha_{i} = 1}} \sum_{i=1}^{n} \left(\alpha_{i} \cdot \max_{\substack{b \in \overline{B} \cup \text{flip}_{J}(\overline{B})}} z^{T} b\right)$$

$$\leq 1 \cdot \max \left(\max_{S \text{ all.}} \Upsilon_{S}^{*}(z), \max_{S \text{ all.}} \Upsilon_{S}^{*}(z_{f(J)})\right).$$

Thus equality holds, and one can easily see that

 $\max\left(\max_{S \text{ all.}} \Upsilon_S^*(z), \max_{S \text{ all.}} \Upsilon_S^*(z_{f(J)})\right)$ is a norm again. Now the condition $\Omega(\beta_{f(J)}) = \Omega(\beta)$ for all $\beta \in \mathbb{R}^p$ forces all Υ_S -norms to have the same symmetrical property, and thus $B_{\Upsilon_S} = \text{flip}_J(B_{\Upsilon_S})$. Therefore the one maximum can be omitted and the claim is proven. For the characterization of the dual of the Υ_S -norm we can just apply Lemma 15.

(4): The function flip $_J$ leads to $g(\beta_J - \beta_{J^c}) = g(\beta)$. Hence

$$g(\beta_{J^c}) = g(\frac{1}{2}(\beta - \beta_J) + \frac{1}{2}\beta_{J^c})$$

$$\leq \frac{1}{2}g(\beta) + \frac{1}{2}g(\beta_J - \beta_{J^c})$$

$$= \frac{1}{2}g(\beta) + \frac{1}{2}g(\beta)$$

$$= g(\beta)$$

Proof of Theorem 1. Then

$$\begin{split} M(\hat{b}_{J} - \hat{\beta}_{J}) &= \sqrt{n} \hat{\Sigma}_{J}^{-1/2} (X_{J} - X_{J^{c}} \hat{B}_{J})^{T} X_{J} / n \cdot \dots \\ & \cdot \left(T_{J}^{-1} (X_{J} - X_{J^{c}} \hat{B}_{J})^{T} (X \beta^{0} - X \hat{\beta} + \epsilon) \right) \\ &= \sqrt{n} \hat{\Sigma}_{J}^{-1/2} (X_{J} - X_{J^{c}} \hat{B}_{J})^{T} \left(\epsilon + X (\beta^{0} - \hat{\beta}) \right) \\ &= \hat{\Sigma}_{J}^{-1/2} (X_{J} - X_{J^{c}} \hat{B}_{J})^{T} \cdot \dots \\ & \cdot \left(X_{J^{c}} (\beta^{0} - \hat{\beta})_{J} + X_{J^{c}} (\beta^{0} - \hat{\beta})_{J^{c}} + \epsilon \right) / \sqrt{n} \\ &= \hat{\Sigma}_{J}^{-1/2} (X_{J} - X_{J^{c}} \hat{B}_{J})^{T} X_{J^{c}} (\beta^{0} - \hat{\beta})_{J^{c}} / \sqrt{n} + \dots \\ & + \hat{\Sigma}_{J}^{-1/2} (X_{J} - X_{J^{c}} \hat{B}_{J})^{T} X_{J} (\hat{\beta} - \beta^{0})_{J} / \sqrt{n} \end{split}$$

We can simplify the term

$$\hat{\Sigma}_J^{-1/2} (X_J - X_{J^c} \hat{B}_J)^T X_J (\hat{\beta} - \beta^0)_J / \sqrt{n} = M(\hat{\beta}_J - \beta_J^0)$$

That is why we can conclude that

$$\begin{split} M(\hat{b}_J - \beta_J^0) &= M(\hat{b}_J - \hat{\beta}_J) + M(\hat{\beta}_J - \beta_J^0) \\ &= \hat{\Sigma}_J^{-1/2} (X_J - X_{J^c} \hat{B}_J)^T \epsilon / \sqrt{n} + \dots \\ &+ \sqrt{n} \hat{\Sigma}_J^{-1/2} (X_J - X_{J^c} \hat{B}_J)^T X_{J^c} (\beta^0 - \hat{\beta})_{J^c} / n \\ &= \hat{\Sigma}_J^{-1/2} (X_J - X_{J^c} \hat{B}_J)^T \epsilon / \sqrt{n} + \underbrace{\lambda Z(\beta^0 - \hat{\beta})_{J^c} / \sqrt{n}}_{\text{Gaussian Random Variable}} + \underbrace{\lambda Z(\beta^0 - \hat{\beta})_{J^c} / \sqrt{n}}_{\text{Remainder Term}} \end{split}$$

where Z comes from the KKT conditions which fulfills:

$$\Psi^*(Z) \le 1$$
$$\operatorname{tr}(Z^T \hat{B}_J) = \Psi(\hat{B}_J).$$

The remainder term can be bounded with the generalized Cauchy Schwartz inequality in the ℓ_{∞} -norm by

$$\begin{split} \lambda \| Z(\beta^0 - \hat{\beta})_{J^c} \|_{\infty} / \sqrt{n} &= \lambda \max_{1 \leq j \leq |J|} Z_j(\beta^0 - \hat{\beta})_{J^c} / \sqrt{n} \\ &\leq \lambda \max_{1 \leq j \leq |J|} g^*(Z_j) g(\beta^0_{J^c} - \hat{\beta}_{J^c}) / \sqrt{n} \\ &\leq \lambda \Psi^*(Z) g(\beta^0_{J^c} - \hat{\beta}_{J^c}) / \sqrt{n} \\ &\leq \lambda g(\beta^0_{J^c} - \hat{\beta}_{J^c}) / \sqrt{n} \quad \text{(KKT conditions.)} \end{split}$$

Dividing everything by σ_0 leads to the result.

Proof of Lemma 3. Let us first observe:

$$\begin{split} \Omega(\beta^{0} - \hat{\beta}) &\leq \Omega(\beta^{0}_{S_{\star}} - \hat{\beta}_{S_{\star}}) + \Omega(\beta^{0}_{S^{*c}} - \hat{\beta}_{S^{*c}}) \\ &\leq \Omega(\beta^{0}_{S_{\star}} - \hat{\beta}_{S_{\star}}) + \Omega^{S^{*c}} (\beta^{0}_{S^{*c}} - \hat{\beta}_{S^{*c}}) \\ &- \Omega^{S^{*c}} (\beta^{0}_{S^{*c}} - \hat{\beta}_{S^{*c}}) + \Omega(\beta^{0}_{S^{*c}} - \hat{\beta}_{S^{*c}}) \\ &\leq \Upsilon_{S_{\star}} (\beta^{0} - \hat{\beta}) + \Delta_{S^{*c}} (\beta^{0} - \hat{\beta}). \end{split}$$

Here we define $\Delta_{S^{*^c}}(\beta) := \Omega(\beta_{S^{*^c}}) - \Omega^{S^{*^c}}(\beta_{S^{*^c}})$. But we are left with another problem, how to bound $\Delta_{S^{*^c}}$. Understanding this distance will give us a bound on how far apart the weakly decomposable norm and the norm from the triangle inequality are. Now let us take the optimal constant $C_{S_{\star}}$, which may depend on the active set of the oracle $|S_{\star}|$, such that $\Omega(\beta_{S^{*^c}}) \leq C_{S_{\star}} \cdot \Omega^{S^{*^c}}(\beta_{S^{*^c}})$, $\forall \beta \in \mathbb{R}^p$. Then with this we can write

$$\Delta_{S^{*^c}}(\beta^0 - \hat{\beta}) \le (C_{S_{\star}} - 1)\Omega^{S^{*^c}}(\beta_{S^{*^c}}^0 - \hat{\beta}_{S^{*^c}}) \le (C_{S_{\star}} - 1)\Upsilon_{S_{\star}}(\beta^0 - \hat{\beta}).$$

In the last inequality we have used the weak decomposability condition. Therefore $\Omega(\beta^0 - \hat{\beta}) \leq C_{S_{\star}} \Upsilon_{S_{\star}}(\beta^0 - \hat{\beta})$.

Proof of Theorem 2. The first part follows directly the proof of Theorem 1, with Ξ-norm instead of Ψ-norm. The remainder term can be bounded with the generalized Cauchy Schwartz inequality in the ℓ_{∞} -norm by

$$\begin{split} \lambda \| Z (\beta^0 - \hat{\beta})_{J^c} \|_{\infty} / \sqrt{n} &= \lambda \max_{1 \leq j \leq |J|} Z_j (\beta^0 - \hat{\beta})_{J^c} / \sqrt{n} \\ &\leq \lambda \max_{1 \leq j \leq |J|} \Omega^* (Z_j) \Omega (\beta^0_{J^c} - \hat{\beta}_{J^c}) / \sqrt{n} \\ &\leq \lambda \Xi^* (Z) \Omega (\beta^0_{J^c} - \hat{\beta}_{J^c}) / \sqrt{n} \\ &\leq \lambda \Omega (\beta^0_{J^c} - \hat{\beta}_{J^c}) / \sqrt{n} \quad \text{(KKT conditions.)} \\ &< \lambda 2 \Omega (\beta^0 - \hat{\beta}) \end{split}$$

The last inequality comes directly from the weak decomposability of the allowed

set J:

$$\Omega(\beta_{J^c}^0 - \hat{\beta}_{J^c}) \leq \Omega\left((\beta_{J^c}^0 - \hat{\beta}_{J^c}) + (\beta_J^0 - \hat{\beta}_J) - (\beta_J^0 - \hat{\beta}_J)\right)
\leq \Omega(\beta^0 - \hat{\beta}) + \Omega(\beta_J^0 - \hat{\beta}_J)
\leq 2\Omega(\beta^0 - \hat{\beta}).$$

Now with the calculation in the proof of Lemma 3 and by dividing everything by σ_0 the proof is finished.

Proof of Lemma 4. First of all, let us see that $l_p \|\beta\|_1$ indeed is a lower bound for all weakly decomposable norms of $\Omega = J_l$. From Stucky and van de Geer [14] we know that for any subset $S \subset \{1, ..., p\}$ we have

$$\Upsilon_S(\beta) = \sum_{j=1}^{|S|} l_j |\beta|_{(j,S)} + \sum_{i=1}^{|S^c|} l_{|S|+i} |\beta|_{(i,S^c)}$$

with $1 \ge l_1 \ge l_2 \ge ... \ge l_p > 0$ and $|\beta|_{(1,S^c)} \ge ... \ge |\beta|_{(r,S^c)}$ being the ordered sequence in $\{\beta_i : i \in S^c\}$. We can now lower bound each l_i and l_j by the minimum of the decreasing sequence, namely l_p . That is why we get the sought lower bound

$$|l_p||\beta||_1 \leq \Upsilon_S(\beta) \leq \Omega(\beta) \quad \forall S \subset \{1,...,p\} \text{ and all } \beta \in \mathbb{R}^p.$$

Therefore $\lambda_p \|\beta\|_1$ is a candidate for the gauge function, but we need to show that this norm is the best lower bounding norm. Assume by contradiction that there is another norm $g(\cdot)$ on \mathbb{R}^p such that

$$|l_p||\beta||_1 \le g(\beta) \le \Upsilon_S(\beta) \quad \forall S \subset \{1,...,p\} \text{ and all } \beta \in \mathbb{R}^p$$

and that there exists $\gamma \in \mathbb{R}^p$ such that $l_p ||\gamma||_1 < g(\gamma)$.

Denote the k-th standard basis vectors in \mathbb{R}^p as e_k . Where e_k is the vector having a one at the k-th entry and zeroes otherwise. Then γ can be written in the standard basis as a combination of the standard basis vectors

$$\gamma = v_1 e_1 + v_2 e_2 + \dots + v_p e_p.$$

From the above assumption and the fact that the set without the k-th index $\{1,...,p\} \setminus \{k\}$, denoted briefly as $\setminus \{k\}$, is an allowed set, we have that for each standard basis vector e_k the following needs to hold true

$$||e_k||_1 \le g(e_k) \le \Upsilon_{\{k\}}(e_k) \quad \forall k \in \{1, ..., p\}.$$

Inserting the values $||e_k||_1 = 1$ and $\Upsilon_{\{k\}}(e_k) = l_p \ \forall k \in \{1,..,p\}$ leads to

$$l_p \le g(e_k) \le l_p$$
.

Therefore we can conclude that $g(e_k) = l_p$ for all $k \in \{1, ..., p\}$. Now applying the triangle inequality the g we have

$$g(\gamma) \le |v_1|g(e_1) + \dots + |v_p|g(e_p) = (|v_1| + \dots + |v_p|)l_p.$$

On the other hand we get $l_p ||\gamma||_1 = l_p(|v_1| + ... + |v_p|)$. This now clearly contradicts our assumption because $l_p ||\gamma||_1 \not \leq g(\gamma) \leq l_p ||\gamma||_1$.

Proof of Lemma 5. By $\Omega(\beta_S) = \sum_{j=1}^{|S|} l_j |\beta|_{(j,S)}$ and upper bounding all $l_j, j = \{1, ..., |S|\}$ we have

$$\Omega(\beta_{S^{*c}})/l_1 \leq \|\beta_{S^{*c}}\|_1.$$

In a similar fashion by $\Omega^{S^c}(\beta_{S^c}) = \sum_{i=1}^{|S^c|} l_{|S|+i} |\beta|_{(i,S^c)}$ and lower bounding all $l_i, i = \{|S|+1,...,p\}$, we get

$$\Omega^{S^{*^c}}(\beta_{S^{*^c}})/l_p \ge \|\beta_{S^{*^c}}\|_1.$$

Combining these two inequalities leads to

$$\Omega^{S^{*^c}}(\beta_{S^{*^c}})l_1/l_p \ge \Omega(\beta_{S^{*^c}}).$$

for the SLOPE penalty $C_{S_{\star}} = l_1/l_p = o(\log(p))$. The last equality comes from the Bonferroni l-sequence choice in Bogdan et al. [3].

Proof of Lemma 6. First we know by Micchelli et al. [9] that $\|\beta\|_1 \leq \Upsilon(\beta)$ for all allowed sets S and all $\beta \in \mathbb{R}^p$. Now in order to show that this is the best lower bounding norm, let us assume by contradiction that there exists another norm $g(\cdot)$ which is strictly better than $\|\cdot\|_1$:

$$\|\beta\|_1 \leq g(\beta) \leq \Upsilon(\beta) \ \forall S \text{ allowed } \forall \beta \in \mathbb{R}^p,$$

 $\exists \gamma \in \mathbb{R}^p \text{ such that } \|\gamma\|_1 < g(\gamma) \leq \Upsilon(\gamma) \ \forall S \text{ allowed.}$

Define the standard basis as $e_k, k \in \{1, ..., p\}$ being the vector having a one at the k-th entry and zero entries otherwise. Let us fix any allowed set S. It is straight forward to check that

$$\Upsilon(e_1) = 1$$
, and $\Upsilon(e_{s+1}) = 1$.

By the assumption we get that

$$1 = ||e_{s+1}||_1 \le g(e_{s+1}) \le \Upsilon(e_{s+1}) = 1 \ \forall S \text{ allowed.}$$

And similarly for the first standard basis vector e_1 we have

$$1 = ||e_1||_1 \le g(e_1) \le \Upsilon(e_1) = 1 \ \forall S \text{ allowed.}$$

Now because $s \in \{1, ..., p-1\}$ we get that:

$$g(e_k) = 1$$
, for any $k \in \{1, ..., p\}$.

So we know the values that g attains for the standard basis. With this we can conduct the following contradiction. The vector γ has a unique representation in the standard basis $\gamma = v_1e_1 + v_2e_2 + ... + v_pe_p$, and therefore we can apply the triangle inequality p times to get:

$$\begin{split} g(\gamma) &\leq |v_1|g(e_1) + |v_2|g(e_2) + \ldots + |v_p|g(e_p) \\ &= |v_1| + |v_2| + \ldots + |v_p| \\ &= ||\gamma||_1 \end{split}$$

This contradicts our assumption that $\|\gamma\|_1 < g(\gamma)$, and the claim is proven. \square

Proof of Lemma 7. For any allowed set S, the weakly decomposable Υ -norm consists of the following two parts

$$\Omega(\beta_{S^c}) = \min_{a_{S^c} \in \mathcal{A}_{S^c}} \frac{1}{2} \left(\sum_{j \in S^c} \left(\frac{\beta_j^2}{a_j} + a_j \right) + s \cdot a_{s+1} \right),$$

$$\Omega^{S^c}(\beta_{S^c}) = \min_{a_{S^c} \in \mathcal{A}_{S^c}} \frac{1}{2} \left(\sum_{j \in S^c} \frac{\beta_j^2}{a_j} + a_j \right).$$

Here we have used that $a_j \geq a_{j+1}$ for all $1 \geq j \leq p-1$. Because of the structure of the cone \mathcal{A} we have

$$\Omega(\beta_{S^c}) = \min_{a_{S^c} \in \mathcal{A}_{S^c}} \frac{1}{2} \left(\sum_{j=s+2}^p \left(\frac{\beta_j^2}{a_j} + a_j \right) + \frac{\beta_{s+1}^2}{a_{s+1}} + (s+1)a_{s+1} \right) \\
\leq \min_{a_{S^c} \in \mathcal{A}_{S^c}} \frac{1}{2} \left(\sum_{j=s+2}^p \left(\frac{\beta_j^2}{a_j} + (s+1)a_j \right) + \frac{\beta_{s+1}^2}{a_{s+1}} + (s+1)a_{s+1} \right) \\
= \sqrt{s+1} \min_{a_{S^c} \in \mathcal{A}_{S^c}} \frac{1}{2} \left(\sum_{j=s+1}^p \frac{\beta_j^2}{\sqrt{s+1}a_j} + \sqrt{s+1}a_j \right).$$

In the second inequality we added $\sum_{j=s+2}^p sa_j \geq 0$, and in the last inequality we take $\sqrt{s+1}$ outside the minimum. Now in this setting we know that for $a_{S^c} \in \mathcal{A}_{S^c}$ we have $a_{s+1} \geq a_{s+2} \geq ... \geq a_p \geq 0$. Furthermore $a_{S^c}' := (\sqrt{s+1}a_{s+1}, \sqrt{s+1}a_{s+2}, ..., \sqrt{s+1}a_p)^T \in \mathcal{A}_{S^c}$, in fact any sequence $a_{S^c} \in \mathcal{A}_{S^c}$ can be displayed by a sequence which is multiplied by $\sqrt{s+1}$. Therefore

$$\Omega(\beta_{S^c}) \leq \sqrt{s+1} \min_{\substack{a'_{S^c} \in \mathcal{A}_{S^c} \\ \leq \sqrt{s+1} \cdot \Omega^{S^c}(\beta_{S^c})}} \frac{1}{2} \left(\sum_{j=s+1}^p \frac{\beta_j^2}{a'_j} + a'_j \right)$$

Proof of Lemma 9. The ℓ_2 -norm does not have any non trivial active sets, and the g-dimensional wedge norm has active sets $S = \{1, ..., s\}$ for any $s \in \{1, ..., g\}$.

Combining theses facts leads to the conclusion that only for active sets of the form $S = \bigcup_{i \in S_a} G_i$ we have weak decomposability:

$$\|\beta_S\|_{qrW} + \|\beta_{S^c}\|_{qrW} \le \|\beta\|_{qrW}.$$

Because of the definition of the group wedge as a composition of the wedge and ℓ_2 -norm this is the best lower bound. For the gauge function g it is easy to see that by applying Lemma 6, we get the Group LASSO.

Proof of Lemma 8.

(1):
$$\|\beta\|_{grW} = 0 \iff \|\beta_{G_i}\|_{\ell_2} = 0 \ \forall i \in \{1, ..., g\} \iff \beta \equiv 0.$$

(2): The following calculations hold true:

$$||a\beta||_{grW} = ||(||a\beta_{G_{s+1}}||_{\ell_2}, ..., ||a\beta_{G_g}||_{\ell_2})^T||_W$$

= $||a(||\beta_{G_{s+1}}||_{\ell_2}, ..., ||\beta_{G_g}||_{\ell_2})^T||_W$
= $a||\beta||_{grW}$.

(3): The triangle inequality holds due to the properties of the wedge and ℓ_2 -norms.

$$\begin{split} &\|\beta + \gamma\|_{grW} = \|(\|\beta_{G_{s+1}} + \gamma_{G_{s+1}}\|_{\ell_2}, ..., \|\beta_{G_g} + \gamma_{G_g}\|_{\ell_2})^T\|_W \\ &\leq \|(\|\beta_{G_{s+1}}\|_{\ell_2} + \|\gamma_{G_{s+1}}\|_{\ell_2}, ..., \|\beta_{G_g}\|_{\ell_2} + \|\gamma_{G_g}\|_{\ell_2})^T\|_W \\ &\leq \|\beta^{\mathcal{G}} + \gamma^{\mathcal{G}}\|_W \\ &\leq \|\beta^{\mathcal{G}}\|_W + \|\gamma^{\mathcal{G}}\|_W = \|\beta\|_{grW} + \|\gamma\|_{grW} \end{split}$$

Proof of Lemma 10. By applying Lemma 7 in this context, together with S_{\star} being the optimal active groups, we immediately get the desired result.

Proof of Lemma 11. By van de Geer [16] we know that for the structured sparsity norms, as introduced in Micchelli et al. [9], it holds that

S is an allowed set
$$\iff \mathcal{A}_S := \{a_S : a \in \mathcal{A}\} \subset \mathcal{A}$$
.

Let us distinguish two cases, in order to proof the lemma.

Case 1: Assume $p \notin S$.

Therefore A_S consists of vectors with the p-th variable set to zero. This means that there exists at least one vector a such that a_S is not in A

$$a_{p,S} = 0 \ngeq \| \begin{pmatrix} a_1 \\ \vdots \\ a_{p-1} \end{pmatrix}_S \|_{\ell_2}.$$

In other words $A_S \nsubseteq A$. Therefore sets S which do not contain p cannot be allowed sets.

<u>Case 2:</u> Assume that the set S satisfies $S \ni p$. For each vector a_S in A_S we have

$$a_{p,S} = a_p \ge \| \begin{pmatrix} a_1 \\ \vdots \\ a_{p-1} \end{pmatrix} \|_{\ell_2} \ge \| \begin{pmatrix} a_1 \\ \vdots \\ a_{p-1} \end{pmatrix}_S \|_{\ell_2}.$$

The first inequality is due to a being in \mathcal{A} . For the second inequality it suffices to see that the ℓ_2 norm can only decrease by setting certain values to zero. therefore we know that any set S which contains p fulfills $\mathcal{A}_S \subset \mathcal{A}$.

Proof of Lemma 12. Again by Micchelli et al. [9] we know that $\|\beta\|_1 \leq \Upsilon(\beta)$ for all allowed sets S and all $\beta \in \mathbb{R}^p$. Define the standard basis as $e_k, k \in \{1, ..., p\}$. Let us fix any allowed set S from Lemma 11. We can calculate that

$$\Upsilon(e_k) = \sqrt{2} \text{ if } k \in S \setminus \{p\}, \Upsilon(e_k) = 1 \text{ if } k \notin S \setminus \{p\},$$

$$\Upsilon(e_p) = 1.$$

Taking the special allowed set $S = \{g\}$ we have

$$1 = ||e_k||_1 \le g(e_k) \le \Upsilon_{\{g\}}(e_k) = 1, \forall k \in \{1, ..., p\}.$$

This leads to $g(e_k) = 1, \forall k \in \{1, ..., p\}$. Therefore we can use the same idea of the proof from Lemma 6, and we get that $g(\cdot) = \|\cdot\|_1$.

Proof of Lemma 13. We have that

$$\Omega^{S^c}(\beta_{S^c}) = \min_{a_{S^c} \in \mathcal{A}_{S^c}} \frac{1}{2} \sum_{j \in S^c} \left(\frac{\beta_j^2}{a_j} + a_j \right) = \|\beta_{S^c}\|_1.$$

This is due to $p \notin S^c$ and therefore the $\{a_j : j \in S^c\}$ can be chosen independently of each other, leading to the minimum $a_j = \beta_j$. Furthermore we have the following upper bound:

$$\Omega(\beta_{S^c}) = \min_{a \in \mathcal{A}} \frac{1}{2} \sum_{j \in S^c} \left(\frac{\beta_j^2}{a_j} + a_j \right) + a_p
\leq \min_{a \in \mathcal{A}} \frac{1}{2} \sum_{j \in S^c} (2\beta_j) + \|\beta_{S^c}\|_2 \text{ with } a_j = \beta_j
= \|\beta_{S^c}\|_1 + \frac{1}{2} \|\beta_{S^c}\|_2
\leq \frac{3}{2} \|\beta_{S^c}\|_1 = \frac{3}{2} \Omega^{S^c} (\beta_{S^c}).$$

Which leads to the desired constant.

Appendix: A refined Sharp Oracle Inequality

Let us first remind us of the definition of the theoretical lambda $\lambda^m := \max\left(\Omega^*(\epsilon^T X_{S_\star}), \Omega^{S_\star^c*}(\epsilon^T X_{S_\star^c})\right)/n = \Upsilon_{S_\star}^*\left(\epsilon^T X\right)/n$. Lemma 16 refines the sharp oracle result from van de Geer [16]. In particular, the sharp oracle inequality from van de Geer [16] measures a variation of the estimation error in the following way $\Omega(\hat{\beta}_{S_\star} - \beta^*) + \Omega^{S_\star^c*}(\hat{\beta}_{S_\star^c})$, with $S_\star = \sup(\beta^*)$. Let us remark here that the optimal oracle parameter β^* may not be equal to β^0 . Therefore we have no guarantee to get an upper bound on the estimation error expressed as $\Upsilon_{S_\star}(\hat{\beta} - \beta^0)$. But this is needed for both confidence frameworks to work. Therefore we will rework Theorem 4.1 from van de Geer [16] to make S and β independent of each other. Let us furthermore define the Ω -effective sparsity as in van de Geer [16] and denote it $\Gamma^2_\Omega(L,S)$.

Lemma 16 (Refined Sharp Oracle Inequality). Assume that $0 \le \delta < 1$, and also that $\frac{\lambda^m}{\lambda} = c$ with 0 < c < 1. We invoke weak decomposability for S and Ω . Here the active set S and parameter vector β can be chosen independently. Then it holds true that

$$\Upsilon_{S_{\star}}(\hat{\beta} - \beta^{0}) \leq \min_{\beta, S, \delta} \left(\Upsilon_{S}(\beta^{0} - \beta) + C_{1} \lambda \Gamma_{\Omega}^{2}(L_{S}, S) + \frac{C_{2}}{\lambda} \|X(\beta - \beta^{0})\|_{n}^{2} + C_{3} \Omega(\beta_{S^{c}}) \right),$$
(8.1)

with $L_S := \frac{\lambda + \lambda^m}{\lambda - \lambda^m} \frac{1 + \delta}{1 - \delta}$, constants $C_1 = \frac{[(1 + \delta)(1 + c)]^2}{2\delta(1 - c)}$, $C_2 = \frac{1}{2\delta(1 - c)}$, $C_3 = \frac{2}{\delta(1 - c)}$ and

$$\begin{split} S_{\star} := \arg\min_{S} \min_{\beta, \delta} \left[\Upsilon_{S}(\beta^{0} - \beta) + C_{1} \lambda \Gamma_{\Omega}^{2}(L_{S}, S) + \dots \right. \\ &+ \frac{C_{2}}{\lambda} \|X(\beta - \beta^{0})\|_{n}^{2} + C_{3} \Omega(\beta_{S^{c}}) \right]. \end{split}$$

Proof. Follows directly from the proof of the main theorem in van de Geer [2014] and the triangle inequality. \Box

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