On Newton Screening

Jian Huang∗ Yuling Jiao† Lican Kang‡ Jin Liu§
Yanyan Liu¶ Xiliang Lu∥ YuanYuan Yang∗∗

February 10, 2020

Abstract

Screening and working set techniques are important approaches to reducing the size of an optimization problem. They have been widely used in accelerating first-order methods for solving large-scale sparse learning problems. In this paper, we develop a new screening method called Newton screening (NS), which is a generalized Newton algorithm with a built-in screening mechanism. We derive an equivalent KKT system for the Lasso and utilize a generalized Newton method to solve the KKT equations. Based on this KKT system, a built-in working set with a relatively small size is first determined using the sum of primal and dual variables generated from the previous iteration, then the primal variable is updated by solving a least-squares problem on the working set and the dual variable updated based on a closed-form expression. Moreover, we consider a sequential version of Newton screening (SNS) with a warm-start strategy. We show that NS possesses an optimal convergence property in the sense that it achieves local convergence in just one step. Under certain regularity conditions on the feature matrix, we show that SNS hits a point on the solution path with the same signs as the underlying true target and achieves a sharp estimation error bound with high probability. Simulation studies and real data analysis support our theoretical results and demonstrate that SNS is faster and more accurate than several state-of-the-art methods for large-scale sparse learning problems in our comparative studies.

∗Department of Statistics and Actuarial Science, University of Iowa, Iowa City, IA 52242 (jianhuang@uiowa.edu)
†School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China. (yulingjiao-math@whu.edu.cn)
‡School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China. (kanglican@whu.edu.cn)
§Center of Quantitative Medicine Duke-NUS Medical School, Singapore. (jin.liu@duke-nus.edu.sg)
¶School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China. (e-mails: liuyy@whu.edu.cn)
∥School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China, and Hubei Key Laboratory of Computational Science (Wuhan University), Wuhan, 430072, China. (xllv.math@whu.edu.cn)
∗∗School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China. (yuanyuanyang.math@whu.edu.cn)
1 Introduction

Sparse learning is an important problem in machine learning, statistics and signal processing. In machine learning and statistics, sparsity is a vital variable/feature selection tool for constructing parsimonious models that admit easy interpretation and better prediction [36, 2]. In signal processing, sparsity represents an important structural property that can be effectively exploited for data acquisition, signal transmission, storage and processing [5, 24]. Since the proposal of Lasso [5, 36], there has been extensive research on its theoretical guarantees with respect to feature selection, estimation and prediction, see, for example, [?] and [38] and the references therein. Computationally, first-order methods such as coordinate descent [10] and proximal gradient descent [6] are workhorses for solving high-dimensional sparse learning models in machine learning and statistics. The computational costs per iteration of vanilla coordinate descent and proximal gradient descent are $O(np)$, as each iteration involves only updating the coordinates of $p$ features with a sample of size $n$. Screening and working set techniques based on correlations or convex duality have been developed for statically or dynamically reducing the size of an optimization problem and accelerating first-order solvers by exploring the sparsity structure of the learning problems [34, 8, 11, 37, 29, 11, 10, 21, 3, 39, 0, 27, 43, 15, 31, 25, 26, 32].

In this paper, we develop a new dynamic screening method called Newton screening (NS). We name the proposed approach Newton screening since it can be considered a generalized Newton method [17, 30, 14] for the Lasso with a built-in screening mechanism. NS is derived from a generalized Newton method for solving an equivalent KKT system for the Lasso problem. By design, at each iteration of the generalized Newton method, a built-in working set with a small size is determined by using the sum of primal and dual variables generated from the previous iteration. Then we sequentially update the primal variable by solving a least squares problem on the working set, and update the dual variable based on a closed-form expression. We show that NS converges in just one step as long as a good initial value is available. To make NS more practical to use, we consider a sequential version of Newton screening (SNS) by combining NS with a continuation strategy on the regularization parameter. We further prove that under a coherence condition for the feature matrix, SNS achieves sharp estimation error bound in $\ell_\infty$ norm with high probability. Moreover, SNS hits a solution with the same signs as the underlying true target as long as the target signal is detectable. We conduct extensive numerical experiments with both simulated and real data to demonstrate the efficiency and accuracy of SNS. Our numerical studies show that SNS is faster and more accurate than several state-of-the-art methods. The MATLAB and R packages are available at [http://faculty.anonymous/list.htm](http://faculty.anonymous/list.htm).

We end this section via introducing some notation used in the remainder of this paper. With $\|\beta\|_q = (\sum_{i=1}^p |\beta_i|^q)^\frac{1}{q}$, $q \in [1, \infty]$, we denote the usual $q$-norm of a vector $\beta = (\beta_1, \ldots, \beta_p)^T \in \mathbb{R}^p$. $\|\beta\|_0$ denotes the number of nonzero elements of $\beta$. $\|X\|$ denotes the operator norm of the matrix $X$ induced by vector with 2-norm. Define $S = \{1, \ldots, p\}$. For any $A \subseteq S$ with length $|A|$, we denote $\beta_A$ (or $X_A \in \mathbb{R}^{n \times |A|}$) as
the subvector (or submatrix) whose entries (or columns) are listed in $A$. $X_{AB}$ denotes submatrix of $X$ whose rows and columns are listed in $A$ and $B$, respectively. We use $\text{supp}(z)$, and $\text{sign}(z)$, and $\text{diag}(z)$, and $1_A$ to denote the support of $z$, the sign of $z$, a diagonal matrix with $z$ being the diagonal, and the indicator function of set $A$, respectively. We use $E$ to denote the identity matrix, and $\lfloor a \rfloor$ denotes the maximum integer no greater than $a$.

2 Derivation of NS

In this section, we describe the proposed NS method in the setting of high-dimensional linear regression. NS can be generalized to solve problems using general convex and differentiable losses with $\ell_1$ / group $\ell_1$ regularization, see Section 6 for a brief discussion. Let $Y = X\beta^* + \epsilon$, where $Y \in \mathbb{R}^n$ is the response vector, $X = [x_1, \ldots, x_p] \in \mathbb{R}^{n \times p}$ is the feature matrix, $\beta^* \in \mathbb{R}^p$ is the target sparse coefficient vector with support $A^*$, and $\epsilon = (\epsilon_1, \ldots, \epsilon_n)^T \in \mathbb{R}^n$ is the random error term. Without loss of generality, we assume that $X$ is normalized such that each feature is $\sqrt{n}$-length. The Lasso [36, 5] estimator reads

$$\beta^* \in \arg \min_{\beta \in \mathbb{R}^{p}} \frac{1}{2n} \|Y - X\beta\|^2 + \lambda \|\beta\|_1, \quad (1)$$

where $\lambda > 0$ is the penalty parameter.

2.1 Motivating NS based on the KKT conditions

We have the following KKT characterization of $\beta^*$.

**Lemma 2.1.** The value $\beta^*$ is a minimizer of (1) if and only if

$$d^* = \frac{X^T(Y - X\beta^*)}{n},$$

$$\beta^* = \Gamma_{\lambda}(\beta^* + d^*), \quad (2)$$

where $\Gamma_{\lambda}(\cdot)$ is the soft-thresholding operator whose $i$th element is given by

$$\Gamma_{\lambda}(\beta)_i = \begin{cases} 
\beta_i - \lambda, & \beta_i > \lambda, \\
\beta_i + \lambda, & \beta_i < -\lambda, \\
0, & |\beta_i| \leq \lambda. 
\end{cases} \quad (3)$$

Let

$$A^* = \text{supp}(\beta^*), I^* = (A^*)^c.$$

From the definition of $\Gamma_{\lambda}(\cdot)$ and (2), we can conclude that

$$A^* = \{i : |\beta_i^* + d_i^*| > \lambda\}, \quad I^* = \{i : |\beta_i^* + d_i^*| \leq \lambda\}, \quad (4)$$
and

\[
\begin{align*}
\beta^0_i & = 0 \\
\delta^0_A & = \lambda \text{sign}(\beta^0_A + d^0_A) \\
\beta^0_A & = (X_A^T X_A/n)^{-1} (X_A^T Y/n - d^0_A) \\
d^0_A & = X_T^T (Y - X_A^T \beta^0_A)/n.
\end{align*}
\] (5)

From (4), we see that the support $A^0$ of the solution is determined by the sum of the primal ($\beta^0$) and dual ($d^0$) variables. Moreover, we can reduce the bias of Lasso by replacing $\lambda$ with $\lambda - \bar{\lambda}$ in (5), where $\bar{\lambda} \in (0, \lambda)$. Let $\{\beta^0, d^0\}$ be an initial guess of $\{\beta^0, d^0\}$. and denote $\{A^0, I^0\}$ as the working set and its complements determined by $\{\beta^0, d^0\}$, i.e.,

\[
A^0 = \{i : |\beta^0_i + d^0_i| > \lambda\}, \quad I^0 = \{i : |\beta^0_i + d^0_i| \leq \lambda\}.
\]

Then we obtain the updated approximation values $\{\beta^i_A, d^i_A, \beta^i_{A^0}, \delta^i_{A^0}\}$ as follows:

\[
\begin{align*}
\beta^i_{A^c} & = 0 \\
\delta^i_A & = (\lambda - \bar{\lambda}) \text{sign}(\beta^i_A + d^i_A) \\
\beta^i_A & = (X_A^T X_A/n)^{-1} (X_A^T Y/n - \delta^i_A) \\
d^i_A & = X_T^T (Y - X_A^T \beta^i_A)/n.
\end{align*}
\] (6)

We can repeat the above procedure iteratively in a way that mimics an oracle solving the KKT equations (2). These are the key steps of the proposed NS algorithm. At each iteration, a small working set is determined using the sum of primal and dual variables generated from the previous iteration. Then we sequentially update the primal variable by solving a least squares problem on the working set and update the dual using an explicit form. The NS algorithm is given in Algorithm 1 below.

**Algorithm 1 NS Algorithm**

1. Input: $\beta^0$, $d^0$, $\lambda$, $\bar{\lambda}$, $k = 0$, $K$
2. for $k = 0, 1, \ldots, K$, do
3. \hspace{1em} $A^k = \{i : |\beta^k_i + d^k_i| > \lambda\}$, \hspace{1em} $I^k = (A^k)^c$.
4. \hspace{1em} $\beta^{k+1}_{A^c} = 0$.
5. \hspace{1em} $d^{k+1}_A = (\lambda - \bar{\lambda}) \text{sign}(\beta^{k+1}_A + d^{k+1}_A)$.
6. \hspace{1em} $\beta^{k+1}_A = (X_A^T X_A/n)^{-1} (X_A^T Y/n - d^{k+1}_A)$.
7. \hspace{1em} $d^{k+1}_A = X_T^T (Y - X_A^T \beta^{k+1}_A)/n$.
8. \hspace{1em} if $A^k = A^k$ or $k \geq K$, stop and denote the last iteration $\beta_A$, $\beta_I$, $d_A$, $d_I$.
9. \hspace{1em} else
10. \hspace{1em} $k = k + 1$
11. \hspace{1em} end if
12. end for
13. Output: $\hat{\beta}(\lambda) = (\beta_A^T, \beta_I^T)^T$ and $\hat{d}(\lambda) = (d_A^T, d_I^T)^T$.

**Remark 2.1.** As we show in Section 3, NS algorithm (Algorithm 1) is actually a gener-
alized Newton method for solving the KKT equations (2) and achieves local convergence in just one step with a computational cost of $O(np)$. Therefore, NS as presented in Algorithm 1 shows that the generalized Newton method has a build-in screening mechanism. This implies that the complexity per iteration of the generalized Newton method is low.

Algorithm 2 SNS Algorithm

1: Input: $\hat{\beta}(\lambda_0) = 0, \tilde{d}(\lambda_0) = X^T Y / n$, $\lambda_0 = \|X^T Y / n\|_{\infty}$, $\alpha$, $M$.
2: for $m = 1, \ldots, M$ do
3: $\lambda = \lambda_m = \lambda_0 \alpha^m$, $\beta^0 = \hat{\beta}(\lambda_{m-1})$, $d^0 = \tilde{d}(\lambda_{m-1})$.
4: Run Algorithm 1 to get $\hat{\beta}(\lambda_m)$ and $\tilde{d}(\lambda_m)$.
5: if $\|\hat{\beta}(\lambda_m)\|_0 < \lfloor n \log p \rfloor$, stop.
6: end for
7: Output: $\{\hat{\beta}(\lambda_1), \hat{\beta}(\lambda_2) \ldots \}$.

2.2 Sequential Newton screening algorithm

To successfully apply Algorithm 1 to estimate the sparse target $\beta^*$, there are two important practical issues, i.e., determining the initial value $(\beta^0, d^0)$ in Algorithm 1 and selecting a proper regularization parameter $\lambda$. In this section, we propose a sequential Newton screening algorithm (SNS) via combining NS with the continuation strategy to provide good initial guesses and simultaneously output a solution path. The idea of sequential screening on the solution path has been used in previous screening and working set methods [11, 37, 41, 40, 21, 28, 25]. Specifically, let $\lambda_m = \lambda_0 \alpha^m$, $\alpha \in (0, 1)$, be a decreasing sequence of regularization parameters, where we set

$$\lambda_0 = \|X^T Y / n\|_{\infty}$$

such that

$$\hat{\beta}(\lambda_0) = 0 \text{ and } \tilde{d}(\lambda_0) = X^T Y / n.$$ 

Then we apply Algorithm 1 on the sequence $\{\lambda_m\}_m$ (the shift parameter $\lambda_m$ in Algorithm 1 varies linearly in $\lambda_m$), with the solution $\{\hat{\beta}(\lambda_m), d(\lambda_m)\}$ being the initial guess for the $\lambda_{m+1}$-problem. We can stop the SNS algorithm and obtain a solution path until $\|\hat{\beta}_{\lambda_m}\|_0 > \lfloor \frac{n}{\log p} \rfloor$ for some $m$. Then we determine the optimal $\lambda$ by a data-driven method such as cross validation, Bayesian information criterion [42] or the voting method [13] without any extra computational overhead. The overall SNS algorithm is described in Algorithm 2. In Section 3.4, we prove that under certain regularity conditions on the feature matrix, with high probability, SNS hits a solution that achieves a sharp estimation error bound and has the same signs as the underlying true target $\beta^*$. 

5
3 Theoretical properties of NS and SNS

3.1 NS as a generalized Newton algorithm

In this subsection, we derive the NS algorithm from the generalized Newton method [17] [30] [14].

Let $z = \left( \begin{array}{c} \beta \\ d \end{array} \right)$ and $F(z) = \left[ \begin{array}{c} F_1(z) \\ F_2(z) \end{array} \right] : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}^{2p}$, where

$$F_1(z) = \beta - \Gamma \lambda (\beta + d),$$
$$F_2(z) = nd - X^T(Y - X\beta).$$

By Lemma 2.1 finding a minimizer of (1) is equivalent to finding a root of $F(z)$. Since $F(z)$ is not Fréchet differentiable, classical Newton method cannot be applied directly. Thus we resort to using generalized Newton algorithm since $F(z)$ is Newton differentiable, see the appendix for the definition, basic property and calculation of Newton derivatives.

Let $A = \{i : |\beta_i + d_i| > \lambda\}, \ I = \{i : |\beta_i + d_i| \leq \lambda\}$.

After permutation, we rewrite $z$ and $F(z)$ such that

$$z = (d^T_A, \beta^T_A, \beta^T_I, d^T_I)^T,$$

and

$$F(z) = \left[ \begin{array}{c} \beta_A - \Gamma \lambda (\beta_A + d_A) \\ \beta_I - \Gamma \lambda (\beta_I + d_I) \\ nd_A - (X^T_A Y - X^T_A X_A \beta_A - X^T_A X_I \beta_I) \\ nd_I - (X^T_I Y - X^T_I X_A \beta_A - X^T_I X_I \beta_I) \end{array} \right].$$

At the $k$th iteration, the generalized Newton method for finding the root of $F(z) = 0$ consists of two steps:

(i) Solve $H_k D^k = -F(z^k)$ for $D^k$, where $H_k$ is an element of $\nabla_N F(z^k)$.

(ii) Update $z^{k+1} = z^k + D^k$, set $k \leftarrow k + 1$ and go to step (i).

The above generalized Newton method for finding a root of a non-smooth equation has the same form as the classical Newton method, except that we choose an element from the Newton derivative $\nabla_N F_N(z^k)$ in step (i) since it is a set-valued mapping by definition.

The next Theorem shows that the NS Algorithm 1 (with $\lambda = 0$) is actually a form of the generalized Newton method.

**Theorem 3.1.** The NS Algorithm 1 with $\lambda = 0$ is equivalent to the generalized Newton iteration.
3.2 Optimal local convergence

We now show that NS achieves optimal local convergence in the sense that it converges locally in just one iteration, which improves the local superliner convergence rate of the generalized Newton method \cite{17,30,14}.

**Theorem 3.2.** Let $\beta^*$ be a minimizer of (1) and let $d^\circ = X^T (Y - X\beta^\circ)/n$. Define

$$A^\circ = \{ i : |\beta^\circ_i + d^\circ_i| > \lambda \}, A^\circ = \{ i : |\beta^\circ_i + d^\circ_i| \geq \lambda \},$$

and

$$\tilde{A} = \{ i : |\beta^\circ_i + d^\circ_i| \neq \lambda \}, C = \min_{i \in \tilde{A}} ||\beta^\circ_i + d^\circ_i| - \lambda|.$$

Suppose the rank of $X_{A^\circ}$ is $|A^\circ|$ and the initial guess $\{\beta^0, d^0\}$ satisfies

$$\|\beta^0 - \beta^\circ\|_\infty + \|d^0 - d^\circ\|_\infty \leq C.$$

Then, $\beta^1 = \beta^\circ$, where $\beta^1$ is the one-step iteration of NS with $\lambda = 0$ in Algorithm 1.

3.3 Computational complexity analysis

In this subsection, we analyze the computational complexity of NS algorithm 1 and SNS algorithm 2. We look at the number of floating point operations per iteration in NS. Clearly it takes $O(p)$ flops to finish step 3-9 in Algorithm 1 except step 6. For step 6, we can solve the linear equation iteratively by conjugate gradient (CG) method initialized with the projection of the previous solution onto the current working set \cite{12}. The main operation of CG per iteration is two matrix-vector multiplication cost $2n|A^k|$ flops. Therefore, we can control the maximum number of CG iterations to be smaller than $p/(2n|A^{k+1}|)$, enabling one to complete step 6 in $O(np)$ flops. The local one-step convergence of NS guarantees that overall cost of NS is $O(np)$, which is the cost per iteration for vanilla first-order Lasso solvers such as coordinate or proximal gradient descent, if a good initial value is provided. Thanks to the continuation strategy in SNS algorithm 2, SNS can be used to obtain the solution path accurately and efficiently at the cost of $O(Mnp)$ with $M$ being the number of knots used on the path, see the numerical results in Section 5.

3.4 Estimation error of SNS

Our SNS algorithm 2 is designed to find a solution path of the Lasso problem (1). In this subsection we show that SNS will hit a solution that stays in a ball centered at $\beta^*$ with an optimal statistical radius. To this end, we need the following model and technical assumptions.

(C1) $|A^*| \leq T$ for some positive integer $T$ and $\|\beta^*_A\|_{\min} \geq 78 \gamma_n$, where $A^* = \text{supp}(\beta^*)$ and $\gamma_n = \sigma \sqrt{\log(p)/n}$.
(C2) $\epsilon \in \mathbb{R}^n$ is a sub-Gaussian random vector, i.e., there exists a constant $\sigma > 0$ such that $\mathbb{E}[\exp(\epsilon^T a)] \leq \exp(||a||^2 \sigma^2 t^2 / 2)$ for $a \in \mathbb{R}^n$, $t \in \mathbb{R}$.

(C3) $T \nu \leq \frac{1}{4}$, where $\nu = \max_{i \neq j} |G_{i,j}|$, with $G_{i,j}$ being the $(i,j)$ element of the Gram matrix $G = X^T X / n$.

**Lemma 3.1.** Suppose that (C1) to (C3) hold. Set $\alpha = \frac{8}{13}$ in SNS algorithm 2. Then there exists an integer $M \in [1, \log(\frac{30 \gamma_n}{\lambda_0})]$ such that $\lambda_M > 30 \gamma_n \geq \lambda_{M+1}$ and $\|\beta^*_A - \beta\|_\infty > \frac{8}{5} \lambda_M$ hold with probability at least $1 - \frac{2}{p}$.

**Theorem 3.3.** Suppose that (C1)-(C3) hold. Set $\alpha = \frac{8}{13}$, $\tilde{\lambda}_m = \frac{13}{15} \lambda_m + 4 \gamma_n$ in SNS algorithm 2 and $K \geq T$ in NS algorithm 1. Then with probability at least $1 - \frac{2}{p}$,

\[
\text{sign}(\hat{\beta}(\lambda_M)) = \text{sign}(\beta^*) \tag{7}
\]

and

\[
\|\hat{\beta}(\lambda_M) - \beta^*\|_\infty < \frac{14}{5} \gamma_n, \tag{8}
\]

where $M$ is determined in Lemma 3.1.

**Remark 3.1.** Condition (C1) assumes that the underlying target $\beta^*$ is sparse and statistically detectable. Condition (C2) is a common assumption for the random noise. Condition (C3) is a coherence condition for the feature matrix. This kind of coherence condition has also been widely used in previous works in bounding the estimation error of greedy and penalized estimators, for example, [22], [4], [7] and [46] assumed $T \nu < \frac{1}{7}$, $\nu < c/ \log(p)$ for a positive constant $c$, $T \nu < 1/4$ and $T \nu \leq 1/4$, respectively.

### 4 Related Works

Our proposed NS is a generalized Newton method for the Lasso with a built-in screening mechanism. Several screening and working set techniques have been proposed to reduce the size of the optimization problem and to accelerate the existing solvers, especially the first-order methods [11, 37, 41, 40, 21, 3, 39, 9, 27, 43, 15, 31, 28, 16, 25, 26, 32].

The above mentioned works on screening and working set remove features from the problem primarily based on the dual information, see [28] for a detailed discussion. In contrast, our NS method selects features using both the primal and the dual information. In addition, the statistical estimation error bound proved in Theorem 3.3 has not been explored in the previous works on screening and working set methods. Computationally, our NS and SNS are simpler and easier to implement than many of the existing methods.

NS and SNS solve the Lasso and estimate the target coefficient directly. Recently, several authors have proposed to take advantages of the fast convergence of the generalized Newton-type methods as an inner solver nested in some (primarily first-order) algorithms. In [19], the authors propose a DC proximal Newton (DCPN) method to solve nonconvex sparse learning problems. The DCPN is based on the multistage convex relaxation scheme that transforms the original nonconvex optimizations into sequences of
Lasso regularized nonlinear regressions. At each stage, a second-order Taylor expansion is used to approximate the nonlinear loss functions, and then a Lasso inner solver is called. [1] proposed using an ADMM algorithm to solve structured convex conic programming, where a nonsmooth Newton method is called to find a fixed point of the residuals of the consecutive ADMM iterations. In [18, 44, 47, 20, 23], the authors used semi-smooth Newton inner solver coupled with an augmented Lagrangian outer loop by fully exploring the second-order sparsity of the learning problem.

5 Simulation studies and real data analysis

In this section, we conduct simulation studies and real data analysis to illustrate the effectiveness of the proposed NS and SNS. We also compare SNS with several state-of-the-art screening/woring set methods such as SIS [8], sequential strong rules (SSR) [37], sequential enhanced dual polytope projection (SEDPP) [39], gap safe rules (GSR) [9], and gap safe rules with dual extrapolation (CELER) [25]. We implemented GSR and CELER in R based on the Python packages https://github.com/EugeneNdiaye and https://github.com/mathurinm/celer, respectively, and use the R packages SIS [35], GLMNET [37] and Biglasso [45] for SIS, SSR and SEDPP, respectively. All the experiments are performed in R version 3.5.1 on a quad-core laptop with an Intel Core i7-5500U CPU (2.40 GHz) and 8 GB RAM running Windows 10 (64 bit).

In all the simulations, the \( n \times p \) feature matrix \( X \) is generated according to the following two settings:

(I) The rows of \( X \) are independently distributed from \( N(0, \Sigma) \), where \( \Sigma_{i,j} = \rho^{|i-j|} \) for \( 1 \leq i, j \leq p \). Here \( 0 < \rho < 1 \) is a measure of the correlation among features.

(II) We first generate an \( n \times p \) random Gaussian matrix \( \tilde{X} \) whose entries are i.i.d. \( \sim N(0,1) \). Then the feature matrix \( X \) is generated with \( x_1 = \tilde{x}_1, x_p = \tilde{x}_p, \) and \( x_j = \tilde{x}_j + \rho(\tilde{x}_{j+1} + \tilde{x}_{j-1}), j = 2, \ldots, p-1 \).

The support \( A^* \) is chosen uniformly from \( S \) with \( |A^*| = T < n \). The nonzero entries are generated via \( \beta^*_i = \theta_i R^{\kappa_i}, \) where \( \theta_i \) are i.i.d. Bernoulli random variables, \( \kappa_i \) are i.i.d. uniform random variables in \([0,1]\), and \( R > 1 \). The response vector is generated based on \( Y = X\beta^* + \epsilon, \) where \( \epsilon \sim N(0, \sigma^2 E) \).

5.1 Accuracy and Efficiency

In this section, we compare SNS with SIS, GSR, SSR, SEDPP and CELER in terms of the average \( \ell_\infty \) absolute error (AE), the average \( \ell_2 \) relative error (RE), the average exact support recovery probability (RP), the mean length of the estimated supports (MEAN), and the average CUP time (Time) (in seconds). We consider two scenarios:

- **X** is generated according to (I) and \( \sigma = 0.2, 0.4, \rho = 0.2 : 0.2 : 0.8, R = 10, n = 300, p = 5000, T = 10.**

- **X** is generated according to and \( \sigma = 0.2, 0.4, \rho = 0.2 : 0.2 : 0.8, n = 600, p = 10000, T = 20.**

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The results reported in Tables 1-2 are based on 100 independent replications. As shown in Tables 1-2, SNS is more accurate in terms of estimation error measured by AE and RE, exact support recovery probability (RP), and mean length of the estimated supports (MEAN) than GSR, SIS, SSR, SEDPP and CELER in all the settings considered here. Specifically, due to the existence of debiased shift parameter in NS, AE and RE of SNS are roughly 10 - 100 times smaller than those of the alternative methods. For support recovery, our SNS is slightly better than others in the scenario of small \( \sigma \) and \( \rho \). However, as the noise and correlation increases, the performance of GSR, SIS, SSR, SEDPP and CELER on RP and MEAN deteriorates dramatically, while SNS still performs well in recovering the true supports. As for computational efficiency, SNS is about 10 times faster than GSR, SIS, SSR and CELER, and is comparable with SEDPP.

### 5.2 Influence of the model parameters

Next we take a closer look at how the model parameters, e.g., sample size \( n \), ambient dimension \( p \), correlation \( \rho \), sparsity level \( T \) and noise level \( \sigma \) influence the performance of SNS and other alternative methods in terms of estimation error and recovery support.
Table 2: Numerical results with $n = 600$, $p = 10000$, $T = 20$, $R = 10$, $\sigma = 0.2$ and 0.4, $\rho = 0.2 : 0.2 : 0.8$ and $X$ follows (II).

| $\rho$ | $\sigma$ | Method | AE ($10^{-2}$) | RE | RP | MEAN | Time(s) |
|--------|----------|--------|----------------|-----|-----|------|---------|
| 0.2    | 0.2      | GSR    | 0.13           | 0.08 | 20.02 | 336.62 |
|        |          | SIS    | 0.20           | 0.98 | 20.02 | 68.16  |
|        |          | SSR    | 0.19           | 0.98 | 20.02 | 31.34  |
|        |          | SEDPP  | 0.13           | 0.97 | 20.03 | 13.45  |
|        |          | CERER  | 0.13           | 0.96 | 20.02 | 49.05  |
| 0.4    | 0.2      | GSR    | 0.15           | 0.91 | 20.01 | 384.08 |
|        |          | SIS    | 0.17           | 0.75 | 20.63 | 31.54  |
|        |          | SSR    | 0.16           | 0.45 | 21.53 | 14.01  |
|        |          | SEDPP  | 0.13           | 2.13 | 0.98 | 49.05  |
|        |          | CERER  | 0.15           | 2.41 | 0.91 | 49.47  |

| $\rho$ | $\sigma$ | Method | AE ($10^{-2}$) | RE | RP | MEAN | Time(s) |
|--------|----------|--------|----------------|-----|-----|------|---------|
| 0.4    | 0.2      | GSR    | 0.45           | 0.88 | 19.39 | 365.82 |
|        |          | SIS    | 0.20           | 0.84 | 20.17 | 66.89  |
|        |          | SSR    | 0.20           | 0.84 | 20.18 | 31.66  |
|        |          | SEDPP  | 0.13           | 0.79 | 20.25 | 13.76  |
|        |          | CERER  | 0.14           | 0.81 | 20.24 | 53.27  |
|        |          | SNS    | 0.03           | 0.42 | 1    | 20.01 | 13.94  |
| 0.4    | 0.2      | GSR    | 0.50           | 0.86 | 19.41 | 587.54 |
|        |          | SIS    | 0.20           | 0.65 | 20.71 | 66.75  |
|        |          | SSR    | 0.18           | 0.64 | 20.58 | 31.10  |
|        |          | SEDPP  | 0.14           | 0.29 | 21.52 | 15.26  |
|        |          | CERER  | 0.15           | 0.64 | 20.49 | 56.54  |
|        |          | SNS    | 0.04           | 0.52 | 1    | 20.01 | 14.08  |
| 0.6    | 0.2      | GSR    | 1.32           | 0.58 | 17.53 | 428.02 |
|        |          | SIS    | 0.21           | 0.56 | 20.52 | 66.22  |
|        |          | SSR    | 0.20           | 0.59 | 20.53 | 32.02  |
|        |          | SEDPP  | 0.14           | 0.43 | 20.79 | 13.70  |
|        |          | CERER  | 0.14           | 0.49 | 20.69 | 57.16  |
|        |          | SNS    | 0.05           | 0.77 | 1    | 20.01 | 14.08  |
| 0.4    | 0.2      | GSR    | 1.40           | 0.58 | 17.48 | 389.31 |
|        |          | SIS    | 0.20           | 0.35 | 21.01 | 65.46  |
|        |          | SSR    | 0.20           | 0.35 | 21.05 | 31.07  |
|        |          | SEDPP  | 0.14           | 0.18 | 21.78 | 15.74  |
|        |          | CERER  | 0.15           | 0.64 | 20.49 | 61.70  |
|        |          | SNS    | 0.06           | 0.82 | 1    | 20.01 | 15.16  |
| 0.8    | 0.2      | GSR    | 1.43           | 0.55 | 17.06 | 313.75 |
|        |          | SIS    | 0.21           | 0.59 | 20.59 | 68.12  |
|        |          | SSR    | 0.20           | 0.55 | 20.63 | 31.65  |
|        |          | SEDPP  | 0.13           | 0.51 | 20.75 | 13.08  |
|        |          | CERER  | 0.14           | 0.52 | 20.71 | 65.94  |
|        |          | SNS    | 0.07           | 1.10 | 1    | 20.01 | 14.68  |
| 0.4    | 0.2      | GSR    | 1.49           | 0.51 | 17.02 | 389.33 |
|        |          | SIS    | 0.20           | 0.45 | 20.45 | 67.13  |
|        |          | SSR    | 0.20           | 0.43 | 20.91 | 30.60  |
|        |          | SEDPP  | 0.14           | 0.22 | 21.39 | 13.82  |
|        |          | CERER  | 0.14           | 0.37 | 21.09 | 69.08  |
|        |          | SNS    | 0.07           | 1.12 | 1    | 20.01 | 15.18  |

To this end, we test all the methods with $X$ generated according to setting (I). The sample size $n$, the feature dimension $p$, the sparsity level $T$, the correlation $\rho$, and the noise level $\sigma$ are set as follows.

- $n = 50 : 50 : 600$, $p = 600$, $T = 10$, $R = 10$, $\sigma = 0.2$, $\rho = 0.5$.
- $n = 200$, $p = 300 : 300 : 3000$, $T = 10$, $R = 10$, $\sigma = 0.2$, $\rho = 0.5$.
- $n = 200$, $p = 600$, $T = 5 : 5 : 30$, $R = 10$, $\sigma = 0.2$, $\rho = 0.5$.
- $n = 200$, $p = 600$, $T = 10$, $R = 10$, $\sigma = 0.1 : 0.1 : 1$, $\rho = 0.5$.

The evaluation measures RP, AE, RE and Time as functions of $n$, $p$, $\rho$, $T$, $\sigma$ are shown in turn in Figures 1-4. For example, the five sub-figures in Figure 1 report the performance of RP of all the six methods represented with six different type of lines as $n$, $p$, $\rho$, $T$, $\sigma$ vary, respectively. We can see that SNS (the black dash star line) is on the top of each sub-figures in Figure 1 and is at the bottom of each sub-figures in Figures 2-4 which
implies that SNS achieves higher support recovery probability, lower estimation error, and faster speed than those of the alternative methods considered in all the settings.

5.3 Real data example

We further demonstrate the proposed SNS algorithm by analyzing the Breast cancer gene expression data set (bcTCGA), which is available from The Cancer Genome Atlas (TCGA) project. We downloaded the logarithm transformed and normalized data from http://myweb.uiowa.edu/pbreheny/data/bcTCGA.html. This data set includes gene expression measurements of 17814 genes from 536 patients. Among the genes in bcTCGA, BRCA1 has been identified that increases the risk of early onset breast cancer. BRCA1 is also likely to interact with many other genes, including tumor suppressors and regulators of the cell division cycle. Thus we let BRCA1 be the response vector \( Y \).

We exclude 491 genes with missing values. Hence, the feature matrix \( X \) is a 536 \( \times \) 17322 matrix. Then we fit a linear model with this data set and use the SNS, GSR, SIS, SSR, SEDPP and CELER for selecting genes that are related to BRCA1. The detailed results are shown in Table 3. In Table 3, SNS, SSR and SEDPP select genes CDC6 and TOP2A, and yield similar estimated coefficients for gene TOP2A. Moreover, both SNS and GSR identify genes genes for ASPN, EHF, GGTA1, IGFBP1 and RGS1, and have similar values of the estimated coefficients for genes ASPN, EHF and RGS1. Finally, both SNS and CELER identify genes for ASPN, BBOX1, CDC6, EHF, FAM77C, GGTA1, IGFBP1, MAGEC2, RGS1, SPANXD and TOP2A, and have similar coefficients for genes BBOX1, EHF, GGTA1, MAGEC2, RGS1 and SPANXD. The biological implications of these findings need to be carefully analyzed, but it is beyond the scope of this paper.

6 Discussion and conclusion

Based on the KKT equations for the Lasso, we develop NS and SNS algorithms for sparse learning in the context of a linear model. An attractive feature of NS is that it can be viewed as a generalized Newton method with built-in screening mechanism, hence it is expected to achieve faster convergence than first-order methods. Indeed, we prove that NS possesses the optimal one-step local convergence. We also analyze its computational complexity and establish sharp estimation error bound of SNS under certain regularity conditions. Simulation studies and real data analysis support our theoretical results and demonstrate that SNS is faster and more accurate than several state-of-the-art methods in our comparative studies.

The proposed NS and SNS algorithms for the least squares loss with the Lasso penalty can be generalized to the problems with a general convex loss and a convex penalty. For example, consider the setting of classification or multi-task learning where we have the objective function

\[
\min_{\beta} L(\beta) + \lambda R(\beta),
\]

where \( L(\beta) \) is a convex and differentiable loss function such as the negative log-likelihood
Table 3: The estimation results on bcTCGA.

| Gene name | number | GSR | SIS | SSR | SEDPP | CELER | SNS |
|-----------|--------|-----|-----|-----|-------|-------|-----|
| ASPN      | 957    | -0.043 | -  | -   | -     | -0.050 | -0.065 |
| BBOX1     | 1213   | -    | -   | -   | -     | -0.022 | -0.021 |
| C17orf53  | 1743   | 0.049 | 0.083 | 0.080 | -     | -     | -   |
| CDC6      | 2727   | 0.064 | -   | -   | -     | -     | -   |
| CDC163    | 2710   | 0.054 | 0.040 | -   | -     | -     | -   |
| CDC25C    | 2964   | 0.098 | 0.025 | 0.027 | -     | -     | -   |
| CDC6      | 2987   | -    | 0.003 | 0.006 | 0.038 | 0.021 |
| CEACAL46  | 3076   | -    | -   | -   | 0.004 | -     | -   |
| CENPQ     | 3105   | 0.009 | 0.012 | -   | 0.041 | -     | -   |
| CXXL13    | 3001   | -    | -   | -   | -     | 0.008 | -   |
| DTL       | 4543   | 0.136 | 0.088 | 0.090 | -     | -     | -   |
| EHF       | 4735   | 0.001 | -   | -   | -     | 0.001 | 0.006 |
| FAM17C    | 5201   | -    | -   | -   | -     | 0.019 | 0.007 |
| FCGBP3A   | 5407   | 0.003 | -   | -   | -     | -0.045 | 0.045 |
| GGTAA1    | 6068   | -0.001 | -   | -   | -     | 0.021 | 0.042 |
| IGFBP1    | 7197   | 0.125 | -   | -   | -     | 0.012 | 0.011 |
| MAGEC2    | 8905   | -    | -   | -   | -     | 0.035 | -   |
| MPHOSPH1  | 9516   | 0.074 | -   | -   | -     | 0.035 | -   |
| NHL2      | 9941   | -    | 0.430 | 0.227 | 0.237 | -     | -   |
| PCCG1     | 11091  | -0.141 | -   | -   | -     | -     | -   |
| POLQ      | 11694  | 0.029 | -   | -   | -     | -     | -   |
| PSME3     | 12146  | -0.182 | 0.071 | 0.075 | -     | -     | -   |
| RBM23     | 12542  | 0.067 | -   | -   | -     | -     | -   |
| RDM1      | 12615  | -    | -   | -   | -     | 0.035 | -   |
| REG1      | 12705  | -0.004 | -   | -   | -     | -0.003 | -0.004 |
| RPS2K1    | 13058  | 0.001 | -   | -   | -     | -     | -   |
| SSCB2A24  | 13288  | -0.002 | -   | -   | -     | -     | -   |
| SPAQ5     | 14296  | -    | 0.010 | 0.014 | -     | -     | -   |
| SPANX5    | 14302  | -    | -   | -   | 0.013 | 0.006 | -   |
| SPSB2     | 14397  | -    | -   | -   | -0.003 | -0.005 | -   |
| TIMELESS  | 15122  | 0.079 | 0.034 | 0.035 | -     | -     | -   |
| TSPAN6S4  | 15432  | -    | -   | -   | 0.009 | -     | -   |
| TOP2A     | 15535  | 0.058 | 0.036 | 0.035 | 0.060 | 0.039 |
| VRBP1     | 16259  | -0.070 | -   | -   | -     | -     | -   |
| VPS25     | 16315  | 0.223 | 0.108 | 0.108 | -     | -     | -   |

for logistic regression, and $\mathcal{R}(\beta)$ is a convex penalty encoding the low complexity structure, e.g., sparsity, group sparsity or low rank. We can derive the KKT conditions similarly to those in Lemma 2.1. Specifically, the KKT system for (9) is

$$
\begin{align*}
\mathbf{d}^\circ &= -\nabla \mathcal{L}(\beta^\circ), \\
\beta^\circ &= \mathcal{T}_R^\lambda(\beta^\circ + \mathbf{d}^\circ),
\end{align*}
$$

where $\mathcal{T}_R^\lambda(\cdot)$ is the proximal operator of the convex regularizer $\mathcal{R}(\cdot)$ [6]. Therefore, we can derive the generalizations of the NS and SNS algorithms based on the above KKT equations. We will consider such generalizations and analyze their numerical and statistical convergence properties in the future work.

Acknowledgements

The authors are grateful to the anonymous referees, the associate editor and the editor for their helpful comments, which have led to a significant improvement on the quality of the paper. The work of Jian Huang is supported in part by the NSF grant DMS-1916199. The work of Y. Jiao was supported in part by the National Science Foundation of China under Grant 11871474 and by the research fund of KLATASDSMOE. The work of J. Liu is supported by Duke-NUS Graduate Medical School WBS: R913-200-098-263 and MOE2016- T2-2-029 from Ministry of Eduction, Singapore. The work of Yanyan Liu is supported in part by the National Science Foundation of China under Grant 11971362. The work of X. Lu is supported by the National Key Research and Development Pro-
Figure 1: RP versus $n, p, \rho, T, \sigma$.

Figure 2: AE versus $n, p, \rho, T, \sigma$.

gram of China (No. 2018YFC1314600), the National Science Foundation of China (No. 91630313 and No. 11871385), and the Natural Science Foundation of Hubei Province
Figure 3: RE versus $n, p, \rho, T, \sigma$.

Figure 4: Time versus $n, p, \rho, T, \sigma$.

(No. 2019CFA007).
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Appendix

In the appendix, we will show the proofs of the theoretical results. In the appendix, we give detailed proofs of Lemmas 2.1 and Lemma 3.1 and Theorems 3.1-3.3 in the paper. To begin with, we recall some backgrounds in convex analysis [33] and describe the concept and some properties of Newton derivative [14].

A.1 Background on convex analysis and Newton derivative

Recall the classical Fermat’s rule [33],

\[ 0 \in \partial f(z^0) \iff z^0 \in \arg\min_{z \in \mathbb{R}^p} f(z). \]

Moreover, a more general case is [6]

\[ w \in \partial f(z) \iff z = \text{Prox}_f(z + w), \]

where Prox is the proximal operator for \( f \) defined as

\[ \text{Prox}_f(z) := \arg\min_{x \in \mathbb{R}^p} \frac{1}{2} \| x - z \|_2^2 + f(x). \]

The proximal operator of \( \lambda \| \cdot \|_1 \) has a closed form, i.e.,

\[ \text{Prox}_{\lambda \| \cdot \|_1}(z) = \Gamma_{\lambda}(x), \]

where \( \Gamma_{\lambda}(\cdot) \) is defined in [3].

Let \( F : \mathbb{R}^m \to \mathbb{R}^l \) be a nonlinear map. [17] [30] [14] generalized classical Newton’s algorithm to find a root of \( F(z) = 0 \) in the scenario that \( F \) is not Fréchet differentiable via introducing the concept of generalized Jacobian [17] [30] or Newton derivative [14].

**Definition.** \( F : \mathbb{R}^m \to \mathbb{R}^l \) is called Newton differentiable at \( x \in \mathbb{R}^m \) if there exists an open neighborhood \( N(x) \) and a family of mappings \( D : N(x) \to \mathbb{R}^{l \times m} \) such that

\[ \lim_{\| h \|_2 \to 0} \frac{\| F(x + h) - F(x) - D(x)(h) \|_2}{\| h \|_2} = 0. \]

The set of maps \( \{ D(z) : z \in N(x) \} \) denoted by \( \nabla_N F(x) \) is called the Newton derivative of \( F \) at \( x \).

It can be easily seen that \( \nabla_N F(x) \) coincides with the Fréchet derivative at \( x \) if \( F \) is continuously Fréchet differentiable. An example that is Newton differentiable but not Fréchet differentiable is the absolute function \( F(z) = |z| \) defined on \( \mathbb{R}^1 \). In fact, let \( G(z + h)h = \frac{z + h}{|z + h|}h \) and \( G(0)h = rh \) with \( r \) be any constant in \( \mathbb{R}^1 \). Then

\[ \nabla_N F(z) = \begin{cases} 
1, & z > 0, \\
-1, & z < 0, \\
r \in \mathbb{R}^1, & z = 0.
\end{cases} \]
follows from the definition of Newton derivative.

Next we recall the chain rule of Newton derivative. Suppose $F_i : \mathbb{R}^m \to \mathbb{R}^1$ is Newton differentiable at $x$ with Newton derivative $\nabla_N F_i(x)$, $i = 1, \ldots, l$. Then $F = (F_1, \ldots, F_l)'$ is also Newton differentiable at $x$ with Newton derivative

$$\nabla_N F(x) = \begin{pmatrix} \nabla_N F_1(x) \\ \nabla_N F_2(x) \\ \vdots \\ \nabla_N F_l(x) \end{pmatrix}.$$  

Furthermore, if $F_1$ and $F_2$ are Newton differentiable at $x$, then the linear combination of them are also Newton differentiable at $x$, i.e., for any $\theta, \gamma \in \mathbb{R}^1$,

$$\nabla_N (\theta F_1 + \gamma F_2)(x) = \theta \nabla_N F_1(x) + \gamma \nabla_N F_2(x).$$

Let $F_1 : \mathbb{R}^s \to \mathbb{R}^l$ be Newton differentiable with Newton derivative $\nabla_N F_1$. Let $L \in \mathbb{R}^{s \times m}$ and define $F(x) = F_1(Lx + z)$. It can be verified that the chain rule holds, i.e., $F(x)$ is Newton differentiable at $x$ with Newton derivative

$$\nabla_N F(x) = \nabla_N F_1(Lx + z)L.$$ 

With the above preparation we can calculate the Newton derivative of the componentwise soft threshold operator $\Gamma_\lambda(x)$.

**Lemma A.1.** $\Gamma_\lambda(\cdot) : \mathbb{R}^p \to \mathbb{R}^p$ is Newton differentiable at any point $x \in \mathbb{R}^p$. And $\text{diag}(b) \in \nabla_N \Gamma_\lambda(x)$, where, $\text{diag}(b)$ is a diagonal matrix with

$$b = [\mathbf{1}_{|x_1|}>\lambda], \ldots, [\mathbf{1}_{|x_p|}>\lambda]^T,$$

and $\mathbf{1}_A$ is the indicator function of set $A$.

**Proof.** Let

$$F_i(x) = \Gamma_\lambda(e'_i x) : x \in \mathbb{R}^p \to \mathbb{R}^1, \quad i = 1, \ldots, p,$$

where the column vector $e_i$ is the $i_{th}$ basis in $\mathbb{R}^p$. Obliviously,

$$\Gamma_\lambda(x) = [F_1(x), \ldots, F_p(x)]^T,$$

$$\Gamma_\lambda(z) = z - |z + \lambda|/2 + |z - \lambda|/2.$$  

Using the fact $\mathbf{1}_{|z|>0} \in \nabla_N |z|$ and chain rule, we get

$$\mathbf{1}_{|z|>0} \in \nabla_N \Gamma_\lambda(z),$$

$$e'_i \mathbf{1}_{|z|>0} \in \nabla_N F_i(x),$$

$$\text{diag}(b) \in \nabla_N \Gamma_\lambda(x).$$

This completes the proof of Lemma A.1. \qed 

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A.2 Proof of Lemma 2.1

Proof. Assume \( \beta^* \) is the minimizer of (1). By the Fermat’s rule, we can get
\[
0 \in X^T (X \beta^* - Y) / n + \lambda \partial \| \beta^* \|_1.
\]
Thus there exists
\[
d^* \in \lambda \partial \| \beta^* \|_1,
\]
and
\[
0 = X^T (X \beta^* - Y) / n + d^*.
\]
Obviously, (10) is equivalent to
\[
0 \in \beta^* - (\beta^* + d^*) + \lambda \partial \| \beta^* \|_1.
\]
Let \( G(\beta) = \frac{1}{2} \| \beta - (\beta^* + d^*) \|^2 + \lambda \| \beta \|_1 \). (11) shows
\[
0 \in \partial G(\beta^*).
\]
By Fermat’s rule, (12) implies
\[
\beta^* \in \arg\min_{\beta \in \mathbb{R}^p} G(\beta).
\]
By the strong convexity of \( G(\beta) \), \( \beta^* \) is the unique minimizer. Then \( \beta^* = \Gamma_\lambda (\beta^* + d^*) \) follows from fact that the proximal mapping of \( \ell_1 \) norm equals to \( \Gamma_\lambda \). Therefore \( \beta^* \) and \( d^* \) satisfies (2).

Conversely, if \( \beta^* \) and \( d^* \) satisfy (2). Then \( \beta^* \) is a minimizer of \( G(\beta) \), i.e., (12)-(10) hold. Then,
\[
0 \in X^T (X \beta^* - Y) / n + \lambda \partial \| \beta^* \|_1.
\]
By Fermat’s rule again, \( \beta^* \) is the minimizer of (1). This completes the proof. \( \square \)

A.3 Proof of Theorem 3.1

Proof. Recall that,
\[
z = (d_A^T, \beta_I^T, \beta_A^T, d_I^T)^T,
\]
and
\[
F(z) = \begin{bmatrix}
\beta_A - \Gamma_\lambda (\beta_A + d_A) \\
\beta_I - \Gamma_\lambda (\beta_I + d_I) \\
\mu d_A - (X_A^T Y - X_A^T X_A \beta_A - X_A^T X_I \beta_I) \\
\mu d_I - (X_I^T Y - X_I^T X_A \beta_A - X_I^T X_I \beta_I)
\end{bmatrix}
\]

22
By Lemma A.1 and chain rule of Newton derivative, we get $F(z)$ is Newton differentiable at any point $z$, and

$$H = \begin{bmatrix} -E_{AA} & 0 & 0 & 0 \\ 0 & E_{II} & 0 & 0 \\ nI_{AA} & X^T_A I & X^T_A X_A & 0 \\ 0 & X^T_I I & X^T_I X_A & nE_{II} \end{bmatrix} \in \nabla N F(z).$$

Given $z^k$ define

$$A^k = \{ j : |\beta_j^k + d_j^k| > \lambda \} , I^k = (A^k)^c.$$

Then

$$H_k = \begin{bmatrix} -E_{A_k A_k} & 0 & 0 & 0 \\ 0 & E_{I_k I_k} & 0 & 0 \\ nI_{A_k A_k} & X^T_{A_k} I_{I_k} & X^T_{A_k} X_{A_k} & 0 \\ 0 & X^T_{I_k} I_{I_k} & X^T_{I_k} X_{A_k} & nE_{I_k I_k} \end{bmatrix} \in \nabla N F(z^k).$$

Let

$$D^k = \begin{pmatrix} D_{A_k}^d \\ D_{A_k}^\beta \\ D_{I_k}^\beta \\ D_{I_k}^d \end{pmatrix}$$

Some algebra shows the generalized Newton iteration

- Solve $H_k D^k = -F(z^k)$ for $D^k$,

- Update $z^{k+1} = z^k + D^k$

can be reformulate as

$$d^k_{A_k} + D_{A_k}^d = \lambda \text{sgn}(\beta_{A_k}^k + d_{A_k}^k), \quad (13)$$

$$\beta_{I_k}^k + D_{I_k}^\beta = 0, \quad (14)$$

$$X^T_{A_k} X_{A_k} (\beta_{A_k}^k + D_{A_k}^\beta) = X^T_{A_k} Y - n(d_{A_k}^k + D_{A_k}^d), \quad (15)$$

$$n(d_{I_k}^k + D_{I_k}^d) = X^T_{I_k} Y - X^T_{I_k} X_{A_k} (\beta_{A_k}^k + D_{A_k}^\beta) - X^T_{I_k} X_{I_k} (\beta_{I_k}^k + D_{I_k}^\beta). \quad (16)$$
and
\[
\begin{pmatrix}
  d_{k+1}^k \\
  \beta_{k+1}^k \\
  \beta_{k+1}^k \\
  d_{k+1}^k 
\end{pmatrix}
= 
\begin{pmatrix}
  d_k^k + D_k^d \\
  \beta_k^k + D_k^d \\
  \beta_k^k + D_k^d \\
  d_k^k + D_k^d 
\end{pmatrix}.
\] (17)

Substituting (13) - (14) into (15)-(16) and using (17) we obtain lines 4-7 in NS Algorithm 1. This completes the proof. □

A.4 Proof of Theorem 3.2

Proof.
\[
\begin{align*}
\beta_i^+ + d_i^+ - \beta_i^- - d_i^- & \\
\leq |\beta_i^+ + d_i^+ - \beta_i^- - d_i^-| & \\
\leq \|\beta_i^+ - \beta_i^-\|_\infty + \|d_i^+ - d_i^-\|_\infty & \\
\leq C & \\
\leq \beta_i^+ + d_i^+ - \lambda, \forall i \in \{j \in \tilde{A} : \beta_j^+ + d_j^+ > \lambda\}
\end{align*}
\]

where the last inequality uses the definition that \( C = \min_{i \in \tilde{A}} |\beta_i^+ + d_i^+ - \lambda| \). This implies that \( \beta_i^+ + d_i^+ > \lambda \Rightarrow \beta_i^- + d_i^- > \lambda \) (similarly, we can show \( \beta_i^+ + d_i^+ < -\lambda \Rightarrow \beta_i^- + d_i^- < -\lambda \)), i.e.,
\[
A^+ \subseteq A^0 = \{i : |\beta_i^0 + b_i^0| > \lambda\}.
\]

Meanwhile, by the same argument we can show that
\[
|\beta_i^0 + d_i^0| < \lambda \Rightarrow |\beta_i^0 + b_i^0| < \lambda,
\]
i.e.,
\[
A^0 \subseteq A = \{i : |\beta_i^+ + d_i^+| \geq \lambda\}.
\]

Then by the second equation of (2) and the definition of \( \Gamma_\lambda(\cdot) \), we get
\[
d_{A^0}^\circ = \lambda \text{sign}(\beta_{A^0}^\circ + d_{A^0}^\circ),
\]
which implies
\[
d_{A^0}^\circ = \lambda \text{sign}(\beta_{A^0}^\circ + d_{A^0}^\circ).
\]

This together with the first equation of (2) and the definition of NS Algorithm imply
\[
X^T_{A^0} X_{A^0} \beta_{A^0}^\circ + nd_{A^0}^\circ = X^T_{A^0} Y = X^T_{A^0} X_{A^0} \beta_{A^0}^1 + nd_{A^0}^1.
\]

Then we get \( X^T_{A^0} X_{A^0} (\beta_{A^0}^\circ - \beta_{A^0}^1) = 0 \), therefore, \( \beta_{A^0}^\circ = \beta_{A^0}^1 \) follows from the above equation and the assumption that the rank of \( X_{A^0} \) is \( |A^0| \). Let \( I_0 = (A^0)^c \), due to \( \beta_{I_0}^1 = 0 \) in NS Algorithm and the fact \( A^0 \subseteq A^0 \), we deduce that \( \beta_{I_0}^1 = 0 = \beta_{I_0}^0 \). Hence, \( \beta^0 = \beta^1 \). This completes the proof of Theorem 3.2. □
A.5 Proof of Lemma 3.1

The proof of Lemma 3.1 are based on the following Lemmas A.2–A.3.

**Lemma A.2.** Let $A, B$ be disjoint subsets of $S = \{1, 2, \ldots, p\}$, with $|A| = a, |B| = b$. Let $\nu$ be the mutual coherence of $X$ defined in (C3). Then we have

$\|X^T_B X_A u\|_\infty \leq na\nu \|u\|_\infty, \forall u \in \mathbb{R}^{|A|}, \quad (18)$

$\|X_A\| = \|X_A^T\| \leq \sqrt{n(1 + (a - 1)\nu)}. \quad (19)$

Furthermore, if $\nu < 1/(a - 1)$, then $\forall u \in \mathbb{R}^{|A|},$

$\|X_A^T X_A u\|_\infty \geq n(1 - (a - 1)\nu)\|u\|_\infty, \quad (20)$

$\|X_A^T X_A u\|_\infty \leq \frac{\|u\|_\infty}{n(1 - (a - 1)\nu)}. \quad (21)$

$\|X_A^T X_A - nI\|_\infty \leq n\nu(a - 1)\|u\|_\infty. \quad (22)$

**Proof.** Let $G = X^T X/n. \forall i \in B, \sum_{j=1} G_{i,j} u_j \leq a\nu\|u\|_\infty$, which implies (18). For any $i \in A$, by using Gerschgorin’s disk theorem, $\|G_{A,A} - G_{i,i}\| \leq \sum_{i \neq j=1}^a |G_{i,j}| \leq (a - 1)\nu$, that is, (19) holds. Let $i \in A$ such that $\|u\|_\infty = |u_i|$. (20) follows that $|\sum_{i=1}^a G_{i,j} u_j| \geq |u_i| - \sum_{i \neq j=1}^a |G_{i,j}| u_i \geq \|u\|_\infty - \nu(a - 1)\|u\|_\infty$. (21) follows directly from (20). And (22) can be showed similarly as the (20). This completes the proof of Lemma A.2.

**Lemma A.3.** Suppose (C2) holds. We have

$P \left( \|X^T \epsilon/n\|_\infty \leq \gamma_n \right) \geq 1 - \frac{2}{p}. \quad (23)$

**Proof.** This lemma follows from the sub-Gaussian assumption (C2) and the union bounds.

**Proof.** We first show that under the assumption of Lemma 3.1

$\lambda_1 > 30\gamma_n \quad (24)$
holds with probability at least \(1 - \frac{2}{p}\). In fact,

\[
\lambda_1 = \lambda_0 \alpha = \alpha \|X^T Y / n\|_{\infty} = \alpha \|X^T (X\beta^* + \epsilon) / n\|_{\infty} \\
\geq \alpha \left(\|X_A^T X_A\beta_A^* / n\|_{\infty} - \|X^T \epsilon / n\|_{\infty}\right) \\
\geq \alpha ((1 - (T - 1)\nu)\|\beta^*\|_{\infty} - \gamma_n) \text{ W.H.P.} \\
\geq \alpha ((1 - 1/4) \cdot 78\gamma_n - \gamma_n) \\
> 30\gamma_n,
\]

where the first inequality is the triangle inequality, the second inequality uses \((20)\) and \((23)\), and the third one follows uses assumption \((C1)-(C3)\). Here in the third line, “W. H. P.” stands for with high probability, that is, with probability at least \(1 - \frac{2}{p}\). Then it follows from \((24)\) and the definition of \(\lambda_m\) that there exists an integer \(M \in [1, \log_\alpha \left(\frac{30\gamma_n}{\lambda_0}\right)\) such that

\[
\lambda_M > 30\gamma_n \geq \lambda_{M+1}
\]

holds with high probability. It follows from assumption \((1)\) and \((25)\) that \(\lambda_{M+1} = \alpha \lambda_M \leq 30\gamma_n \leq \frac{13}{15} \|\beta_A^*\|_{\min}, \text{ which implies that with high probability } \|\beta_A^*\|_{\min} > \frac{5}{3} \lambda_M\) holds. This completes the proof of Lemma 3.1.

**A.6 Proof of Theorem 3.3**

The proof of Theorem 3.3 is based on the following Lemmas A.4-A.5.

**Lemma A.4.** Suppose assumption \((C3)\) holds. Let \(A^k, I^k, \beta^{k+1}, d^{k+1}\) are generated by Algorithm 1 with \(\lambda > \frac{13}{15} \lambda + 4\gamma_n\). Denote \(E^k = A^* \setminus A^k\) and \(i_k = \{i \in E^k : |\beta_i^*| = \|\beta_{E^k}\|_{\infty}\}\). If \(A^k \subset A^*\), then with probability at least \(1 - \frac{2}{p}\), we have

\[
\|\beta_{A^k}^{k+1} + d_{A^k}^{k+1} - \beta_{A^k}^*\|_{\infty} < \frac{1}{3} |\beta_{A^k}^*| + \frac{2}{45} \lambda,
\]

(26)

\[
|\beta_{i_k}^{k+1} + d_{i_k}^{k+1}| > |\beta_{i_k}^*| - \frac{1}{3} |\beta_{i_k}^*| - \frac{2}{45} \lambda, \quad \forall i \in A^k,
\]

(27)

\[
|d_{i_k}^{k+1}| < \frac{1}{3} |\beta_{i_k}^*| + \frac{2}{45} \lambda, \quad \forall i \in I^k,
\]

(28)

\[
|d_{i_k}^{k+1}| > \frac{2}{3} |\beta_{i_k}^*| - \frac{2}{45} \lambda.
\]

(29)

**Proof.** Since \(\beta^{k+1}, d^{k+1}\) are generated by Algorithm 1, \(A^k \subset A^*\), \(E^k = A^* \setminus A^k\) and
\(Y = X_{A^k} \beta_{A^k} + \epsilon\) we have

\[
\begin{align*}
\beta_{A^k}^{k+1} &= (X_{A^k}^T X_{A^k})^{-1} \\
& \cdot (X_{A^k}^T (X_{A^k} \beta_{A^k} + X_{E^k} \beta_{E^k}^* + \epsilon) - n d_{A^k}^{k+1})
\end{align*}
\]

(30)

and

\[
\begin{align*}
\|\beta_{A^k}^{k+1} + d_{A^k}^{k+1} - \beta_{A^k}^*\|_\infty \\
\leq \|X_{A^k}^T (X_{A^k} \beta_{A^k} + X_{E^k} \beta_{E^k}^* + \epsilon)\|_\infty \\
+ \|X_{A^k}^T X_{A^k} - n I\| d_{A^k}^{k+1}\|_\infty \\
\leq \frac{n\nu|E^k|\beta_{A^k}^*| + \|X_{A^k}^T \epsilon\|_\infty}{n(1 - (|X^k| - 1)\nu)} + \frac{n\nu(|A^k| - 1)(\lambda - \beta_{A^k})}{n(1 - \nu(|X^k| - 1))}
\end{align*}
\]

\[
\begin{align*}
& \leq \frac{T\nu|\beta_{A^k}^*| + \gamma_n}{1 - T\nu} + \frac{T\nu(\lambda - \beta_{A^k})}{1 - T\nu} \text{ W.H.P} \\
& \leq \frac{1}{3}|\beta_{A^k}^*| + \frac{2}{45}\lambda,
\end{align*}
\]

where the first inequality uses (30) and the triangle inequality, the second inequality uses (18), (21) and (22), the third inequality uses (23), the last inequality uses assumption (C3). Thus, (26) holds. Then, (27) follows from (26) and the triangle inequality, \(\forall i \in I_k\),

\[
|d_{A^k}^{k+1}| = |x_i^T (X_{A^k} (\beta_{A^k}^* - \beta_{A^k}^{k+1} - d_{A^k}^{k+1}) \\
+ X_{A^k} d_{A^k}^{k+1} + X_{E^k} \beta_{E^k}^* + \epsilon)/n|
\leq |x_i^T X_{A^k} (\beta_{A^k}^* - \beta_{A^k}^{k+1} - d_{A^k}^{k+1})|/n
\leq |x_i^T X_{A^k} d_{A^k}^{k+1} + X_{E^k} \beta_{E^k}^* + \epsilon|/n
\leq \nu|A^k|\|\beta_{A^k}^{k+1} + d_{A^k}^{k+1} - \beta_{A^k}^*\|_\infty
\leq \nu|A^k|\|\beta_{A^k}^{k+1} + d_{A^k}^{k+1} - \beta_{A^k}^*\|_\infty
\leq \frac{1}{4} \left( \frac{1}{3} |\beta_{A^k}^*| + \frac{2}{45}\lambda \right) + \frac{1}{30}\lambda + \frac{1}{4} |\beta_{A^k}^*|
\leq \frac{1}{3} |\beta_{A^k}^*| + \frac{2}{45}\lambda,
\]

where the first equality uses (30), the first inequality is the triangle inequality, the second inequality is due to (18) and (23), and the third inequality uses (13) and (26), i.e., (28).
holds. Observing \( i_k \in E^k \) and (30), we get

\[
|d_i^{k+1}| = |x_i^T (X_{A^k} (\beta_{A^k}^{k+1} - \beta_{A^k}^{k+1} - d_{A^k}^{k+1}) + X_{A^k} d_{A^k}^{k+1} + x_i \beta_i + X_{E^{k \setminus i}} \beta_{E^{k \setminus i}} + \epsilon) / n |
\]

\[
\geq |\beta_{i_k}^*| - |x_i^T X_{A^k} (\beta_{A^k}^{k+1} - \beta_{A^k}^{k+1} - d_{A^k}^{k+1})| / n
\]

\[
- |x_i^T (X_{A^k} d_{A^k}^{k+1} + X_{E^{k \setminus i}} \beta_{E^{k \setminus i}} + \epsilon)| / n
\]

\[
\geq |\beta_{i_k}^*| - \nu |A^k| \|\beta_{A^k}^{k+1} - d_{A^k}^{k+1} - \beta_{A^k}^{\infty} - \epsilon| - \nu |A^k| \nu |A^k| |\beta_{i_k}^*| - \gamma_n \text{ W.H.P}
\]

\[
> |\beta_{i_k}^*| - \frac{1}{4} |\beta_{i_k}^*| + \frac{2}{45} \lambda
\]

\[
= \frac{2}{3} |\beta_{i_k}^*| - \frac{2}{45} \lambda,
\]

where the first inequality is the triangle inequality, the second inequality is due to (18) and (23), and the third one uses (28) and (26), i.e., (29) holds. This completes the proof of Lemma A.4. \( \square \)

**Lemma A.5.** Suppose assumption (C3) holds. Let \( \kappa = \frac{8}{5} \) and \( \tau = \kappa + 1 \). Denote \( E^k = A^* \setminus A^k \), \( i_k = \{ i \in I^k : |\beta_i^*| = \|\beta_{E^k}^{k+1}\|_{\infty} \} \) and \( S_{\lambda, \tau} = \{ i : |\beta_i^*| \geq \lambda \tau \} \). If \( S_{\lambda, \tau} \subset A^k \subset A^* \) then \( S_{\lambda, \tau} \subset A^k \subset A^* \). Meanwhile, if \( S_{\lambda, \kappa+1} \subset A^k \subset A^* \) and \( S_{\lambda, \kappa} \not\subset A^k \) then \( |\beta_{i_k}^*| > |\beta_{i_{k+1}}^*| \).

**Proof.** Assume \( S_{\lambda, \tau} \subset A^k \subset A^* \). Since \( E^k = A^* \setminus A^k \) and \( i_k \in E^k \), we get \( i_k \not\in A^k \) which implies \( |\beta_{i_k}^*| < \lambda \tau \). \( \forall i \in S_{\lambda, \tau} \subset A^k \), by using (27) we have

\[
|\beta_i^{k+1} + d_i^{k+1}| > |\beta_i^*| - \frac{1}{3} |\beta_{i_k}^*| - \frac{2}{45} \lambda
\]

\[
> \frac{2}{3} \lambda \tau - \frac{2}{45} \lambda
\]

\[
> \lambda,
\]

which implies \( i \in A^{k+1} \), i.e., \( S_{\lambda, \tau} \subset A^{k+1} \) holds. \( \forall i \in (A^*)^c \subset I^k \). By using (28) we get

\[
|\beta_i^{k+1} + d_i^{k+1}| = |d_i^{k+1}|
\]

\[
\leq \frac{1}{3} |\beta_{i_k}^*| + \frac{2}{45} \lambda
\]

\[
\leq \frac{1}{3} \lambda \tau + \frac{2}{45} \lambda
\]

\[
\leq \lambda
\]

i.e., \( i \not\in A^{k+1} \) which implies \( A^{k+1} \subset A^* \). Next we turn to the second assertion. Assume \( S_{\lambda, \kappa+1} \subset A^k \subset A^* \), \( S_{\lambda, \kappa} \not\subset A^k \). It suffices to show all the elements of \( |\beta_i^*| > \|\beta_{E^k}^{k+1}\|_{\infty} \) larger than \( |\beta_{i_k}^*| > \lambda \tau \) move into \( A^{k+1} \). It follows from the definition of \( S_{\lambda, \kappa}, S_{\lambda, \kappa+1} \) and \( i_k \in E^k = A^* \setminus A^k \)
that $i_k \in S_{\lambda, \kappa} \setminus S_{\lambda, \kappa+1}$, i.e., $|\beta^*_m| \in [\lambda \kappa, \lambda(\kappa + 1))$. By using (29) we have

$$|\beta^{k+1}_k + d^{k+1}_k| = |d^{k+1}_k|$$

$$> \frac{2}{3} |\beta^*_k| - \frac{2}{45} \lambda$$

$$> \frac{2}{3} \lambda \kappa - \frac{2}{45} \lambda$$

$$> \lambda,$$

which implies $i_k \in A^{k+1}$. Let $i \in A^k$ satisfies $|\beta^*_i| \geq |\beta^*_m|$. Then it follows from (27) that

$$|\beta^{k+1}_i + d^{k+1}_i| > |\beta^*_i| - \frac{1}{3} |\beta^*_m| - \frac{2}{45} \lambda$$

$$\geq \frac{2}{3} |\beta^*_i| - \frac{2}{45} \lambda$$

$$\geq \frac{2}{3} \lambda \kappa - \frac{2}{45} \lambda$$

$$> \lambda,$$

which implies $i \in A^{k+1}$. This completes the proof of Lemma A.5.

Proof. Let $\overline{\lambda}_m = \frac{11}{12} \lambda_m + 4 \gamma_n$. By using Lemma 3.1 and the definition of $\lambda_m$ and we get $\lambda_m > \overline{\lambda}_m$ for $m = 0, 1, \ldots, M$. At the $m_{th}$ knot of Algorithm 2 with $\lambda_0, \alpha, K, M$, suppose it takes Algorithm 1 $k_m$ iterations to get the solution $(\hat{\beta}(\lambda_m), \hat{d}(\lambda_m))$, where the initial values of Algorithm 1 is $(\beta^0, d^0) = (\hat{\beta}(\lambda_{m-1}), \hat{d}(\lambda_{m-1}))$ and $k_m \leq K$ by the definition of Algorithm 1. We denote the approximate primal solution pair and active set generated in Algorithm 1 with $(\beta^0, d^0) = (\hat{\beta}(\lambda_{m-1}), \hat{d}(\lambda_{m-1}))$ and $A^k_{m}$, respectively, $k = 0, 1, \ldots, k_m$. By the construction of Algorithm 1, we have $(\beta^0, d^0) = (\hat{\beta}(\lambda_{m-1}), \hat{d}(\lambda_{m-1}))$, i.e., the solution at the $m_{th}$ stage is the initial value for the $m + 1$ stage which implies

$$A^k_m \subseteq A^0_{m+1}$$

We claim that

$$S_{\lambda, \kappa+1} \subseteq A^0_m \subseteq A^*, m = 0, 1, \ldots, M,$$

$$S_{\lambda, \kappa} \subseteq A^k_m \subseteq A^*, m = 0, 1, \ldots, M.$$

We prove the above two claims by mathematical induction. First we show that $\emptyset =
$S_{\lambda, \kappa+1} \subseteq A_0^* \subseteq A^*$. Let $|\beta^*_i| = \|\beta^*\|_\infty$.

$$\begin{align*}
(\kappa + 1)\lambda_0 &= \frac{13}{5} \|X^T \mathbf{Y}/n\|_\infty = \frac{13}{5} \|X^T (X\beta^* + \epsilon)/n\|_\infty \\
&\geq \frac{13}{5} (\|X_A^* X_{A\beta^*}/n\|_\infty - \|X^T \epsilon/n\|_\infty ) \\
&\geq \frac{13}{5} ((1 - (T - 1)\nu)|\beta^*_i| - \gamma_n), \quad \text{W.H.P} \\
&> \frac{13}{5} \left( 4 |\beta^*_i| - \gamma_n \right) \\
&> |\beta^*_i|, \quad \text{by}\ (35)
\end{align*}$$

where the first inequality is the triangle equation and the second inequality uses (20) and (23), the third inequality uses assumption (C3), and the last inequality is derived from assumption (C1). This implies $\emptyset = S_{\lambda_0, \kappa+1}$. By the construction of Algorithm 2, we get $A_0^* = \{ j : |x_j^T \mathbf{Y}/n| > \lambda_0 = \|X^T \mathbf{Y}/n\|_\infty \} = \emptyset$. Therefore, (33) holds when $m = 0$.

Now we suppose (33) holds for some $m \geq 0$. Thus, by the first assertion of Lemma A.5, we get $S_{\lambda, \kappa+1} \subseteq A_k^m \subseteq A^*, k = 0, 1, \ldots, k_m$. (36)

By the stopping rule of Algorithm 1, it holds either $A_{k_m}^m = A_{k_m-1}^m$ or $k_m = K \geq T$ when it stops. In both cases, by using (36) and the second assertion of Lemma A.5 we get $S_{\lambda, \kappa} \subseteq A_{k}^m \subseteq A^*$, i.e., (34) holds for this given $m$. Observing the relation $S_{\lambda_{m+1}, \kappa+1} = S_{\lambda_{m}, \kappa}$ and (31)-(32), we get $S_{\lambda_{m+1}, \kappa+1} \subseteq A_{k_{m+1}}^m \subseteq A^*$, i.e., (33) holds for $m + 1$. Therefore, (33)-(34) are verified by mathematical induction on $m$. That is all the active set generated in SNS and contained in $A^*$. Therefore, by Lemma 3.1 we get $A^* \subseteq S_{\lambda, \kappa} \subseteq A_{k}^m \subseteq A^*$, i.e.,

$$\text{supp}(\hat{\beta}(\lambda_M)) = A^* \quad \text{(37)}$$
Then,

\[
\|\beta^* - \hat{\beta}(\lambda_M)\|_\infty \\
= \|\beta_{A^*}^* - (X_{A^*}^TX_{A^*})^{-1}(X_{A^*}^TY - n\bar{d}(\lambda_M)A^*)\|_\infty \\
= \|\beta_{A^*}^* - (X_{A^*}^TX_{A^*})^{-1}(X_{A^*}^T(\lambda_M^*X_{A^*}^*A^*) + \epsilon) \\
- n\bar{d}(\lambda_M)A^*)\|_\infty \\
\leq \frac{\|X_{A^*}^T\epsilon\|_\infty + n(\lambda_M - \lambda_M)}{n(1 - T\nu)} \\
\leq \frac{2\lambda_{M}/15 - 3\gamma_n}{1 - 1/4} \text{ W.H.P.} \\
\leq \frac{14}{3} \gamma_n,
\]

where the first inequality uses (21), the second inequality uses (23) and assumption (C3), and last inequality uses Lemma 3.1 i.e., (8) holds. The sign consistency (7) directly follows from (37), (8) and assumption (C1). This completes the proof of Theorem 3.3. \qed