

## A Proof of Theorem 2

*Proof.* By standard conditions for optimality,  $\hat{\beta}$  is a critical point if and only if there exists a subgradient  $\hat{z} \in \partial \|\hat{\beta}\|_1 := \{\hat{z} \in \mathbb{R}^p | \hat{z}_j = \text{sgn}(\hat{\beta}_j) \text{ for } \hat{\beta}_j \neq 0, |\hat{z}_j| \leq 1 \text{ otherwise}\}$  such that  $\partial_{\hat{\beta}} L(\beta) = 0$ . Because  $\partial_{\beta} \frac{1}{2} |\beta|^\top R |\beta| = \text{Diag}(R|\beta|)z$ , the condition  $\partial_{\hat{\beta}} L(\beta) = 0$  yields

$$-\frac{1}{n} X^\top (y - X\hat{\beta}) + \lambda \hat{z} + \lambda \alpha \text{Diag}(R|\hat{\beta}|) \hat{z} = 0. \quad (\text{A.1})$$

Substituting  $y = X\beta^* + \epsilon$  in (A.1), we have

$$-\frac{1}{n} X^\top (X(\beta^* - \hat{\beta}) + \epsilon) + \lambda \hat{z} + \lambda \alpha \text{Diag}(R|\hat{\beta}|) \hat{z} = 0. \quad (\text{A.2})$$

Let the true active set  $S = \{1, \dots, s\}$  and inactive set  $S^c = \{s+1, \dots, p\}$  without loss of generality, then (A.2) is turned into

$$\frac{1}{n} X_S^\top X_S (\hat{\beta}_S - \beta_S^*) + \frac{1}{n} X_S^\top X_{S^c} \hat{\beta}_{S^c} - \frac{1}{n} X_S^\top \epsilon + \lambda \hat{z}_S + \lambda \alpha \text{Diag}(R_{SS}|\hat{\beta}_S|) \hat{z}_S = 0, \quad (\text{A.3})$$

$$\frac{1}{n} X_{S^c}^\top X_S (\hat{\beta}_S - \beta_S^*) + \frac{1}{n} X_{S^c}^\top X_{S^c} \hat{\beta}_{S^c} - \frac{1}{n} X_{S^c}^\top \epsilon + \lambda \hat{z}_{S^c} + \lambda \alpha \text{Diag}(R_{S^c S}|\hat{\beta}_S|) \hat{z}_{S^c} = 0. \quad (\text{A.4})$$

Hence, there exists a critical point with correct sign recovery if and only if there exists  $\hat{\beta}$  and  $\hat{z}$  such that (A.3), (A.4),  $\hat{z} \in \partial \|\hat{\beta}\|_1$  and  $\text{sgn}(\hat{\beta}) = \text{sgn}(\beta^*)$ . The latter two conditions can be written as

$$\hat{z}_S = \text{sgn}(\beta_S^*), \quad (\text{A.5})$$

$$|\hat{z}_{S^c}| \leq 1, \quad (\text{A.6})$$

$$\text{sgn}(\hat{\beta}_S) = \text{sgn}(\beta_S^*), \quad (\text{A.7})$$

$$\hat{\beta}_{S^c} = 0. \quad (\text{A.8})$$

The condition (A.5) and (A.8) yield

$$\frac{1}{n} X_S^\top X_S (\hat{\beta}_S - \beta_S^*) - \frac{1}{n} X_S^\top \epsilon + \lambda \text{sgn}(\beta_S^*) + \lambda \alpha \text{Diag}(R_{SS}|\hat{\beta}_S|) \text{sgn}(\beta_S^*) = 0, \quad (\text{A.9})$$

$$\frac{1}{n} X_{S^c}^\top X_S (\hat{\beta}_S - \beta_S^*) - \frac{1}{n} X_{S^c}^\top \epsilon + \lambda \hat{z}_{S^c} + \lambda \alpha \text{Diag}(R_{S^c S}|\hat{\beta}_S|) \hat{z}_{S^c} = 0. \quad (\text{A.10})$$

Since

$$\begin{aligned} \text{Diag}(R_{SS}|\hat{\beta}_S|) \text{sgn}(\beta_S^*) &= \text{Diag}(\text{sgn}(\beta_S^*)) R_{SS} |\hat{\beta}_S| \\ &= \text{Diag}(\text{sgn}(\beta_S^*)) R_{SS} \text{Diag}(\text{sgn}(\beta_S^*)) \hat{\beta}_S, \end{aligned}$$

(A.9) can be rewritten as

$$U(\hat{\beta}_S - \beta_S^*) + V = 0,$$

where

$$U := \frac{1}{n} X_S^\top X_S + \lambda \alpha \text{Diag}(\text{sgn}(\beta_S^*)) R_{SS} \text{Diag}(\text{sgn}(\beta_S^*)),$$

$$V := \lambda \text{sgn}(\beta_S^*) + \lambda \alpha \text{Diag}(\text{sgn}(\beta_S^*)) R_{SS} \text{Diag}(\text{sgn}(\beta_S^*)) \beta_S^* - \frac{1}{n} X_S^\top \epsilon.$$

If we assume  $U$  is invertible, we obtain

$$\hat{\beta}_S = \beta_S^* - U^{-1}V. \quad (\text{A.11})$$

Substituting this in (A.10), we have

$$\frac{1}{n} X_{S^c}^\top X_S (-U^{-1}V) - \frac{1}{n} X_{S^c}^\top \epsilon + \lambda \hat{z}_{S^c} + \lambda \alpha \text{Diag}(R_{S^c S}|\beta_S^* - U^{-1}V|) \hat{z}_{S^c} = 0,$$

that is,

$$(1 + \alpha \text{Diag}(R_{S^c S} |\beta_S^* - U^{-1}V|)) \lambda \hat{z}_{S^c} = \frac{1}{n} X_{S^c}^\top X_S U^{-1}V + \frac{1}{n} X_{S^c}^\top \epsilon. \quad (\text{A.12})$$

Combining (A.6), (A.7), (A.11) and (A.12), we have the following conditions:

$$\begin{aligned} \text{sgn}(\beta_S^* - U^{-1}V) &= \text{sgn}(\beta_S^*), \\ \left| \frac{1}{n} X_{S^c}^\top X_S U^{-1}V + \frac{1}{n} X_{S^c}^\top \epsilon \right| &\leq \lambda (1 + \alpha R_{S^c S} |\beta_S^* - U^{-1}V|). \end{aligned}$$

□

## B Proof of Theorem 3

First, we prepare the following lemma.

**Lemma B.1.** Suppose that Assumption 1 and

$$\frac{1}{n} \sum_{i=1}^n X_{ij}^2 \leq 1 \quad (\forall j = 1, \dots, p),$$

are satisfied. For  $\forall \delta > 0$ , let  $\gamma_n := \gamma_n(\delta)$  be

$$\gamma_n := \sigma \sqrt{\frac{2 \log(2p/\delta)}{n}}.$$

Then, we have that

$$P \left( \left\| \frac{1}{n} X^\top \epsilon \right\|_\infty \geq \gamma_n \right) \leq \delta.$$

*Proof.* The assertion can be shown in the standard way. First notice that

$$\begin{aligned} P \left( \left\| \frac{1}{n} X^\top \epsilon \right\|_\infty \geq \gamma \right) &= P \left( \max_{1 \leq j \leq p} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i X_{ij} \right| \geq \gamma \right) \\ &= P \left( \bigcup_{1 \leq j \leq p} \left\{ \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i X_{ij} \right| \geq \gamma \right\} \right) \\ &\leq \sum_{j=1}^p P \left( \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i X_{ij} \right| \geq \gamma \right) \leq p \max_{1 \leq j \leq p} P \left( \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i X_{ij} \right| \geq \gamma \right). \end{aligned}$$

Since  $\frac{1}{n} \sum_{i=1}^n X_{ij}^2 \leq 1$ ,  $\xi_i = X_{ij} \epsilon_i$  satisfies  $E[e^{t\xi_i}] \leq e^{\sigma^2 t^2/2} \forall t \in \mathbb{R}$ . Hence, applying Hoeffding's inequality, we obtain the assertion. □

Then, we derive Theorem 3.

*Proof.* By  $L_{\lambda_n}(\hat{\beta}) \leq L_{\lambda_n}(\beta^*)$  and  $y = X\beta^* + \epsilon$ , it holds that

$$\begin{aligned} \frac{1}{2n} \|X(\hat{\beta} - \beta^*) - \epsilon\|_2^2 + \lambda_n \psi(\hat{\beta}) &\leq \frac{1}{2n} \|\epsilon\|_2^2 + \lambda_n \psi(\beta^*) \\ \Rightarrow \frac{1}{2n} \|X(\hat{\beta} - \beta^*)\|_2^2 + \lambda_n \psi(\hat{\beta}) &\leq \frac{1}{n} \epsilon^\top X(\hat{\beta} - \beta^*) + \lambda_n \psi(\beta^*), \end{aligned} \quad (\text{B.1})$$

where  $\psi(\beta) = \lambda_n (\|\beta\|_1 + \frac{\alpha}{2} |\beta^\top R \beta|)$ . By Lemma B.1, it holds that

$$P \left( \left\| \frac{1}{n} X^\top \epsilon \right\|_\infty > \gamma_n \right) \leq \delta.$$

Hereafter, we assume that the event  $\{\| \frac{1}{n} X^\top \epsilon \|_\infty \leq \gamma_n\}$  is happening.

Then, if  $\gamma_n \leq \lambda_n/3$ , by (B.1),

$$\begin{aligned} \frac{1}{2n} \|X(\hat{\beta} - \beta^*)\|_2^2 + \lambda_n \psi(\hat{\beta}) &\leq \frac{1}{n} \|\epsilon^\top X\|_\infty \|\beta^* - \hat{\beta}\|_1 + \lambda_n \psi(\beta^*) \\ &\leq \gamma_n \|\beta^* - \hat{\beta}\|_1 + \lambda_n \psi(\beta^*) \leq \frac{1}{3} \lambda_n \|\beta^* - \hat{\beta}\|_1 + \lambda_n \psi(\beta^*). \end{aligned} \quad (\text{B.2})$$

Since

$$\|\hat{\beta} - \beta^*\|_1 = \|\hat{\beta}_S - \beta_S^*\|_1 + \|\hat{\beta}_{S^c} - \beta_{S^c}^*\|_1 = \|\hat{\beta}_S - \beta_S^*\|_1 + \|\hat{\beta}_{S^c}\|_1,$$

and

$$\begin{aligned} |\beta_S^*|^\top R_{SS} |\beta_S^*| - |\hat{\beta}_S|^\top R_{SS} |\hat{\beta}_S| &\leq \sum_{(j,k) \in S \times S} R_{jk} |\beta_j^* \beta_k^* - \hat{\beta}_j \hat{\beta}_k| \\ &\leq 2 \sum_{(j,k) \in S \times S} R_{jk} |\beta_j^* (\beta_k^* - \hat{\beta}_k)| + \sum_{(j,k) \in S \times S} R_{jk} |(\beta_j^* - \hat{\beta}_j) (\beta_k^* - \hat{\beta}_k)| \\ &= 2 |\beta_S^*|^\top R_{SS} |\beta_S^* - \hat{\beta}_S| + |\beta_S^* - \hat{\beta}_S|^\top R_{SS} |\beta_S^* - \hat{\beta}_S| \\ &\leq 2 \|R_{SS} |\beta_S^*|\|_\infty \|\beta_S^* - \hat{\beta}_S\|_1 + D \|\beta_S^* - \hat{\beta}_S\|_1^2, \end{aligned}$$

we obtain that

$$\begin{aligned} &\frac{1}{2n} \|X(\hat{\beta} - \beta^*)\|_2^2 + \lambda_n \left( \|\hat{\beta}_S\|_1 + \|\hat{\beta}_{S^c}\|_1 + \frac{\alpha}{2} |\hat{\beta}_S|^\top R_{SS} |\hat{\beta}_S| + \frac{\alpha}{2} \sum_{(j,k) \notin S \times S} R_{jk} |\hat{\beta}_j \hat{\beta}_k| \right) \\ &\leq \frac{1}{3} \lambda_n (\|\hat{\beta}_S - \beta_S^*\|_1 + \|\hat{\beta}_{S^c}\|_1) + \lambda_n \left( \|\beta_S^*\|_1 + \frac{\alpha}{2} |\beta_S^*|^\top R_{SS} |\beta_S^*| \right) \\ \Rightarrow &\frac{1}{2n} \|X(\hat{\beta} - \beta^*)\|_2^2 + \lambda_n \left( \frac{2}{3} \|\hat{\beta}_{S^c}\|_1 + \frac{\alpha}{2} \sum_{(j,k) \notin S \times S} R_{jk} |\hat{\beta}_j \hat{\beta}_k| \right) \\ &\leq \frac{1}{3} \lambda_n \|\hat{\beta}_S - \beta_S^*\|_1 + \lambda_n \left( \|\beta_S^*\|_1 - \|\hat{\beta}_S\|_1 + \alpha \|R_{SS} |\beta_S^*|\|_\infty \|\beta_S^* - \hat{\beta}_S\|_1 + \frac{\alpha D}{2} \|\beta_S^* - \hat{\beta}_S\|_1^2 \right) \\ \Rightarrow &\frac{1}{2n} \|X(\hat{\beta} - \beta^*)\|_2^2 + \lambda_n \left( \frac{2}{3} \|\hat{\beta}_{S^c}\|_1 + \frac{\alpha}{2} \sum_{(j,k) \notin S \times S} R_{jk} |\hat{\beta}_j \hat{\beta}_k| \right) \\ &\leq \lambda_n \left( \frac{4}{3} \|\hat{\beta}_S - \beta_S^*\|_1 + \alpha \|R_{SS} |\beta_S^*|\|_\infty \|\beta_S^* - \hat{\beta}_S\|_1 + \frac{\alpha D}{2} \|\beta_S^* - \hat{\beta}_S\|_1^2 \right). \end{aligned} \quad (\text{B.3})$$

On the other hand, (B.2) also gives

$$\begin{aligned} \|\hat{\beta}_S\|_1 + \|\hat{\beta}_{S^c}\|_1 &\leq \frac{1}{3} (\|\hat{\beta}_S - \beta_S^*\|_1 + \|\hat{\beta}_{S^c}\|_1) + \|\beta_S^*\|_1 + \frac{\alpha}{2} |\beta_S^*|^\top R_{SS} |\beta_S^*| \\ \Rightarrow \frac{2}{3} \|\hat{\beta}_S - \beta_S^*\|_1 + \frac{2}{3} \|\hat{\beta}_{S^c}\|_1 &\leq 2 \|\beta_S^*\|_1 + \frac{\alpha}{2} |\beta_S^*|^\top R_{SS} |\beta_S^*| \\ \Rightarrow \|\hat{\beta}_S - \beta_S^*\|_1 &\leq 3 \|\beta_S^*\|_1 + \frac{3}{4} \alpha |\beta_S^*|^\top R_{SS} |\beta_S^*| \\ \Rightarrow \|\hat{\beta}_S - \beta_S^*\|_1 &\leq \left( 3 + \frac{3}{4} \alpha \|R_{SS} |\beta_S^*|\|_\infty \right) \|\beta_S^*\|_1. \end{aligned}$$

Therefore, (B.3) gives

$$\begin{aligned} &\frac{2}{3} \|\hat{\beta}_{S^c}\|_1 + \frac{\alpha}{2} \sum_{(j,k) \notin S \times S} R_{jk} |\hat{\beta}_j \hat{\beta}_k| \\ &\leq \left( \frac{4}{3} + \alpha \|R_{SS} |\beta_S^*|\|_\infty + \frac{3}{2} \alpha D \|\beta_S^*\|_1 \left( 1 + \frac{\alpha}{4} \|R_{SS} |\beta_S^*|\|_\infty \right) \right) \|\hat{\beta}_S - \beta_S^*\|_1. \end{aligned} \quad (\text{B.4})$$

The second term of the left side is evaluated as

$$\begin{aligned} \sum_{(j,k) \notin S \times S} R_{jk} |\hat{\beta}_j \hat{\beta}_k| &= \sum_{j \in S^c, k \in S^c} R_{jk} |\hat{\beta}_j \hat{\beta}_k| + 2 \sum_{j \in S, k \in S^c} R_{jk} |(\hat{\beta}_j - \beta_S^* + \beta_S^*) \hat{\beta}_k| \\ &= |\hat{\beta}_{S^c}|^\top R_{S^c S^c} |\hat{\beta}_{S^c}| + 2 |\hat{\beta}_{S^c}|^\top R_{S^c S} |\hat{\beta}_S - \beta_S^* + \beta_S^*|. \end{aligned}$$

Hence, (B.4) gives

$$\begin{aligned} & \frac{2}{3} \|\hat{\beta}_{S^c}\|_1 + \frac{\alpha}{2} |\hat{\beta}_{S^c}|^\top R_{S^c S^c} |\hat{\beta}_{S^c}| + \alpha |\hat{\beta}_{S^c}|^\top R_{S^c S} |\hat{\beta}_S - \beta_S^* + \beta_S^*| \\ & \leq \left( \frac{4}{3} + \alpha \|R_{SS} \beta_S^*\|_\infty + \frac{3}{2} \alpha D \|\beta_S^*\|_1 \left( 1 + \frac{\alpha}{4} \|R_{SS} \beta_S^*\|_\infty \right) \right) \|\hat{\beta}_S - \beta_S^*\|_1 \\ \Rightarrow & \|\hat{\beta}_{S^c}\|_1 + \frac{3}{4} \alpha |\hat{\beta}_{S^c}|^\top R_{S^c S^c} |\hat{\beta}_{S^c}| + \frac{3}{2} \alpha |\hat{\beta}_{S^c}|^\top R_{S^c S} |\hat{\beta}_S - \beta_S^* + \beta_S^*| \\ & \leq \left( 2 + \frac{15}{4} \alpha D \|\beta_S^*\|_1 + \frac{9}{16} (\alpha D \|\beta_S^*\|_1)^2 \right) \|\hat{\beta}_S - \beta_S^*\|_1. \end{aligned} \quad (\text{B.5})$$

If  $\alpha \leq \frac{1}{4D \|\beta_S^*\|_1}$ , we have

$$\|\hat{\beta}_{S^c}\|_1 + \frac{3}{4} \alpha |\hat{\beta}_{S^c}|^\top R_{S^c S^c} |\hat{\beta}_{S^c}| + \frac{3}{2} \alpha |\hat{\beta}_{S^c}|^\top R_{S^c S} |\hat{\beta}_S - \beta_S^* + \beta_S^*| \leq 3 \|\hat{\beta}_S - \beta_S^*\|_1.$$

Therefore, we can see that

$$\Delta\beta \in \mathcal{B}(S, C, C'),$$

where  $\Delta\beta = \hat{\beta} - \beta^*$ ,  $C = 3$  and  $C' = \frac{3}{2}$ . By applying the definition of  $\phi_{\text{GRE}}$  to (B.3), it holds that

$$\frac{\phi_{\text{GRE}}}{2} \|\hat{\beta} - \beta^*\|_2^2 \leq \lambda_n \left( \frac{4}{3} + \frac{5}{2} \alpha D \|\beta_S^*\|_1 + \frac{3}{8} (\alpha D \|\beta_S^*\|_1)^2 \right) \|\hat{\beta}_S - \beta_S^*\|_1$$

Because  $\|\hat{\beta}_S - \beta_S^*\|_1^2 \leq s \|\hat{\beta}_S - \beta_S^*\|_2^2$ , we have

$$\begin{aligned} \|\hat{\beta} - \beta^*\|_2 &\leq \frac{\left( \frac{8}{3} + 5\alpha D \|\beta_S^*\|_1 + \frac{3}{4} (\alpha D \|\beta_S^*\|_1)^2 \right) \sqrt{s} \lambda_n}{\phi_{\text{GRE}}} \\ \Rightarrow \|\hat{\beta} - \beta^*\|_2^2 &\leq \frac{\left( \frac{8}{3} + 5\alpha D \|\beta_S^*\|_1 + \frac{3}{4} (\alpha D \|\beta_S^*\|_1)^2 \right)^2 s \lambda_n^2}{\phi_{\text{GRE}}^2} \leq \frac{16s \lambda_n^2}{\phi_{\text{GRE}}^2} \end{aligned} \quad (\text{B.6})$$

This concludes the assertion.  $\square$

### C Corollary of Theorem 3

For comparison with IIIasso and Lasso, we use the following a little bit stricter bound.

**Corollary C.1.** *Suppose the same assumption of Theorem 3 except for  $\alpha \leq \frac{1}{4D \|\beta_S^*\|_1}$  and Assumption GRE( $S, 3, \frac{3}{2}$ ). Instead, suppose that Assumption GRE( $S, C, \frac{3}{2}$ ) (Definition 1) where  $C = 2 + \frac{15}{4} \alpha D \|\beta_S^*\|_1 + \frac{9}{16} (\alpha D \|\beta_S^*\|_1)^2$  is satisfied. Then, it holds that*

$$\|\hat{\beta} - \beta^*\|_2^2 \leq \frac{\left( \frac{8}{3} + 5\alpha D \|\beta_S^*\|_1 + \frac{3}{4} (\alpha D \|\beta_S^*\|_1)^2 \right)^2 s \lambda_n^2}{\phi_{\text{GRE}}^2},$$

with probability  $1 - \delta$ .

*Proof.* This is derived basically in the same way as Theorem 3. From (B.5), we can see directly that

$$\Delta\beta \in \mathcal{B}(S, C, C'),$$

where  $\Delta\beta = \hat{\beta} - \beta^*$ ,  $C = 2 + \frac{15}{4} \alpha D \|\beta_S^*\|_1 + \frac{9}{16} (\alpha D \|\beta_S^*\|_1)^2$  and  $C' = \frac{3}{2}$ . This and (B.6) concludes the assertion.  $\square$

From this corollary, we can compare Lasso and IILasso with  $R_{SS} = O$ .

- If  $\alpha = 0$ , we have

$$\|\hat{\beta} - \beta^*\|_2^2 \leq \frac{64s\lambda_n^2}{9\phi_{\text{GRE}}^2},$$

with  $\mathcal{B}(S, C, C')$  where  $C = 2$  and  $C' = 0$ . This is a standard Lasso result.

- If  $D = 0$ , we have

$$\|\hat{\beta} - \beta^*\|_2^2 \leq \frac{64s\lambda_n^2}{9\phi_{\text{GRE}}^2},$$

with  $\mathcal{B}(S, C, C')$  where  $C = 2$  and  $C' = \frac{3}{2}$ . Since  $\phi_{\text{GRE}}$  is the minimum eigenvalue restricted by  $\mathcal{B}(S, C, C')$ ,  $\phi_{\text{GRE}}$  of IILasso is larger than that of Lasso.

## D Proof of Theorem 4

*Proof.* Let

$$\check{\beta} := \arg \min_{\beta \in \mathbb{R}^p: \beta_{S^c} = 0} \|y - X\beta\|_2^2.$$

That is,  $\check{\beta}$  is the least squares estimator with the true non-zero coefficients. Let  $\tilde{\beta}$  be a local optimal solution. For  $0 < h < 1$ , letting  $\beta(h) := \tilde{\beta} + h(\check{\beta} - \tilde{\beta})$ , then it holds that

$$\begin{aligned} L_{\lambda_n}(\beta(h)) - L_{\lambda_n}(\tilde{\beta}) &= \frac{h^2 - 2h}{2n} \|X(\tilde{\beta} - \check{\beta})\|_2^2 - \frac{h}{n} (X\tilde{\beta} - y)^\top X(\tilde{\beta} - \check{\beta}) \\ &\quad + \lambda_n(\|\beta(h)\|_1 - \|\tilde{\beta}\|_1) + \frac{\lambda_n \alpha}{2} (|\beta(h)^\top R| - |\tilde{\beta}^\top R|). \end{aligned} \quad (\text{D.1})$$

First we evaluate the term  $\frac{1}{n} (X\tilde{\beta} - y)^\top X(\tilde{\beta} - \check{\beta}) = \frac{1}{n} (X\tilde{\beta} - y)^\top X_S(\tilde{\beta}_S - \check{\beta}_S) + \frac{1}{n} (X\tilde{\beta} - y)^\top X_{S^c}(\tilde{\beta}_{S^c} - \check{\beta}_{S^c})$  as follows:

- (1) Since  $\check{\beta}$  is the least squares estimator and  $\frac{1}{n} X_S^\top X_S$  is invertible by the assumption, we have

$$\check{\beta}_S = (X_S^\top X_S)^{-1} X_S^\top y, \quad \check{\beta}_{S^c} = 0.$$

Therefore,

$$\frac{1}{n} X_S^\top (X\tilde{\beta} - y) = \frac{1}{n} X_S^\top (X_S(X_S^\top X_S)^{-1} X_S^\top - I)y.$$

Here,  $I - X_S(X_S^\top X_S)^{-1} X_S^\top$  is the projection matrix to the orthogonal complement of the image of  $(X_S^\top X_S)^\top$ . Hence,  $\frac{1}{n} (X\tilde{\beta} - y)^\top X_S(\tilde{\beta}_S - \check{\beta}_S) = 0$ .

- (2) Noticing that

$$\begin{aligned} \frac{1}{n} X_{S^c}^\top (X\tilde{\beta} - y) &= -\frac{1}{n} X_{S^c}^\top (I - X_S(X_S^\top X_S)^{-1} X_S^\top) y \\ &= -\frac{1}{n} X_{S^c}^\top (I - X_S(X_S^\top X_S)^{-1} X_S^\top) (X_S \beta_S^* + \epsilon) \\ &= -\frac{1}{n} X_{S^c}^\top (I - X_S(X_S^\top X_S)^{-1} X_S^\top) \epsilon, \end{aligned}$$

where we used  $(I - X_S(X_S^\top X_S)^{-1} X_S^\top) X_{S^c} = 0$  in the last line. Because  $(I - X_S(X_S^\top X_S)^{-1} X_S^\top)$  is a projection matrix, we have  $\|(I - X_S(X_S^\top X_S)^{-1} X_S^\top) X_j\|_2^2 \leq \|X_j\|_2^2$ . This and Lemma B.1 gives

$$\left\| \frac{1}{n} X_{S^c}^\top (X\tilde{\beta} - y) \right\|_\infty \leq \gamma_n,$$

with probability  $1 - \delta$ . Hence, let  $V := \text{supp}(\tilde{\beta}) \setminus S$ , then we have

$$\left| \frac{1}{n} (\tilde{\beta}_{S^c} - \check{\beta}_{S^c})^\top X_{S^c}^\top (X\tilde{\beta} - y) \right| \leq \gamma_n \|\tilde{\beta}_{S^c} - \check{\beta}_{S^c}\|_1 = \gamma_n \|\tilde{\beta}_V\|_1.$$

where we used the assumption  $V \subseteq S^c$  and  $\check{\beta}_V = 0$ .

Combining these inequalities and the assumption  $\lambda_n \geq \gamma_n$ , we have that

$$\left| \frac{1}{n} (X\check{\beta} - y)^\top X(\tilde{\beta} - \check{\beta}) \right| \leq \lambda_n \|\tilde{\beta}_V\|_1. \quad (\text{D.2})$$

As for the regularization term, we evaluate each term of  $\lambda_n(\|\beta(h)\|_1 - \|\tilde{\beta}\|_1) + \frac{\lambda_n}{2}(|\beta(h)|^\top R|\beta(h)| - |\tilde{\beta}|^\top R|\tilde{\beta}|)$  in the following.

(i) Evaluation of  $\|\beta(h)\|_1 - \|\tilde{\beta}\|_1$ . Because of the definition of  $\beta(h)$ , it holds that

$$\begin{aligned} \|\beta(h)\|_1 - \|\tilde{\beta}\|_1 &= \|\tilde{\beta} + h(\check{\beta} - \tilde{\beta})\|_1 - \|\tilde{\beta}\|_1 \\ &= \|\tilde{\beta}_S + h(\check{\beta}_S - \tilde{\beta}_S)\|_1 - \|\tilde{\beta}_S\|_1 + \|\tilde{\beta}_V + h(\check{\beta}_V - \tilde{\beta}_V)\|_1 - \|\tilde{\beta}_V\|_1 \\ &= \|\tilde{\beta}_S + h(\check{\beta}_S - \tilde{\beta}_S)\|_1 - \|\tilde{\beta}_S\|_1 + (1-h)\|\tilde{\beta}_V\|_1 - \|\tilde{\beta}_V\|_1 \\ &\leq h\|\check{\beta}_S - \tilde{\beta}_S\|_1 - h\|\tilde{\beta}_V\|_1. \end{aligned} \quad (\text{D.3})$$

(ii) Evaluation of  $|\beta(h)|^\top R|\beta(h)| - |\tilde{\beta}|^\top R|\tilde{\beta}|$ . Note that

$$\begin{aligned} &|\beta(h)_j|_{R_{jk}}|\beta(h)_k| - |\tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| \\ &= |(1-h)\tilde{\beta}_j + h\check{\beta}_j|_{R_{jk}}|(1-h)\tilde{\beta}_k + h\check{\beta}_k| - |\tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| \\ &\leq (1-h)^2|\tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| + h(1-h)(|\check{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| + |\tilde{\beta}_j|_{R_{jk}}|\check{\beta}_k|) \\ &\quad + h^2|\check{\beta}_j|_{R_{jk}}|\check{\beta}_k| - |\tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| \\ &= -2h|\tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| + h(|\check{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| + |\tilde{\beta}_j|_{R_{jk}}|\check{\beta}_k|) + O(h^2) \\ &= h(|\check{\beta}_j| - |\tilde{\beta}_j|)_{R_{jk}}|\tilde{\beta}_k| + |\tilde{\beta}_j|_{R_{jk}}(|\check{\beta}_k| - |\tilde{\beta}_k|) + O(h^2). \end{aligned} \quad (\text{D.4})$$

If  $j, k \in S$ , then the right hand side of Eq. (D.4) is bounded by

$$\begin{aligned} &h(|\check{\beta}_j - \tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k - \tilde{\beta}_k| + |\tilde{\beta}_j - \tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k - \tilde{\beta}_k|) \\ &\quad + h(|\check{\beta}_j - \tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k| + |\tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k - \tilde{\beta}_k|) + O(h^2). \end{aligned}$$

If  $j \in V$  and  $k \in S$ , then the right hand side of Eq. (D.4) is bounded by

$$h|\tilde{\beta}_j|_{R_{jk}}(|\tilde{\beta}_k| - |\tilde{\beta}_k|) + O(h^2) \leq h|\tilde{\beta}_j|_{R_{jk}}|\tilde{\beta}_k - \tilde{\beta}_k| + O(h^2).$$

If  $j \in V$  and  $k \in V$ , then the right hand side of Eq. (D.4) is bounded by

$$0 + O(h^2) = O(h^2).$$

Based on these evaluations, we have

$$\begin{aligned} &|\beta(h)|^\top R|\beta(h)| - |\tilde{\beta}|^\top R|\tilde{\beta}| \\ &\leq 2h \left( |\check{\beta}_S - \tilde{\beta}_S|^\top R_{SS}|\check{\beta}_S - \tilde{\beta}_S| + |\check{\beta}_S - \tilde{\beta}_S|^\top R_{SS}|\tilde{\beta}_S| + |\tilde{\beta}_V|^\top R_{VS}|\check{\beta}_S - \tilde{\beta}_S| \right) + O(h^2) \\ &\leq 2h \left( |\check{\beta} - \tilde{\beta}|^\top R|\check{\beta} - \tilde{\beta}| + |\check{\beta}_S - \tilde{\beta}_S|^\top R_{SS}|\tilde{\beta}_S| \right) + O(h^2) \\ &\leq 2h\bar{D}(\|\check{\beta} - \tilde{\beta}\|_2^2 + \|\tilde{\beta}\|_2\|\check{\beta}_S - \tilde{\beta}_S\|_2) + O(h^2). \end{aligned}$$

Here, we will show later in Eq. (D.6) that  $\|\check{\beta} - \beta^*\|_2 \leq \sqrt{s}\lambda_n/\phi$ , and thus it follows that

$$\|\tilde{\beta}\|_2 \leq \|\beta^*\|_2 + \sqrt{s}\lambda_n/\phi.$$

Therefore, we obtain that

$$\begin{aligned} &|\beta(h)|^\top R|\beta(h)| - |\tilde{\beta}|^\top R|\tilde{\beta}| \\ &\leq 2h\bar{D} \left( \|\check{\beta} - \tilde{\beta}\|_2^2 + (\|\beta^*\|_2 + \sqrt{s}\lambda_n/\phi)\|\check{\beta}_S - \tilde{\beta}_S\|_2 \right) + O(h^2). \end{aligned} \quad (\text{D.5})$$

Applying the inequalities (D.2), (D.3) and (D.5) to (D.1) yields that

$$\begin{aligned}
& L_{\lambda_n}(\beta(h)) - L_{\lambda_n}(\tilde{\beta}) \\
& \leq h \left\{ -\frac{1}{n} \|X(\check{\beta} - \tilde{\beta})\|_2^2 + \lambda_n \|\tilde{\beta}_S - \check{\beta}_S\|_1 - (\lambda_n - \gamma_n) \|\tilde{\beta}_V\|_1 \right. \\
& \quad \left. + \lambda_n \alpha \bar{D} [\|\check{\beta} - \tilde{\beta}\|_2^2 + (\|\beta^*\|_2 + \sqrt{s} \lambda_n / \phi) \|\check{\beta}_S - \tilde{\beta}_S\|_2] \right\} + O(h^2) \\
& \leq h \left\{ -\phi \|\check{\beta} - \tilde{\beta}\|_2^2 + \lambda_n \|\tilde{\beta}_S - \check{\beta}_S\|_1 \right. \\
& \quad \left. + \lambda_n \alpha \bar{D} [\|\check{\beta} - \tilde{\beta}\|_2^2 + (\|\beta^*\|_2 + \sqrt{s} \lambda_n / \phi) \|\check{\beta}_S - \tilde{\beta}_S\|_2] \right\} + O(h^2) \\
& \leq h \left\{ (-\phi + \lambda_n \alpha \bar{D}) \|\check{\beta} - \tilde{\beta}\|_2^2 \right. \\
& \quad \left. + \lambda_n \left( \|\tilde{\beta}_S - \check{\beta}_S\|_1 + \alpha \bar{D} (\|\beta^*\|_2 + \sqrt{s} \lambda_n / \phi) \|\check{\beta}_S - \tilde{\beta}_S\|_2 \right) \right\} + O(h^2),
\end{aligned}$$

where we used the assumption  $\lambda_n > \gamma_n$  in the second inequality.

Since we have assumed  $\alpha < \min \left\{ \frac{\sqrt{s}}{2\bar{D}\|\beta^*\|_2}, \frac{\phi}{2\bar{D}\lambda_n} \right\}$ , the right hand side is further bounded by

$$h \left\{ -\frac{\phi}{2} \|\check{\beta} - \tilde{\beta}\|_2^2 + 2\lambda_n \sqrt{s} \|\check{\beta}_S - \tilde{\beta}_S\|_2 \right\} + O(h^2).$$

Because of this, if  $\|\check{\beta} - \tilde{\beta}\|_2 > \frac{4\sqrt{s}\lambda_n}{\phi}$ , then the first term becomes negative, and we conclude that, for sufficiently small  $\eta > 0$ , it holds that

$$L_{\lambda_n}(\beta(h)) < L_{\lambda_n}(\tilde{\beta}),$$

for all  $0 < h < \eta$ . In other word,  $\tilde{\beta}$  is not a local optimal solution. Therefore, we must have

$$\|\check{\beta} - \tilde{\beta}\|_2 \leq \frac{4\sqrt{s}\lambda_n}{\phi}$$

Finally, notice that  $\|\tilde{\beta} - \beta^*\|_2^2 \leq (\|\tilde{\beta} - \check{\beta}\|_2 + \|\beta^* - \check{\beta}\|_2)^2$  and

$$\begin{aligned}
\|\tilde{\beta} - \beta^*\|_2^2 &= \|(X_S^\top X_S)^{-1} X_S^\top y - \beta_S^*\|_2^2 = \|(X_S^\top X_S)^{-1} X_S^\top (X_S \beta_S^* + \epsilon) - \beta_S^*\|_2^2 \\
&= \|(X_S^\top X_S)^{-1} X_S^\top \epsilon\|_2^2 \leq \phi^{-2} \left\| \frac{1}{n} X_S^\top \epsilon \right\|_2^2 \leq \phi^{-2} s \gamma_n^2 \leq \phi^{-2} s \lambda_n^2, \tag{D.6}
\end{aligned}$$

which concludes the assertion.  $\square$

## E Optimization for Logistic Regression

We derive coordinate descent algorithm of ILLasso for the binary objective variable. The objective function is

$$L(\beta) = -\frac{1}{n} \sum_i (y_i X^i \beta - \log(1 + \exp(X^i \beta))) + \lambda \left( \|\beta\|_1 + \frac{\alpha}{2} |\beta|^\top R |\beta| \right),$$

where  $X^i$  is the  $i$ -th row of  $X = [1, X_1, \dots, X_p]$  and  $\beta = [\beta_0, \beta_1, \dots, \beta_p]$ . Forming a quadratic approximation with the current estimate  $\tilde{\beta}$ , we have

$$\bar{L}(\beta) = -\frac{1}{2n} \sum_{i=1}^n w_i (z_i - X^i \beta)^2 + C(\tilde{\beta}) + \lambda \left( \|\beta\|_1 + \frac{\alpha}{2} |\beta|^\top R |\beta| \right),$$

where

$$\begin{aligned}
z_i &= X^i \tilde{\beta} + \frac{y_i - \bar{p}(X^i)}{\bar{p}(X^i)(1 - \bar{p}(X^i))}, \\
w_i &= \bar{p}(X^i)(1 - \bar{p}(X^i)), \\
\bar{p}(X^i) &= \frac{1}{1 + \exp(-X^i \tilde{\beta})}.
\end{aligned}$$

---

**Algorithm E.1** CDA for Logistic IIIasso

---

```
for  $\lambda = \lambda_{\max}, \dots, \lambda_{\min}$  do  
  initialize  $\beta$   
  while until convergence do  
    update the quadratic approximation using the current parameters  $\bar{\beta}$   
    while until convergence do  
      for  $j = 1, \dots, p$  do  
         $\beta_j \leftarrow \frac{1}{\frac{1}{n} \sum_{i=1}^n w_i X_{ij}^2 + \lambda \alpha R_{jj}} S \left( \frac{1}{n} \sum_{i=1}^n w_i (z_i - X_{i,-j} \beta_{-j}) X_{ij}, \lambda (1 + \alpha R_{j,-j} |\beta_{-j}|) \right)$   
      end for  
    end while  
  end while  
end for
```

---

To derive the update equation, when  $\beta_j \neq 0$ , differentiating the quadratic objective function with respect to  $\beta_j$  yields

$$\begin{aligned} \partial_{\beta_j} \bar{L}(\beta) &= -\frac{1}{n} \sum_{i=1}^n w_i (z_i - X^i \beta) X_{ij} + \lambda (\text{sgn}(\beta_j) + \alpha R_j^\top |\beta| \text{sgn}(\beta_j)) \\ &= -\frac{1}{n} \sum_{i=1}^n w_i (z_i - X_{i,-j} \beta_{-j}) X_{ij} + \left( \frac{1}{n} \sum_{i=1}^n w_i X_{ij}^2 + \lambda R_{jj} \right) \beta_j + \lambda (1 + \alpha R_{j,-j} |\beta_{-j}|) \text{sgn}(\beta_j). \end{aligned}$$

This yields

$$\beta_j \leftarrow \frac{1}{\frac{1}{n} \sum_{i=1}^n w_i X_{ij}^2 + \lambda \alpha R_{jj}} S \left( \frac{1}{n} \sum_{i=1}^n w_i (z_i - X_{i,-j} \beta_{-j}) X_{ij}, \lambda (1 + \alpha R_{j,-j} |\beta_{-j}|) \right).$$

These procedures amount to a sequence of nested loops. The whole algorithm is described in Algorithm E.1.