SNAP: A semismooth Newton algorithm for pathwise optimization with optimal local convergence rate and oracle properties

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Abstract

We propose a semismooth Newton algorithm for pathwise optimization (SNAP) for the LASSO and Enet in sparse, high-dimensional linear regression. SNAP is derived from a suitable formulation of the KKT conditions based on Newton derivatives. It solves the semismooth KKT equations efficiently by actively and continuously seeking the support of the regression coefficients along the solution path with warm start. At each knot in the path, SNAP converges locally superlinearly for the Enet criterion and achieves an optimal local convergence rate for the LASSO criterion, i.e., SNAP converges in one step at the cost of two matrix-vector multiplication per iteration. Under certain regularity conditions on the design matrix and the minimum magnitude of the nonzero elements of the target regression coefficients, we show that SNAP hits a solution with the same signs as the regression coefficients and achieves a sharp estimation error bound in finite steps with high probability. The computational complexity of SNAP is shown to be the same as that of LARS and coordinate descent algorithms per iteration. Simulation studies and real data analysis support our theoretical results and demonstrate that SNAP is faster and accurate than LARS and coordinate descent algorithms.

Keywords: KKT conditions, LASSO, Newton derivative, semismooth functions, sign consistency, superlinear convergence

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1 Introduction

In this paper, we propose a semismooth Newton algorithm for pathwise optimization (SNAP) for regularized high-dimensional regression problems. We consider the linear regression model

\[ y = X\beta^\dagger + \eta, \]  

(1.1)

where \( y \in \mathbb{R}^n \) is a response vector, \( X \in \mathbb{R}^{n \times p} \) is a design matrix, \( \beta^\dagger = (\beta_1^\dagger, \ldots, \beta_p^\dagger)' \in \mathbb{R}^p \) is a vector of underlying regression coefficients, and \( \eta \in \mathbb{R}^n \) is a vector of random errors. We assume without loss of generality that \( y \) is centered and the columns of \( X \) are centered and \( \sqrt{n} \)-normalized. For this model, the LASSO (Tibshirani, 1996; Chen et al., 1998a) solves

\[
\min_{\beta \in \mathbb{R}^p} L_\lambda(\beta) := \frac{1}{2n} \| X\beta - y \|^2_2 + \lambda \| \beta \|_1, 
\]

(1.2)

where \( \lambda > 0 \) is a penalty parameter. Closely related to the LASSO is the elastic net (Enet) (Zou and Hastie, 2005), which solves

\[
\min_{\beta \in \mathbb{R}^p} J_{\lambda,\alpha}(\beta) := L_\lambda(\beta) + \frac{\alpha}{2n} \| \beta \|^2_2, \quad \alpha > 0.
\]

(1.3)

This can be viewed as a regularized form of (1.2). Since \( J_{\lambda,\alpha}(\cdot) \) is strongly convex for \( \alpha > 0 \), the Enet solution \( \hat{\beta}_{\lambda,\alpha} \) is unique. This enables us to characterize the unique minimum 2-norm LASSO solution (1.2) as the limit of \( \hat{\beta}_{\lambda,\alpha} \) as \( \alpha \rightarrow 0^+ \) (Proposition 3.2). In high-dimensional settings, it is nontrivial to efficiently solve (1.2) and (1.3) numerically since they are large scale nondifferentiable optimization problems.

The key ingredient of SNAP is a semismooth Newton algorithm (SNA), which is derived based on a suitable formulation of the KKT conditions. At each step in the iteration, the SNA works by first estimating the support of the solution based on a combination of the primal and dual information, and then finding the values of the nonzero coefficients on the support. Interestingly, our analysis shows that the SNA can be formally derived as a Newton algorithm based on the notion of Newton derivatives for nondifferentiable functions (Kummer, 1988; Qi and Sun, 1993; Ito and Kunisch, 2008).

SNAP proceeds by running SNA along a grid of \( \lambda \) values: \( \{\lambda_t = \lambda_0 \gamma^t\}_{t=0,1,\ldots,N} \) with the continuation strategy and warm start, where \( \gamma \in (0,1) \), \( \lambda_0 > 0 \) and the integer \( N \) are user given parameters. It is easy to implement and computationally stable. Moreover, our simulation studies indicate that SNAP is nearly problem independent, in the sense that the computational cost of using SNAP to approximate the solution path is \( O(Nnp) \), independent of the following aspects of the model, including the ambient dimension, sparsity level, correlation structure of the predictors, range of the magnitude of the nonzero regression coefficients and the noise level.

1.1 Contributions

The most popular algorithms for solving \( \ell_1 \)-regularized problems in the literature are mainly first order methods. It is natural to ask whether we can develop a second order
method, i.e., Newton type method, which is a workhorse in low dimensional estimation, for such nonsmooth optimization problems which converges faster than first order methods. We give a definitive answer to this question via proposing the SNAP algorithm and developed a MATLAB package snap, which is available at http://faculty.zuel.edu.cn/tjyjxxy/jyl/list.htm.

We show that, for the LASSO, the SNA converges locally in just one step, which is obviously the best possible local convergence rate for any algorithms (Theorem 3.3). For the Enet, it converges locally superlinearly (Theorem 3.2). To the best of our knowledge, these are the best convergence rates for LASSO and Enet regularized regression problems with $p \gg n$ in the literature. Our computational complexity analysis shows that the cost of each iteration in SNA is $O(np)$, which is the same as most existing LASSO solvers, including LARS and coordinate descent algorithms. Hence, the overall cost of using SNA to find the unique minimizer of $J_{\lambda,\alpha}(\beta)$ is still $O(np)$ due to its superlinear convergence if it is warm started.

Another contribution of this paper is that we establish the statistical properties of SNAP in the Gaussian noise case. Specifically, we show that under certain regularity conditions on the design matrix $X$, the solution sequence generated by SNAP enjoys the sign consistency property in finite steps if the minimum magnitude of the nonzero elements of $\beta^\dagger$ is of the order $O(\sigma \sqrt{2 \log(p)/n})$, which is the optimal magnitude of detectable signal. We also establish a sharp upper bound in supreme norm for the estimation error of the solution sequence.

1.2 Related work

Osborne et al. (2000) showed that the LASSO solution path is continuous and piecewise linear as a function of $\lambda$. They proposed a Homotopy algorithm that defines an active set of nonzero variables at the current vertex then moves to a new vertex by adding a new variable to or removing an existing one from the active set. Efron et al. (2004) proposed the LARS algorithm to trace the whole solution path of (1.2) by omitting the removing steps in the Homotopy algorithm. Donoho and Tsaig (2008) showed that, in the noiseless case with $\eta = 0$ and under certain conditions on $X$ and $\beta^\dagger$, LARS (Homotopy) algorithm has the “$\|\beta^\dagger\|_0$-step” convergence property with the cost of $O(\|\beta^\dagger\|_0 np)$. However, the convergence property of LARS is unknown when the noise vector $\eta$ is nonzero in the $p > n$ settings. Further connections of SNA with LARS, sure independence screening (Fan and Lv, 2008), and active set tricks for accelerating coordinate descent (Tibshirani et al., 2012) are discussed in Section 5.

Several authors have adopted a Gauss-Seidel type coordinate descent algorithm (CD-GS) (Fu, 1998; Friedman et al., 2007; Wu and Lange, 2008; Li and Osher, 2009), as well as Jacobi type coordinate descent (CD-J), or iterative thresholding (Daubechies et al., 2004; She, 2009) to solve (1.2). For the CD-GS proposed in Friedman et al. (2007), the results of Tseng (2001), Saha and Tewari (2013) and Yun (2014) only ensure the
convergence and sublinear convergence rate of the sequence of the objective functions $\{L_\lambda(\beta^k), k = 1, 2, \ldots\}$, but not the sequence of the solutions $\{\beta^k, k = 1, 2, \ldots\}$. Since in high-dimensional settings with $p \gg n$, the global minimizers $\hat{\beta}_\lambda$ are generally not unique, hence, it is not clear which minimizer the sequence $\{\beta^k, k = 1, 2, \ldots\}$ generated from CD-GS iterations converges to. The CD-GS proposed in Li and Osher (2009) and Tseng and Yun (2009) with refined sweep rules is guaranteed to converge. Other widely used algorithms include proximal gradient descent (Nesterov, 2005, 2013; Agarwal et al., 2012; Xiao and Zhang, 2013), alternative direction method of multiplier (ADMM) (Boyd et al., 2011; Chen et al., 2017; Han et al., 2017), among others. For more comprehensive reviews of the literature on the related topics, see the review papers by Tropp and Wright (2010), and Parikh and Boyd (2014).

Agarwal et al. (2012) considered the statistical properties of the proximal gradient descent path. But their analysis required knowing $\|\beta^I\|_1$, which is unknown or hard to estimate in practice. Although this can be remedied by using the techniques developed by Xiao and Zhang (2013), it does not achieve the sharp error bound as SNAP does.

1.3 Notation

Some notation used throughout this paper are defined below. With $\|\beta\|_q = \left(\sum_{i=1}^{p} |\beta_i|^q\right)^{\frac{1}{q}}$ we denote the usual $q$ ($q \in [1, \infty]$) norm of a vector $\beta = (\beta_1, \beta_2, \ldots, \beta_p)' \in \mathbb{R}^p$. $\|\beta\|_0$ denotes the number of nonzero elements of $\beta$. $X'$ denotes the transpose of the covariate matrix $X \in \mathbb{R}^{n \times p}$ and $\|X\|$ denotes the operator norm of $X$ induced by vector with 2-norm. $1$ or $0$ denote a vector $\in \mathbb{R}^p$ or a matrix with elements all 1 or 0. Define $S = \{1, \ldots, p\}$. For any $A, B \subseteq S$ with length $|A|, |B|$, we denote $\beta_A \in \mathbb{R}^{|A|}$ (or $X_A \in \mathbb{R}^{|A| \times p}$) as the sub-vector (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 supp($z$), sgn($z$) to denote the support and sign of a vector $z$, respectively. We use $I$, $G$ and $\tilde{y}$ to denote the identity matrix, the regularized Gram matrix $X'X + \alpha I$ and $X' y$, respectively.

1.4 Organization

In Section 2 we provide a heuristic and intuitive derivation of SNA for solving (1.3) (including (1.2) as a special case by setting $\alpha = 0$) and describe SNA for pathwise optimization (SNAP). In Section 3 we establish the locally superlinear convergence rate of SNA for (1.3) and local one-step convergence for (1.2), and analyze the computational complexity of SNA. In Section 4 we provide the conditions for the finite-step sign consistency of SNAP and the upper bounds for the estimation error. In Section 5 we discuss the relations of SNA with LARS, SIS, and active set tricks for accelerating coordinate descent. The implementation detail and numerical comparison with LARS and coordinate descent methods are given in Section 6. We conclude in Section 7 with some comments and future work. The proofs of the main results and some background on Newton derivatives used
for deriving SNA are included in the appendices.

2 A general description of SNAP

In this section we first give an intuitive description of the SNA for computing the LASSO and Enet solutions at a given $\lambda$ and $\alpha$. We then describe the SNAP, which uses SNA for computing the solution paths with warm start and a continuation strategy.

2.1 Motivating SNA based on the KKT conditions

The key idea in the proposed algorithm is to iteratively identify the active set in the optimization using both the primal and dual information, then solve the problem on the active set. Here the primal is simply $\beta$ and its dual is $d = (\tilde{y} - G\beta)/n$. Recall $\tilde{y} = X'y$ and $G = X'X + \alpha I$. For the LASSO, the expression of $d$ simplifies to $d = X'(y - X\beta)/n$, i.e., the correlation vector between the predictors and the residual. For any given $(\lambda, \alpha)$, the KKT conditions (Proposition 3.3) assert that $\hat{\beta}_{\lambda,\alpha}$ is the unique Enet solution if and only if the pair $\{\hat{\beta}_{\lambda,\alpha}, \hat{d}_{\lambda,\alpha}\}$ satisfies

$$
\begin{cases}
\hat{d}_{\lambda,\alpha} = (\tilde{y} - G\hat{\beta}_{\lambda,\alpha})/n, \\
\hat{\beta}_{\lambda,\alpha} = T_\lambda(\hat{\beta}_{\lambda,\alpha} + \hat{d}_{\lambda,\alpha}),
\end{cases}
$$

where $T_\lambda(x)$ is the soft-threshold operator (Donoho and Johnstone, 1995) acting on $x$ component wise, that is, $T_\lambda(x) = (T_\lambda(x_1), \ldots, T_\lambda(x_p))'$ with

$$
T_\lambda(x) = x - \frac{|x + \lambda|}{2} + \frac{|x - \lambda|}{2}, x \in \mathbb{R}.
$$

The KKT conditions in (2.1) are stated in equalities using the soft-threshold operator, rather than in the usual inequality form or in terms of set-valued subdifferentials. This is the basis for our derivation of the SNA, which seeks to solve these nonsmooth equations.

To simplify the notation we drop the subscripts of $(\hat{\beta}_{\lambda,\alpha}, \hat{d}_{\lambda,\alpha})$ and write them as $(\hat{\beta}, \hat{d})$, when it does not cause any confusion. By the second equation of (2.1) and the definition of the soft-threshold operator, we have

$$
\hat{\beta}_B = 0,
$$

$$
\hat{d}_A = \lambda \text{sgn}(\hat{\beta}_A + \hat{d}_A),
$$

where

$$
A = \left\{ j \in S : |\hat{\beta}_j + \hat{d}_j| > \lambda \right\} \quad \text{and} \quad B = \left\{ j \in S : |\hat{\beta}_j + \hat{d}_j| \leq \lambda \right\}.
$$

Substituting (2.3) into the first equation of (2.1) and observing $G_{AA}$ is invertible, we can solve the resulting linear system to get

$$
\hat{\beta}_A = G_{AA}^{-1}(\tilde{y}_A - n\hat{d}_A),
$$

$$
\hat{d}_B = (\tilde{y}_B - G_{BA}\hat{\beta}_A)/n.
$$
Therefore, $\{\hat{\beta}, \hat{d}\}$ can be obtained from (2.3)-(2.4) and (2.6)-(2.7) if $A$ is known.

This naturally leads to the follow iterative algorithm for computing $\{\hat{\beta}, \hat{d}\}$. Let $\{\beta^k, d^k\}$ be the primal and dual approximation of $\{\hat{\beta}, \hat{d}\}$ at the $k$th iteration. Based on (2.5), we approximate the active and inactive sets by

$$A_k = \{ j \in S : |\beta^k_j + d^k_j| > \lambda \} \quad \text{and} \quad B_k = \{ j \in S : |\beta^k_j + d^k_j| \leq \lambda \}. \quad (2.8)$$

Based on (2.3)-(2.4) and (2.6)-(2.7) we obtain the updated approximation $\{\beta^{k+1}, d^{k+1}\}$,

$$\beta^{k+1}_{Ak} = 0, \quad (2.9)$$
$$d^{k+1}_{Ak} = (\lambda - \bar{\lambda})\text{sgn}(\beta^k_{Ak} + d^k_{Ak}), \quad (2.10)$$
$$\beta^{k+1}_{Ak} = G^{-1}_{AkAk}(\bar{y}_{Ak} - n d^{k+1}_{Ak}), \quad (2.11)$$
$$d^{k+1}_{Bk} = (\bar{y}_{Bk} - G_{BkAk}\beta^{k+1}_{Ak})/n. \quad (2.12)$$

In (2.10) we introduce a (small) shifting parameter $\bar{\lambda}$ with $0 \leq \bar{\lambda} < \lambda$ and use a slightly more general version of (2.4), replacing $\lambda$ with $\lambda - \bar{\lambda}$ in (2.4). For $\bar{\lambda} > 0$, we solve a less shrunk version of the Enet. For the solution sequence $\{\beta^k, k \geq 1\}$ with a suitable $\bar{\lambda} > 0$, we show that it achieves finite-step sign consistency and sharp estimation error bound (Theorem 4.1).

Summing up the above discussion, we get the SNA for minimizing (1.3) in Algorithm 1 below, where we write $\hat{\beta}(\lambda) = \hat{\beta}_{\lambda, \alpha}$ for a fixed $\alpha$.

**Algorithm 1** ($\hat{\beta}(\lambda), \hat{d}(\lambda)) \leftarrow \text{SNA}(\beta^0, d^0, \lambda, \bar{\lambda}, K)$

1: Input: $X, y, \alpha, \lambda, \bar{\lambda}, K$, initial guess $\beta^0, d^0$, $A_{-1} = \text{supp}(\beta^0)$. Set $k = 0$.
2: Compute $\bar{y} = X' y$ and store it.
3: for $k = 0, 1, \cdots, K$ do
4: Compute $A_k, B_k$ using (2.8).
5: If $A_k = A_{k-1}$ or $k \geq K$.
6: Stop and denote the last iteration by $\beta_{\hat{A}}, \beta_{\hat{B}}, d_{\hat{A}}, d_{\hat{B}}$.
7: Else
8: Compute $\{\beta^{k+1}, d^{k+1}\}$ using (2.9) - (2.12).
9: $k := k + 1$.
10: End
11: end for
12: Output: $\hat{\beta}(\lambda) = \begin{pmatrix} \beta_{\hat{A}} \\ \beta_{\hat{B}} \end{pmatrix}$ and $\hat{d}(\lambda) = \begin{pmatrix} d_{\hat{A}} \\ d_{\hat{B}} \end{pmatrix}$

**Remark 2.1.** In the algorithm, we use a safeguard maximum number of iterations $K$ that can be defined by the user. We usually set $K \leq 5$ due to the locally superlinear/one-step convergence of SNA.
Each line in Algorithm 1 consists of simple vector and matrix multiplications, except (2.11) in line 6, where we need to invert a $|A_k| \times |A_k|$ matrix. Note that $A_k$ is usually a small subset of $S$ if Algorithm 1 is warm started. Intuitively, at the $k$th step in the iteration, this algorithm tries to identify $A_k$, an approximation of the underlying support by using the estimated coefficients with a proper adjustment $d_k$ determined by the KKT, and solves a low-dimensional adjusted least squares problem on $A_k$. Therefore, with a good starting estimation of $A_k$, which is guaranteed by using a continuation strategy with warm start described below, Algorithm 1 can find a good solution in a few steps.

In Section 3, we derive Algorithm 1 formally from the semismooth Newton method and show that its convergence rate is locally superlinear for the Enet and locally one step for the LASSO.

### 2.2 Solution path approximation

We are often interested in the whole solution path $\hat{\beta}(\lambda) \equiv \hat{\beta}_{\lambda, \alpha}$ of (1.3) for $\lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}]$ and some given $\alpha \geq 0$. Here we approximate the solution path by computing $\hat{\beta}(\lambda)$ on a given finite set $\Lambda = \{\lambda_0, \lambda_1, ..., \lambda_N\}$ for some integer $N$, where $\lambda_0 > \cdots > \lambda_N > 0$. Obviously, $\hat{\beta}(\lambda) = 0$ satisfies (2.1) and (2.1) if $\lambda \geq \|X'y/n\|_{\infty}$. Hence we set $\lambda_{\text{max}} = \lambda_0 = \|X'y/n\|_{\infty}$, $\lambda_t = \lambda_0 \gamma^t$, $t = 0, 1, ..., N$, and $\lambda_{\text{min}} = \lambda_0 \gamma^N$, where $\gamma \in (0, 1)$.

We adopt a simple continuation technique with warm start in computing the solution path. This strategy has been successfully used for computing the LASSO and Enet paths (Friedman et al., 2007; Jiao et al., 2017). We use the solution at $\lambda_t$ as the initial value for computing the solution at $\lambda_{t+1}$. The shift parameter $\lambda_t$ can be vary at different path knots $\lambda_t$, so here we use $\lambda_t$ to demonstrate this. We summarize this in the following SNAP algorithm.

**Algorithm 2** $\hat{\beta}(\Lambda) \leftarrow \text{SNAP}(\lambda_0, \gamma, N, K)$

1: Input: $\lambda_0 = \|X'y/n\|_{\infty}, \hat{\beta}(\lambda_{-1}) = 0, \hat{\beta}(\lambda_{-1}) = X'y/n, \gamma, N, K$.
2: for $t = 0, 1, ..., N$ do
3: Set $\lambda_t = \lambda_0 \gamma^t$ and $(\beta^0, d^0) = (\hat{\beta}(\lambda_{t-1}), \hat{d}(\lambda_{t-1}))$.
4: \((\hat{\beta}(\lambda_t), \hat{d}(\lambda_t)) \leftarrow \text{SNA}(\beta^0, d^0, \lambda_t, \lambda_t, K)\)
5: end for
6: Output: $\hat{\beta}(\Lambda) = [\hat{\beta}(\lambda_0), ..., \hat{\beta}(\lambda_N)]$.

When running SNAP with warm start (Algorithm 2), SNA (Algorithm 1) usually converges in a few steps, since SNA converge locally superlinearly or locally in one step and warm start provides a good initial value.
3 Derivation of SNA and convergence analysis

3.1 KKT conditions

In this subsection, we first discuss the relationship between the minimizers of (1.2) and (1.3). We then characterize the unique minimizer (1.3) by its KKT system.

**Proposition 3.1.** Let $M_\lambda$ be the set of the LASSO solutions given in (1.2). Then $M_\lambda$ is nonempty, convex and compact.

In general, the uniqueness of the LASSO solution (the minimizer of (1.2)) cannot be guaranteed in the $p \gg n$ settings. But the one in $M_\lambda$ with the minimum Euclidean norm denoted by $\widehat{\beta}_\lambda$ is unique. We have the following relation between $\widehat{\beta}_\lambda$ and the Enet solutions $\widehat{\beta}_{\lambda,\alpha}$.

**Proposition 3.2.** For $\alpha > 0$, the Enet (1.3) admits a unique minimizer denoted by $\widehat{\beta}_{\lambda,\alpha}$. Furthermore, $\|\widehat{\beta}_{\lambda,\alpha} - \widehat{\beta}_\lambda\|_2 \to 0$ as $\alpha \to 0^+$.

By Proposition 3.2, a good numerical solution of (1.3) is a good approximation of the minimum 2-norm minimizer of (1.2) for a sufficiently small $\alpha$.

**Proposition 3.3.** Let $\widehat{\beta}_{\lambda,\alpha} \in \mathbb{R}^p$ be the Enet solution, which is the unique minimizer of $J_{\lambda,\alpha}$ in (1.3) for $\alpha > 0$. Then there exists a $\widehat{\mathbf{d}}_{\lambda,\alpha} \in \mathbb{R}^p$ such that (2.1) hold. Conversely, if there exists $\widehat{\beta}_{\lambda,\alpha} \in \mathbb{R}^p$ and $\widehat{\mathbf{d}}_{\lambda,\alpha} \in \mathbb{R}^p$ satisfying (2.1), then $\widehat{\beta}_{\lambda,\alpha}$ is the unique minimizer of $J_{\lambda,\alpha}$ in (1.3).

The KKT equations (2.1) with $\alpha = 0$ also characterize the LASSO solution (1.2), except that the solution may not be unique.

Here the KKT conditions are formulated in terms of equalities (2.1), which are different from but equivalent to the usual inequality form

$$\widehat{\mathbf{d}}_A = \lambda \text{sgn}(\widehat{\beta}_A),$$

$$\|\widehat{\mathbf{d}}_A\|_\infty \leq \lambda,$$

where, $\widehat{\mathbf{d}} = (X'y - G\widehat{\beta})/n$ and $A = \text{supp}(\widehat{\beta})$. The reason we adopt the equation form (2.1) is that we can transform the minimization problem (1.3) into a root finding problem, which help us derive SNA formally under the framework of semismooth Newton method.

3.2 SNA as a Newton algorithm

We now formally derive the SNA based on the KKT conditions by using the semismooth Newton method (Kummer, 1988; Qi and Sun, 1993; Ito and Kunisch, 2008) for finding a root of a nonsmooth equation. This enables us to prove its locally superlinear convergence stated in Theorem 3.2 below. The definition and related property on Newton derivative are given in Appendix A.
Let 
\[ z = \begin{pmatrix} \beta \\ d \end{pmatrix} \] 
and 
\[ F(z) = \begin{bmatrix} F_1(z) \\ F_2(z) \end{bmatrix} : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}^{2p}, \]
where
\[ F_1(z) := \beta - T_\lambda (\beta + d), \]
\[ F_2(z) := G\beta + nd - \tilde{y}. \]

By Proposition 3.3, to find the minimizer of (1.3), it suffices to find a root of 
\[ F(z). \]

Although the classical Newton algorithm cannot be applied directly since 
\[ F(z) \] is not Fréchet differentiable, we can resort to semismooth Newton algorithm since 
\[ F(z) \] is Newton differentiable.

Let 
\[ A := \{ i \in S : |\beta_i + d_i| \geq \lambda \}, \quad B := \{ i \in S : |\beta_i + d_i| < \lambda \}. \]

We reorder \((\beta', d')\) such that 
\[ z = (d'_A, \beta'_A, \beta'_B, d'_B)' \]. We also reorder \(F_1(z)\) and \(F_2(z)\) accordingly,
\[
F(z) = \begin{bmatrix}
\beta_A - T_\lambda (\beta_A + d_A) \\
\beta_B - T_\lambda (\beta_B + d_B) \\
G_{AA}\beta_A + G_{AB}\beta_B + nd_A - \tilde{y}_A \\
G_{BA}\beta_A + G_{BB}\beta_B + nd_B - \tilde{y}_B
\end{bmatrix}.
\]

We have the following result concerning the Newton derivative of \(F\).

**Theorem 3.1.** \( F(z) \) is Newton differentiable at any point \( z \). And
\[
H := \begin{bmatrix}
-I_{AA} & 0 & 0 & 0 \\
0 & I_{BB} & 0 & 0 \\
nI_{AA} & X'AX_B & G_{AA} & 0 \\
0 & G_{BB} & X'BX_A & nI_{BB}
\end{bmatrix} \in \nabla_N F(z). \tag{3.1}
\]

Furthermore, \( H \) is invertible and \( H^{-1} \) is uniformly bounded with
\[
\|H^{-1}\| \leq 1 + 2(n + 1 + \alpha + \|X\|^2)/\alpha.
\]

At the \( k \)th iteration, the semismooth Newton method for finding the root of \( F(z) = 0 \) consists of two steps.

1. Solve \( H_k D_k = -F(z^k) \) for \( D_k \), where \( H_k \) is an element of \( \nabla_N F(z^k) \).
2. Update \( z^{k+1} = z^k + D_k \), set \( k \leftarrow k + 1 \) and go to step (1).
This has the same form as the classical Newton method, except that here we use an element of \( \nabla_N F(Z^k) \) in step (1). Indeed, the key to the success of this method is to find a suitable and invertible \( H_k \). We state this method in Algorithm 3.

**Algorithm 3** SNA for finding a root of \( F(z) \)

1: Input: \( X, y, \lambda, \alpha \), initial guess \( z^0 = \begin{pmatrix} \beta^0 \\ d^0 \end{pmatrix} \). Set \( k = 0 \).

2: for \( k = 0, 1, 2, 3, \ldots \) do

3: Choose \( H_k \in \nabla_N F(z^k) \).

4: Get the semismooth Newton direction \( D_k \) by solving

\[
H_k D_k = -F(z^k).
\] (3.2)

5: Update

\[
z^{k+1} = z^k + D^k.
\] (3.3)

6: Check Stop condition

   If stop

   Denote the last iteration by \( \hat{z} \).

   Else

   \( k := k + 1 \).

7: end for

8: Output: \( \hat{z} \) as an estimate of the roots of \( F(z) \).

**Remark 3.1.** When \( A_k = A_{k+1} \) holds for some \( k \), Algorithm 1 converges. Hence it is natural to stop Algorithm 1 accordingly. A common condition that can be used as a stop rule of Algorithm 3 is when \( \|F(z^k)\|_2 \) is sufficiently small, since this algorithm is a root finding process. Therefore we can use both stopping rules in Algorithm 1 due to the equivalence of Algorithm 1 and Algorithm 3. We also stop Algorithm 1 when the iteration number \( k \) exceeds a prespecified integer \( K \).

It can be verified that Algorithm 1 with \( \overline{\lambda} = 0 \) is just Algorithm 3 written in a form for easy computational implementation. The details are given in Appendix C. Thus it is indeed a semismooth Newton method. The more compact form of Algorithm 3 is better suited for its convergence analysis.

**Theorem 3.2.** Let \( H_k \) in Algorithm 3 be given in (A.42). Then the sequence \( \{\beta^k, k = 1, 2, \ldots\} \) generated based on Algorithm 3 (and Algorithm 1 with \( \overline{\lambda} = 0 \)) converges locally and superlinearly to \( \hat{\beta}_{\lambda, \alpha} \), the unique minimizer of (1.3).

Theorem 3.2 shows the local supperlinear convergence rate of SNA, which is a superior property of Newton type algorithms to first order methods.
Theorem 3.3. For a given \( \lambda > 0 \), let \( \hat{\beta} \equiv \hat{\beta}_\lambda \) be a minimizer of (1.2), 
\[ \hat{d} = X'(y - X\hat{\beta})/n, \]
\[ A = \{ i : |\hat{\beta}_i + \hat{d}_i | > \lambda \}, \] 
\[ \tilde{A} = \{ i : |\hat{\beta}_i + \hat{d}_i | \neq \lambda \}, \] 
and 
\[ C = \min_{i \in \tilde{A}} ||\hat{\beta}_i + \hat{d}_i | - \lambda | > 0. \] 
Suppose \( \text{rank}(X_A) = |A| \) and the initial guess \( \beta^0, d^0 \) satisfies 
\[ \| \hat{\beta} - \beta^0 \|_\infty + \| \hat{d} - d^0 \|_\infty \leq C. \] 
Then, \( \beta^1 = \hat{\beta} \), where \( \beta^1 \) is generated by Algorithm 3 with \( \alpha = 0 \) and \( \lambda = 0 \).

Theorem 3.3 shows that the SNA has an optimal local convergence rate in the sense that it converges in just one step, which improves the locally supper linear convergence rate of semismooth Newton method, see for example, Kummer (1988), Qi and Sun (1993) and Ito and Kunisch (2008).

3.3 Computational complexity analysis

We now consider the computational complexity of SNA (Algorithm 1). We look at the number of floating point operations per iteration. Clearly it takes \( O(p) \) flops to finish step 4-7 in Algorithm 1. For step 8, we solve the linear equation iteratively by conjugate gradient (CG) method initialized with the projection of the previous solution onto the current active set (Golub and Van Loan, 1996). The main operation of iteration of CG is two matrix-vector multiplication cost \( 2n|A_k| \) flops Therefore we can control the number of CG iterations smaller than \( p/(2|A_{k+1}|) \) to make that \( O(np) \) flops will be enough for step 8. For step 9, calculation of the matrix-vector product costs \( np \) flops. So the the overall cost per iteration of Algorithm 1 is \( O(np) \) which is also the cost for state-of-the-art first order LASSO solvers. The local superlinear/one step convergence of SNA guaranteed that a good solution can be found in only a few iteration if it is warm started. Therefore, at each knot of the path, the whole cost of SNA can be still \( O(np) \) if we use the continuation strategy. So Algorithm 2 (SNAP) can get the solution path accurately and efficiently at the cost of \( O(Nnp) \) with \( N \) be the number of knot on the path, see the numerical results in Section 6.

4 Error bounds and finite-step sign consistency

As shown in Theorems 3.2 and 3.3, SNA converges locally superlinearly for Enet and converges in one step for LASSO. In this section we prove that the simple warm start technique makes the SNAP converge globally under certain mutual coherence conditions on \( X \) and a condition on the minimum magnitude of the nonzero components of \( \beta^\dagger \). Specifically, we show that SNAP hits a solution with the same sign as \( \beta^\dagger \) and attains a sharp statistical error bound in finitely many steps with high probability if we properly design the path \( \{ \lambda_t = \lambda_0 \gamma^t \}_{t=0,1,...,N} \) and run SNA along it with warm start.

We only consider the LASSO, so we set \( \alpha = 0 \) and \( G = X'X \). The mutual coherence \( \nu \) defined as \( \nu = \max_{i \neq j} |G_{i,j}|/n \) (Donoho and Huo, 2001; Donoho et al., 2006) characterizes the minimum angle between different columns of \( X/\sqrt{n} \). Let \( A^\dagger = \text{supp}(\beta^\dagger) \) and \( T = ...
Let $|A\dagger|$. Define $|\beta\dagger|_{\min} = \min\{|\beta\dagger_j| : j \in A\dagger\}$. Denote the universal threshold value by $\lambda_u = \sigma \sqrt{2 \log(p)/n}$. Let $\delta_u = 3\lambda_u$, $\lambda_0 = \|X'y/n\|_\infty$, and $\lambda_t = \lambda_0 \gamma^t$, $t = 0, 1, ...$

We make the following assumptions on the design matrix $X$, the target coefficient $\beta\dagger$, and the noise vector $\eta$.

(A1) The mutual coherence satisfies $T\nu \leq \frac{1}{4}$.

(A2) The smallest nonzero regression coefficient satisfies $|\beta\dagger|_{\min} \geq 78\lambda_u$.

(A3) $\eta$ satisfies $\eta \sim N(0, \sigma^2 I_n)$.

**Lemma 4.1.** Suppose that (A1) to (A3) hold. There exists an integer $N \in [1, \log(\gamma(\frac{108}{\lambda_0})))$ such that $\lambda_N > 10\delta_u \geq \lambda_{N+1}$ and $|\beta\dagger|_{\min} > \frac{8\lambda_N}{5}$ hold with probability at least $1 - \frac{1}{2\sqrt{\pi} \log(p)}$.

**Theorem 4.1.** Suppose that (A1) to (A3) hold. Then with probability at least $1 - \frac{1}{2\sqrt{\pi} \log(p)}$, SNAP($\lambda_0, \gamma, N, K$) with $\gamma = \frac{8}{13}$, $N$ determined in Lemma 4.1, $K \geq T$, and $\lambda = \frac{9}{10} \lambda_t + \delta_u$ at the $t_{th}$ knot, has a finite step sign consistency property and achieves a sharp estimation error, i.e.,

$$\text{sgn}(\hat{\beta}(\lambda_N)) = \text{sgn}(\beta\dagger),$$

(4.1)

and

$$\|\hat{\beta}(\lambda_N) - \beta\dagger\|_\infty < \frac{23}{6}\lambda_u.$$  

(4.2)

**Remark 4.1.** From the proof of Theorem 4.1 we can see that SNAP (Algorithm 3) with $\lambda = 0$ can recover $\beta\dagger$ exactly by letting $\lambda_t \rightarrow 0$ in the case $\eta = 0$. However, if the observation contains noise we have to set the shift parameter $\lambda$ in SNAP to be nonzero which reduce the amount of shrinkage of LASSO.

The properties of LASSO have been studied by many authors. For example, Zhao and Yu (2006) and Meinshausen and Bühlmann (2006) showed that LASSO is sign consistent under a strong irrepresentable condition, which is a little weaker than (A1). They also required $|\beta\dagger|_{\min}$ be bounded below by $O(n^{-c/2})$ with $c \in (0, 1)$, which is stronger than (A2). Zhang and Huang (2008) required $X$ satisfy a sparse Rieze condition, which may be weaker than (A1); and $|\beta\dagger|_{\min}$ larger than $O(\sqrt{T}\lambda_u)$, which is stronger than (A2). Wainwright (2009) assumed a condition stronger than the strong irrepresentable condition to guarantee the uniqueness of LASSO and its sign consistency with a condition on $|\beta\dagger|_{\min}$ similar to (A1). Lounici (2008) and Candès and Plan (2009) assumed the mutual coherence conditions with $T\nu < 1/7$ and $\nu < c/\log(p)$ for a constant $c$, respectively; and their requirements for $|\beta\dagger|_{\min}$ are similar to (A1) with different constants. In deriving the $\ell_2$ and $\ell_\infty$ error bounds of the LASSO, Donoho et al. (2006) and Zhang (2009) assumed $T\nu < 1/4$ and $T\nu \leq 1/4$, respectively. The latter is exactly (A1). However, these existing results do not imply the finite-step sign consistency property established in Theorem 4.1.
All the results mentioned above concern the minimizer of the LASSO problem, but they did not directly address the statistical properties of the sequence generated by a specific solver. So there is a gap between those theoretical results and the computational solutions. There has been efforts to close this gap. For example, Agarwal et al. (2012) considered the statistical properties of the proximal gradient descent path. But their analysis required knowing $\|\beta^\dagger\|_1$, which is hard to estimate in practice. Xiao and Zhang (2013) remedied this, but their result does not achieve the sharp error bound like SNAP does. Also, the technique used for deriving the statistical properties of SNAP (a Newton type method), is quite different from the proximal gradient method (a gradient type method).

5 Connections LARS, SIS and active set tricks for accelerating coordinate descent

The key idea in SNAP is using the Newton type method SNA to iteratively identify the active set using both the primal and dual information, then solve the problem on the active set. In this section we discuss the connections between SNAP with other three dual active set methods, i.e., LARS, SIS (Fan and Lv, 2008), and sequential strong rule SSR (active set tricks for accelerating coordinate descent) (Tibshirani et al., 2012).

LARS (Efron et al., 2004) also does not solve (1.2) exactly since it omits the removing procedure of Homotopy (Osborne et al., 2000). As discussed in Donoho and Tsaig (2008), the LARS algorithm can be formulated as

$$\beta_{B_k}^{k+1} = \mathbf{0},$$

$$\beta_{A_k}^{k+1} = (X_{A_k}^\prime X_{A_k})^{-1}(\bar{\mathbf{y}}_{A_k} - \bar{\lambda}^k \text{sgn}(d_{A_k}^k)),$$

where $A_k$ is the set of the indices of the variables with highest correlation with the current residual, $B_k = (A_k)^c$, $\bar{\lambda}^k = \|d^k\|_\infty - \gamma_k$, $d^k = X'(y - X\beta^k)/n$, and $\gamma_k$ is the step size to the next breakpoint on the path (Efron et al., 2004; Donoho and Tsaig, 2008). Comparing Algorithm 2 (SNAP) (by setting $K = 0$) with the above reformulation of the LARS algorithm, we see that both SNAP and LARS can be understood as approaches for estimating the support of the underlying solution, which is the essential aspect in fitting sparse, high-dimensional models. So, SNAP and LARS share some similarity both in formulation and in spirit although they were derived from different perspectives. However, the definitions of the active set in SNAP is based on the sum of primal approximation (current approximation $\beta^k$) and the dual approximation (current correlation $d^k = X'(y - X\beta^k)/n$) while LARS is based on dual only. The following low-dimensional small noise interpretation may clarify the difference between the two active set definitions. If $X'X/n \approx \text{identity}$ and $\eta \approx 0$ we get

$$d^k = X'(y - X\beta^k)/n = X'(X\beta^k + \eta - X\beta^k)/n \approx \beta^\dagger - \beta^k + X'\eta/n \approx \beta^\dagger - \beta^k$$
\[
\beta^k + d^k \approx \beta^i.
\]

In addition, LARS selects variables one by one while SNAP can select more than one variable at each iteration. Also, the adjusted least squares fits on the active sets in SNAP and LARS are different. Under certain conditions on \( X \) both of them recover \( \beta^\dagger \) exactly in the noise free case (Donoho and Tsaig, 2008) even when \( p > n \). But the convergence or consistency of LARS is unknown when the noise vector \( \eta \neq 0 \).

Given a starting point \( \lambda_0 \), SNA is initialized with \( \beta^0 = 0, d^0 = X'y/n \). Therefore,
\[
A_0 = \{ j : |\beta^0_j + d^0_j| > \lambda_0 \} = \{ j : |x'_j y/n| > \lambda_0 \}.
\]

Thus the first active set generated by SNAP contains the features that coorelated with \( y \) larger than \( \lambda_0 \), which are the same as those from the sure independence screening (Fan and Lv, 2008) with parameter \( \lambda_0 \) and include the one selected by the first step of LARS. We then use (2.9) - (2.12) to obtain \( \{ \beta^1, d^1 \} \), and update the active set to \( A_1 \) using (2.8). Clearly, for \( k \geq 1 \), \( A_k \) are determined not just by the correlation \( d^k \), but by the primal (\( \beta^k \)) and dual (\( d^k \)) together.

Tibshirani et al. (2012) proposed a sequential strong rule (SSR) for discarting predictors in LASSO-type problems. At point \( \lambda_t \) on the solution path, this rule discards the \( j \)th predictor if
\[
|\hat{d}_j(\lambda_{t-1})| < 2\lambda_t - \lambda_{t-1},
\]
where \( \hat{d}_j(\lambda) = x'_j (y - X\hat{\beta}(\lambda))/n \) for the LASSO penalty. They define active set
\[
A_k = \{ j : |d_j(\lambda_{t-1})| \geq 2\lambda_t - \lambda_{t-1} \},
\]
and set \( \hat{\beta}(\lambda_t)_{B_k} = 0 \) for \( B_k = A_k \) and solve the LASSO problem on \( A_k \). By combining with a simple check of the KKT condition, it speeds up the computation considerably. So SNA shares some similarity in spirit with SSR in that both methods seek to identify an active set and solve a smaller optimization problem, although they are derived from quite different perspectives. However, there are some important differences. First, the active sets are determined differently. Specifically, SSR determines the active set only based on the dual approximation; while SNA uses both primal and dual approximation. Second, SNA does not need the unit slope assumption, and additional check of the KKT conditions is not needed (The cost of check KKT is \( O(np) \)). Third, as far as we know, the statistical properties of the solution sequence generated from SSR are unknown, while error bounds and sign consistency are established under suitable conditions for the solution sequence generated from the SNAP.

6 Numerical examples

In this section, we present numerical examples to evaluate the performance of the proposed SNAP algorithm 2 for solving LASSO. All experiments are performed in MATLAB.
6.1 Comparison with existing popular algorithms

Both the LARS (Efron et al., 2004; Donoho and Tsaig, 2008) and the CD (Friedman et al., 2007, 2010) are popular algorithms capable of efficiently computing the LASSO solution, hence we compare the proposed SNAP with these two algorithms. In implementation, we consider two solvers: (1) SolveLasso, the Matlab code for LARS with the LASSO modification, available online at http://sparselab.stanford.edu/SparseLab_files/Download_files/SparseLab21-Core.zip; (2) glmnet, the Fortran based Matlab package using CD, available online at https://github.com/distrep/DMLT/tree/master/external/glmnet. The parameters in the solvers are the default values as their online versions. In addition to the default stopping parameters in the solvers, we stop LARS (SolveLasso), CD (glmnet) and SNAP if the number of nonzero elements at some iteration is larger than a given fixed quantity such as \( n/\log(p) \) or even larger \( 0.5n \), since the upper bound of the estimated sparsity level of LASSO is \( O(n/\log(p)) \) when \( n \ll p \) (Candès et al., 2006; Candès and Tao, 2006).

6.2 Tuning parameter selection

To choose a proper value of \( \lambda \) in (1.2) is a crucial issue for LASSO problems, since it balances the tradeoff between the data fidelity and the sparsity level of the solution. In practice, the Bayesian information criterion (BIC) is a widely used selector for the tuning parameter selection, due to its model selection consistency under some regularity conditions. We refer the readers to Wang et al. (2007); Chen and Chen (2008); Wang et al. (2009); Chen and Chen (2012); Kim et al. (2012); Wang et al. (2013) and references therein for more details. In this paper, we use a modified BIC (MBIC) from Kim et al. (2012) to choose \( \lambda \), which is given as

\[
\hat{\lambda} = \arg \min_{\lambda \in \Lambda} \left\{ \frac{1}{2n} \| X \hat{\beta}(\lambda) - y \|_2^2 + |\hat{A}(\lambda)| \frac{\log(n) \log(p)}{n} \right\}, \tag{6.1}
\]

where \( \Lambda = \{ \lambda_t \}_t \) is the candidate set for \( \lambda \), and \( \hat{A}(\lambda) = \{ j : \hat{\beta}(\lambda) \neq 0 \} \) is the model identified by \( \hat{\beta}(\lambda) \). Besides, the high-dimensional BIC (HBIC) in Wang et al. (2013) defined by

\[
\hat{\lambda} = \arg \min_{\lambda \in \Lambda} \left\{ \log \left( \frac{\| X \hat{\beta}(\lambda) - y \|_2^2}{n} \right) + |\hat{A}(\lambda)| \frac{\log(n) \log(p)}{n} \right\} \tag{6.2}
\]

is also a good candidate for the selection of \( \lambda \). Unless otherwise specified, the MBIC (6.1) is the default one to select \( \lambda \).
6.3 Simulation

6.3.1 Implementation setting

The $n \times p$ design matrix $X$ is generated as follows.

(i) Classical Gaussian matrix with correlation parameter $\rho$. The rows of $X$ are drawn independently from $N(0, \Sigma)$ with $\Sigma_{jk} = \rho^{|j-k|}$, $1 \leq j, k \leq p$, $\rho \in (0, 1)$.

(ii) Random Gaussian matrix with auto-correlation parameter $\nu$. First we generate a random Gaussian matrix $\tilde{X} \in \mathbb{R}^{n \times p}$ with its entries following i.i.d. $N(0, 1)$. Then we define a matrix $X \in \mathbb{R}^{n \times p}$ by setting $X_1 = \tilde{X}_1$, $X_j = \tilde{X}_j + \nu \star (\tilde{X}_{j-1} + \tilde{X}_{j+1})$, $j = 2, ..., p-1$, and $X_p = \tilde{X}_p$.

The elements of the error vector $\eta$ are generated independently with $\eta_i \sim N(0, \sigma^2)$, $i = 1, 2, ..., n$. Let $A^\dagger = \text{supp}(\beta^\dagger)$ be the support of $\beta^\dagger$, and let $R^\dagger = \max\{|\beta^\dagger_{A^\dagger}|\} / \min\{|\beta^\dagger_{A^\dagger}|\}$ be the range of magnitude of nonzero elements of $\beta^\dagger$. The underlying regression coefficient vector $\beta^\dagger \in \mathbb{R}^p$ is generated in a way that $A^\dagger$ is a randomly chosen subset of $S$ with $|A^\dagger| = T$. As in Becker et al. (2011), Shi et al. (2018b) and Shi et al. (2018a), each nonzero entry of $\beta^\dagger$ is generated as follows:

$$\beta^\dagger_j = \xi_{1j} 10^{\xi_{2j}},$$

where $j \in A^\dagger$, $\xi_{1j} = \pm 1$ with probability $\frac{1}{2}$ and $\xi_{2j}$ is uniformly distributed in $[0, 1]$. Then the observation vector $y = X\beta^\dagger + \eta$. For convenience, we use $(n, p, \rho, \sigma, T, R^\dagger)$ and $(n, p, \nu, \sigma, T, R^\dagger)$ to denote the data generated as above, respectively.

6.3.2 The behavior of the SNAP algorithm

6.3.2.1 The algorithm parameters of SNAP We study the influence of the free parameters $N$ and $K$ in the SNAP algorithm on the exact support recovery probability (Probability for short), that is, the percentage of the estimated model $\hat{A}$ agrees with the true model $A^\dagger$. To this end, we independently generate 20 datasets from $(n = 200, p = 1000, \rho = 0.1, \sigma = 0.01, T = 5 \div 30, R^\dagger = 10)$ for each combination of $(N, K)$. Here $5 \div 30$ means the sparsity level starts from 5 to 30 with an increment of 5. The numerical results are summarized in Figure 1, which consider the following two settings: (a) $K = 1$, and varying $N \in \{40, 60, 80, 100\}$; (b) $N = 100$, and varying $K \in \{1, 2, 3\}$.

It is observed from Figure 1 that the influence of $K$ is very mild on the exact support recovery probability and $K = 1$ generally works well in practice, due to the locally superlinear convergence of SNA and the continuation technique with warm start on the solution path, which is consistent with the conclusions in Section 2. It is also found in Figure 1 that Larger $N$ values make the algorithm have better exact support recovery probability, but the enhancement decreases as $N$ increases. Thus, unless otherwise specified, we set $(N, K) = (100, 1)$ for the SNAP solver.
6.3.2.2 The MBIC selector for SNAP We illustrate the performance of the MBIC selector (6.1) for SNAP with simulated data \((n = 400, p = 2000, \rho = 0.5, \sigma = 0.1, T = 10, R^1 = 10)\). The results are summarized in Figure 2. It can be observed from Figure 2 that the MBIC selector performs very well for the SNAP algorithm on the continuation solution path introduced in Section 2.2.

Figure 2: Plots for SNAP using the MBIC selector with data \((n = 400, p = 2000, \rho = 0.5, \sigma = 0.1, T = 10, R^1 = 10)\): MBIC curve (left panel), the solution path (middle panel), and the comparison between the underlying true parameter \(\beta^\dagger\) and the selected solution \(\hat{\beta}(\hat{\lambda})\) (right panel). The red vertical line in the middle panel shows the solutions selected by MBIC.

6.3.2.3 The local superlinear convergence of SNAP To gain further insight into the SNAP algorithm, we illustrate the convergence behavior of the algorithm using the simulated data as that of Figure 2. Let \(\tilde{A}_t = \{j : \tilde{\beta}_j(\lambda_t) \neq 0\}\), where \(\tilde{\beta}(\lambda_t)\) is the solution to the \(\lambda_t\)-problem. Set \((N, K) = (100, 5)\). The convergence history is shown in Figure 3, which presents the change of the active sets and the number of iterations for each fixed \(\lambda_t\) along the path \(\lambda_0 > \lambda_1 > \cdots > \hat{\lambda}\). It is observed in Figure 3 that
\( \hat{A}_t \subset A^1 \), and the size \(|\hat{A}_t|\) increases monotonically as the path proceeds and eventually equals the true model size \(|A^\dagger|\). In particular, for each \( \lambda_{t+1} \) problem with \( \hat{\beta}(\lambda_t) \) as the initial guess, SNAP generally reaches convergence within two iterations (typically one, noting that the maximum number of iterations \( K = 5 \) here). This is attributed to the local superlinear/one step convergence of the algorithm for LASSO, which is consistent with the results in Theorem 3.3. Hence, the overall procedure is very efficient.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Convergence behavior of SNAP with data \((n = 400, p = 2000, \rho = 0.5, \sigma = 0.1, T = 10, R^\dagger = 10)\): the change of the active sets (left panel) and the number of iterations (right panel) for each \( \lambda_t \)-problem along the path. \( \hat{A}_t \setminus A^\dagger \) (\( A^\dagger \setminus \hat{A}_t \)) denotes the set difference of sets \( \hat{A}_t \) and \( A^\dagger \) (\( \hat{A}_t \) and \( \hat{A}_t \)). In the left panel, the vertical axis is the size of sets; in the right panel, the vertical axis is the number of iterations.}
\end{figure}

6.3.3 Efficiency and accuracy

To evaluate the efficiency and accuracy of the proposed SNAP algorithm, we independently generate \( M = 100 \) datasets from two settings: (i) the classical Gaussian matrix with \((n, p, \rho, \sigma, T, R^\dagger) = (600, 3000, 0.3 : 0.2 : 0.7, 0.2 : 0.2 : 0.4, 40, 10)\); (ii) the random Gaussian matrix with \((n, p, \nu, \sigma, T, R^\dagger) = (1000, 10000, 0.3 : 0.2 : 0.7, 0.2 : 0.2 : 0.4, 50, 10)\). Based on \( M \) independent runs, we compare SNAP with CD and LARS in terms of the average CPU time (Time, in seconds), the estimated average model size (MS) \( M^{-1} \sum_{m=1}^{M} |\hat{A}^{(m)}| \), the proportion of correct models (CM, in percentage terms) \( M^{-1} \sum_{m=1}^{M} I\{\hat{A}^{(m)} = A^\dagger\} \), the average \( \ell_\infty \) absolute error (AE) \( M^{-1} \sum_{m=1}^{M} \|\hat{\beta}^{(m)} - \beta^\dagger\|_\infty \), and the average \( \ell_2 \) relative error (RE) \( M^{-1} \sum_{m=1}^{M} (\|\hat{\beta}^{(m)} - \beta^\dagger\|_2 / \|\beta^\dagger\|_2) \). The measure Time reflects the efficiency of the solvers, while measures MS, CM, AE and RE evaluate the accuracy (quality) of the solutions. Simulation results are summarized in Table 6.1.
and Table 6.2, respectively.

**Table 6.1:** Simulation results for the classical Gaussian matrix with \( n = 600, \ p = 3000, \ T = 40 \) and \( R^\dagger = 10 \) based on 100 independent runs. The numbers in the parentheses are the corresponding standard errors.

| \( \rho \) | \( \sigma \) | Method | Time | MS | CM | AE | RE |
|---|---|---|---|---|---|---|---|
| 0.3 | 0.2 | CD | 0.2287(0.0060) | 41.35(1.1135) | 23%(0.4230) | 0.1270(0.0286) | 0.0172(0.0042) |
| | | LARS | 0.2066(0.0336) | 41.25(1.1315) | 29%(0.4560) | 0.1208(0.0273) | 0.0163(0.0039) |
| | | SNAP | 0.1784(0.0111) | 40.07(0.2932) | 94%(0.2387) | 0.0808(0.0192) | 0.0105(0.0030) |
| 0.4 | | CD | 0.2233(0.0023) | 42.71(1.5973) | 8%(0.2727) | 0.2041(0.0349) | 0.0275(0.0047) |
| | | LARS | 0.2121(0.0316) | 42.14(3.0978) | 13%(0.3380) | 0.2672(0.6802) | 0.0344(0.0767) |
| | | SNAP | 0.1569(0.0041) | 40.23(0.4894) | 80%(0.4020) | 0.1528(0.0309) | 0.0200(0.0046) |
| 0.5 | 0.2 | CD | 0.2272(0.0025) | 42.74(1.8836) | 11%(0.3145) | 0.1484(0.0454) | 0.0193(0.0057) |
| | | LARS | 0.2086(0.0318) | 42.53(2.0863) | 15%(0.3589) | 0.1808(0.2411) | 0.0223(0.0317) |
| | | SNAP | 0.1746(0.0036) | 40.19(0.4861) | 84%(0.3685) | 0.0925(0.0319) | 0.0117(0.0039) |
| 0.4 | | CD | 0.2236(0.0027) | 44.48(2.1057) | 0%(0.0000) | 0.2333(0.0616) | 0.0299(0.0066) |
| | | LARS | 0.2162(0.0364) | 43.58(5.0835) | 1%(0.1000) | 0.3518(0.9235) | 0.0427(0.1029) |
| | | SNAP | 0.1548(0.0039) | 40.62(1.8138) | 55%(0.5000) | 0.1693(0.0439) | 0.0213(0.0045) |
| 0.7 | 0.2 | CD | 0.2280(0.0023) | 47.96(3.2315) | 0%(0.0000) | 0.2062(0.0956) | 0.0223(0.0061) |
| | | LARS | 0.2325(0.0037) | 47.85(3.4855) | 0%(0.0000) | 0.3177(0.6256) | 0.0255(0.0219) |
| | | SNAP | 0.1737(0.0047) | 41.25(1.2340) | 34%(0.4761) | 0.1274(0.0596) | 0.0136(0.0040) |
| 0.4 | | CD | 0.2249(0.0023) | 50.59(3.6517) | 0%(0.0000) | 0.3323(1.5000) | 0.0349(0.0881) |
| | | LARS | 0.2437(0.0310) | 50.61(5.4028) | 0%(0.0000) | 0.5283(0.7663) | 0.0463(0.0679) |
| | | SNAP | 0.1561(0.0040) | 41.92(1.4885) | 16%(0.3685) | 0.2337(0.0914) | 0.0245(0.0054) |

For each \( (\rho, \sigma) \) combination, it can be observed from Table 6.1 that SNAP has better speed performance than CD and LARS. With \( \rho \) fixed, the CPU time of CD and SNAP slightly decreases as \( \sigma \) increases, while higher \( \sigma \) increases the timing of LARS in general. Given \( \sigma \), the CPU time of CD and SNAP is relatively robust with respect to \( \rho \), while that of LARS generally increases as \( \rho \) increases. According to MS, all solvers tend to overestimate the true model and SNAP usually selects a smaller model, while SNAP can select the correct model far more frequently than CD and LARS in terms of CM. The errors of all solvers AE and RE are small, which means they all can produce estimates that are very close to the true values of \( \beta^\dagger \), while the AE and RE of SNAP are smaller than that of the other two, indicating that SNAP is generally more accurate than CD and LARS. Unsurprisingly, larger \( \rho \) or \( \sigma \) will degrade the accuracy of all solvers. In addition, it is shown from Table 6.1 that SNAP generally has smaller (or comparable) standard errors, especially in accuracy metrics MS, AE and RE, which means the results of SNAP are stable and robust. Similar phenomena also hold for the random Gaussian matrix setting in Table 6.2. In particular, since the value of \( p \) is large in Table 6.2, the timing advantage of SNAP is more obvious, which implies that SNAP is capable of handling much larger data sets. In summary, SNAP behaves very well in simulation studies and generally outperforms the state-of-the-art solvers such as LARS and CD in terms of both
efficiency and accuracy.

Table 6.2: Simulation results for the random Gaussian matrix with \( n = 1000, \ p = 10000, \ T = 50 \) and \( R^\dagger = 10 \) based on 100 independent runs. The numbers in the parentheses are the corresponding standard errors.

| \( \nu \) | \( \sigma \) | Method | Time | MS | CM | AE | RE |
|---|---|---|---|---|---|---|---|
| 0.3 | 0.2 | CD | 1.6607(0.0185) | 51.59(1.5511) | 26%(0.4408) | 0.0902(0.0229) | 0.0121(0.0027) |
| | | LARS | 1.0458(0.1729) | 51.48(1.5007) | 29%(0.4560) | 0.0859(0.0215) | 0.0116(0.0027) |
| | | SNAP | 0.8685(0.0289) | 50.08(3.0755) | 93%(0.2564) | 0.0553(0.0133) | 0.0072(0.0017) |
| 0.4 | CD | 1.6416(0.0074) | 52.76(1.8916) | 9%(0.2876) | 0.1403(0.0314) | 0.0184(0.0031) |
| | LARS | 1.1354(0.2245) | 52.40(2.0792) | 12%(0.3266) | 0.1560(0.2001) | 0.0204(0.0272) |
| | SNAP | 0.7764(0.0149) | 50.28(0.5519) | 76%(0.4292) | 0.1007(0.0217) | 0.0128(0.0022) |
| 0.5 | 0.2 | CD | 1.6719(0.0058) | 55.71(2.6678) | 0%(0.0000) | 0.0959(0.0583) | 0.0111(0.0028) |
| | LARS | 1.1819(0.2301) | 55.59(3.3937) | 0%(0.0000) | 0.2002(0.4392) | 0.0164(0.0377) |
| | SNAP | 0.8980(0.0108) | 50.82(1.0767) | 49%(0.5024) | 0.0559(0.0320) | 0.0064(0.0019) |
| 0.4 | CD | 1.6504(0.0064) | 57.86(3.0847) | 0%(0.0000) | 0.1583(1.0685) | 0.0164(0.0044) |
| | LARS | 1.3180(0.2388) | 56.85(4.2530) | 0%(0.0000) | 0.1954(0.4346) | 0.0220(0.0584) |
| | SNAP | 0.8098(0.0172) | 51.20(1.1192) | 31%(0.4648) | 0.1091(0.0674) | 0.0112(0.0028) |
| 0.7 | 0.2 | CD | 1.6962(0.0100) | 65.22(4.6113) | 0%(0.0000) | 0.1411(0.1521) | 0.0114(0.0060) |
| | LARS | 1.4585(0.2683) | 64.90(7.2202) | 0%(0.0000) | 0.5015(1.0900) | 0.0249(0.0411) |
| | SNAP | 0.9439(0.0506) | 53.09(1.7529) | 6%(0.2387) | 0.0858(0.1374) | 0.0068(0.0100) |
| 0.4 | CD | 1.6715(0.0090) | 67.12(4.8996) | 0%(0.0000) | 0.1880(0.2146) | 0.0156(0.0082) |
| | LARS | 1.5399(0.2448) | 67.07(6.4499) | 0%(0.0000) | 0.5493(0.9422) | 0.0271(0.0299) |
| | SNAP | 0.8441(0.0889) | 52.84(3.3536) | 6%(0.2387) | 0.1907(0.5365) | 0.0187(0.0611) |

6.4 Application

We analyze the breast cancer data which comes from breast cancer tissue samples deposited to The Cancer Genome Atlas (TCGA) project and compiles results obtained using Agilent mRNA expression microarrays to illustrate the application of the SNAP algorithm in high-dimensional settings. This data, which is named bcTCGA, is available at [http://myweb.uiowa.edu/pbreheny/data/bcTCGA.RData](http://myweb.uiowa.edu/pbreheny/data/bcTCGA.RData). In this bcTCGA dataset, we have expression measurements of 17814 genes from 536 patients (all expression measurements are recorded on the log scale). There are 491 genes with missing data, which we have excluded. We restrict our attention to the 17323 genes without missing values. The response variable \( y \) measures one of the 17323 genes, a numeric vector of length 536 giving expression level of gene BRCA1, which is the first gene identified that increases the risk of early onset breast cancer, and the design matrix \( X \) is a 536 \( \times \) 17322 matrix, which represents the remaining expression measurements of 17322 genes. Because BRCA1 is likely to interact with many other genes, it is of interest to find genes with expression levels related to that of BRCA1. This has been studied by using different methods in the recent literature; see, for example, Tan and Huang (2016); Yi and Huang (2017); Lv et al. (2018); Breheny (2018); Shi et al. (2018a). In this subsection, we apply
methods CD (glmnet), LARS (SolveLasso) and SNAP, coupled with the HBIC selector, to analyze this dataset.

First, we analyze the complete dataset of 536 patients. The genes selected by each method along with their corresponding nonzero coefficient estimates, the CPU time (Time, in seconds), the model size (MS) and the prediction error (PE) calculated by $n^{-1}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$ are provided in Table 6.3. It can be seen from Table 6.3 that SNAP runs faster than LARS and CD, while the PE by SNAP is smaller than that by LARS and CD, which demonstrates that SNAP performs better than the other two solvers in terms of both efficiency and accuracy. Further, CD, LARS and SNAP identify 7, 9 and 4 genes respectively, with 3 identified probes in common, namely, C17orf53, NBR2 and TIMELESS. Although the magnitudes of estimates for the common genes are not equal, they have the same signs, which suggests similar biological conclusions.

Table 6.3: The genes identified by CD, LARS and SNAP that correlated with BRCA1 based on the complete dataset of bcTCGA ($n = 536, p = 17322$). The zero entries correspond to variables omitted.

| No. | Term | Gene    | CD    | LARS | SNAP |
|-----|------|---------|-------|------|------|
| 1   | $\beta_{1743}$ | C17orf53 | 0.1008 | 0.0983 | 0.4140 |
| 2   | $\beta_{2739}$ | CCDC56  | 0      | 0.0108 | 0    |
| 3   | $\beta_{2964}$ | CDC25C  | 0      | 0.0136 | 0    |
| 4   | $\beta_{4543}$ | DTL     | 0.0764 | 0.0844 | 0    |
| 5   | $\beta_{9230}$ | MFGE8   | 0      | 0      | -0.1168 |
| 6   | $\beta_{9941}$ | NBR2    | 0.1519 | 0.1885 | 0.4673 |
| 7   | $\beta_{12146}$ | PSME3   | 0.0480 | 0.0615 | 0    |
| 8   | $\beta_{15122}$ | TIMELESS | 0.0157 | 0.0279 | 0.2854 |
| 9   | $\beta_{15535}$ | TOP2A   | 0.0259 | 0.0331 | 0    |
| 10  | $\beta_{16315}$ | VPS25   | 0.1006 | 0.1083 | 0    |

|     | Time   | MS | PE   |
|-----|--------|----|------|
|     | 3.5436 | 7  | 0.3298 |
|     | 2.1070 | 9  | 0.3023 |
|     | 0.7884 | 4  | 0.2345 |

To further evaluate the performance of the three methods, we implement the cross validation (CV) procedure similar to Huang et al. (2008, 2010); Tan and Huang (2016); Yi and Huang (2017); Lv et al. (2018); Shi et al. (2018a). We conduct 100 random partitions of the data. For each partition, we randomly choose 3/4 observations and 1/4 observations as the training and test data, respectively. We compute the CPU time (Time, in seconds) and the model size (MS, i.e., the number of selected genes) using the training data, and calculate the prediction error (PE) based on the test data. Table 6.4 presents the average values over 100 random partitions, along with corresponding
standard deviations in the parentheses.

**Table 6.4**: The CPU time (Time), model size (MS) and prediction error (PE) averaged across 100 random partitions of the bcTCGA data (numbers in parentheses are standard deviations)

| Method | Time   | MS     | PE     |
|--------|--------|--------|--------|
| CD     | 2.0598(0.0393) | 8.72(3.3667) | 0.3503(0.0764) |
| LARS   | 0.5861(0.3625)  | 7.90(3.5689)  | 0.3514(0.0831)  |
| SNAP   | 0.6554(0.0906)  | 6.10(3.0830)  | 0.2742(0.0593)  |

Due to the CV procedure, the working sample size decreases to $n_{CV} = \frac{3}{4}n$. Hence, the CPU time of three solvers in Table 6.4 decrease accordingly compared with the counterpart in Table 6.3. Obviously, it is shown in Table 6.4 that SNAP is still running faster than CD, and is quite comparable to LARS in speed. Compared to LARS, the CPU time of SNAP is less sensitive to the sample size, which means SNAP has more potential than LARS to be applied to a larger volume of noisy data. Also, as clearly shown in the Table 6.4, SNAP selects fewer genes and has a smaller PE, which implies that SNAP could provide a more targeted list of the gene sets. Based on 100 random partitions, we report the selected genes and their corresponding frequency (Freq) in Table 6.5, where the genes are ordered such that the frequency is decreasing. To save space, we only list genes with frequency greater than or equal to 5 counts. It is observed from Table 6.5 that some genes such as NBR2, C17orf53, DTL and VPS25 have quite high frequencies (Freq $\geq 80$) with all three solvers, which largely implies these genes are related to BRCA1. Combining the findings in Table 6.5 and taking into account the small MS and PE of SNAP in Table 6.4, we have a strong belief that genes NBR2 and C17orf53 selected by SNAP are particularly associated with BRCA1.

7 Concluding Remarks

Starting from the KKT conditions we developed SNA for computing the LASSO and Enet solutions in high-dimensional linear regression models. We approximate the whole solution paths using SNAP by utilizing the continuation technique with warm start. SNAP is easy to implement, stable, fast and accurate. We established the locally superlinear of SNA for the Enet and local one-step convergence for the LASSO. We provided sufficient conditions under which SNAP enjoys the sign consistency property in finite steps. Moreover, SNAP has the same computational complexity as LARS and CD. Our simulation studies demonstrate that SNAP is competitive with these state-of-the-art solvers in accuracy and outperforms them in efficiency. These theoretical and numerical results suggest that SNAP is a promising new method for dealing with large-scale $\ell_1$-regularized linear regression problems.

We have only considered the linear regression model with convex penalties. It would
Table 6.5: Frequency table for 100 random partitions of the bcTCGA data. To save space, only the genes with \( \text{Freq} \geq 5 \) are listed.

| CD    | LARS | SNAP |
|-------|------|------|
| Gene  | Freq | Gene  | Freq | Gene  | Freq |
| C17orf53 | 98   | C17orf53 | 93   | NBR2 | 95   |
| DTL   | 91   | NBR2   | 89   | C17orf53 | 91   |
| NBR2  | 91   | VPS25  | 87   | DTL  | 32   |
| VPS25 | 90   | DTL    | 86   | MFGES| 29   |
| PSME3 | 77   | PSME3  | 73   | CCDC56 | 25   |
| TOP2A | 73   | TOP2A  | 67   | CDC25C | 23   |
| TIMELESS | 49  | TIMELESS | 41  | TUBG1 | 23   |
| CCDC56 | 41   | CCDC56 | 33   | LMNB1| 18   |
| CDC25C | 35   | CDC25C | 30   | GNL1 | 18   |
| CENPK | 26   | CENPK  | 24   | TIMELESS | 16   |
| SPRY2 | 20   | RDM1   | 20   | VPS25 | 16   |
| SPAG5 | 18   | CDC6   | 17   | TOP2A | 15   |
| RDM1  | 18   | TUBG1  | 15   | ZYX  | 14   |
| TUBG1 | 17   | SPRY2  | 15   | KIAA0101 | 14   |
| CDC6  | 17   | C16orf59 | 12 | KHDRBS1 | 12   |
| UHRF1 | 16   | CCDC43 | 11   | PSME3 | 11   |
| C16orf59 | 13 | UHRF1  | 10   | SPAG5 | 10   |
| CCDC43 | 13   | SPAG5  | 10   | TUBA1B | 8   |
| ZWINT | 9    | NSF    | 9    | FGFR1 | 8    |
| KIAA0101 | 9  | KIAA0101 | 8   | CMTM5 | 7    |
| NSF   | 8    | ZWINT  | 5    | SYNGR4 | 5   |
| MLX   | 6    |       |      |       |      |
| TRAIP | 5    |       |      |       |      |

It would also be interesting to extend the idea of SNAP to problems with nonconvex penalties such as SCAD (Fan and Li, 2001) and MCP (Zhang, 2010). Coordinate descent algorithms for these penalties have been considered by Breheny and Huang (2011) and Mazumder et al. (2011). In our paper we adopt simple continuation strategy to globalize SNA, globalization via smoothing Newton methods (Chen et al., 1998b; Qi and Sun, 1999; Qi et al., 2000) is also an interesting future work.

We have implemented SNAP in a Matlab package snap, which is available at http://faculty.zuel.edu.cn/tjyjxxy/jyl/list.htm.

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Appendices

A Background on convex analysis and Newton derivative

In order to derive the KKT system (2.1) and prove the locally superlinear convergence of Algorithm 1, we recall some background in convex analysis (Rockafellar, 1970) and describe the concept and some properties of Newton derivative (Kummer, 1988; Qi and Sun, 1993; Ito and Kunisch, 2008).

The standard Euclidean inner product for two vectors \(z, w \in \mathbb{R}^p\) is defined by \(\langle z, w \rangle := \sum_{i=1}^{p} z_i w_i\). The class of all proper lower semicontinuous convex functions on \(\mathbb{R}^p\) is denoted by \(\Gamma_0(\mathbb{R}^p)\). The subdifferential of \(f : \mathbb{R}^p \to \mathbb{R}^1\) denoted by \(\partial f\) is a set-value mapping defined as

\[
\partial f(z) := \{w \in \mathbb{R}^p : f(v) \geq f(z) + \langle w, v - z \rangle, \text{for all } v \in \mathbb{R}^p\}.
\]

If \(f\) is convex and differentiable it holds that

\[
\partial f(z) = \nabla f(z)
\]  

(A.1)

Furthermore, if \(f, g \in \Gamma_0(\mathbb{R}^p)\) then

\[
\partial(f + g)(z) = \partial f(z) + \partial g(z)
\]  

(A.2)

Recall the classical Fermat’s rule (Rockafellar, 1970),

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

(A.3)

Moreover, a more general case is (Combettes and Wajs, 2005)

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

(A.4)

where \(\text{Prox}_f\) is the proximal operator for \(f \in \Gamma_0(\mathbb{R}^p)\) defined as

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

Here we should mention that the proximal operator of \(\lambda \|\cdot\|_1\) is given in a closed form by the componentwise soft-threshold operator, i.e.,

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

(A.5)
where $T_\lambda(x)$ is defined in (2.2).

Let $F : \mathbb{R}^m \rightarrow \mathbb{R}^l$ be a nonlinear map. Chen et al. (2000) generalized classical Newton’s algorithm for finding a root of $F(z) = 0$ when $F$ is not Fréchet differentiable but only Newton differentiable (Ito and Kunisch, 2008).

**Definition 7.1.** $F : \mathbb{R}^m \rightarrow \mathbb{R}^l$ is called Newton differentiable at $x \in \mathbb{R}^m$ if there exists an open neighborhood $N(x)$ and a family of mappings $D : N(x) \rightarrow \mathbb{R}^{l \times m}$ such that

$$
\|F(x + h) - F(x) - D(x + h)h\|_2 = o(\|h\|_2) \quad \text{for} \quad \|h\|_2 \rightarrow 0.
$$

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 $F(x) = |x|$ 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

$$
\nabla_N F(z) = \begin{cases} 
1, & z > 0, \\
-1, & z < 0, \\
r \in \mathbb{R}^1, & z = 0.
\end{cases}
$$

(A.6) follows from the definition of Newton derivative.

Suppose $F_i : \mathbb{R}^m \rightarrow \mathbb{R}^1$ 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

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

(A.7) 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 $\theta, \gamma \in \mathbb{R}^1$,

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

(A.8)

Let $F_1 : \mathbb{R}^s \rightarrow \mathbb{R}^l$ 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

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

(A.9) With the above preparation we can calculate the Newton derivative of the componentwise soft threshold operator $T_\lambda(x)$. 

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Lemma 7.1. $T_\lambda(\cdot) : \mathbb{R}^p \to \mathbb{R}^p$ is Newton differentiable at any point $x \in \mathbb{R}^p$. And $\text{diag}(b) \in \nabla N T_\lambda(x)$, where $\text{diag}(b)$ is a diagonal matrix with $$b = (1_{\{|x_1| > \lambda\}}, \ldots, 1_{\{|x_p| > \lambda\}})'$$ and $1_A$ is the indicator function of set $A$.

This lemma is used in the derivation of the SNA given in Subsection 3.2.

Proof of Lemma 7.1. As shown in (A.6), $1_{\{|z| > 0\}} \in \nabla N |z|$. Then, it follows from (A.8)-(9) that the scalar function $T_\lambda(z) = z - |z + \lambda|/2 + |z - \lambda|/2$ is Newton differentiable by with $$1_{\{|z| > \lambda\}} \in \nabla N T_\lambda(z). \quad (A.10)$$

Let $$F_i(x) = T_\lambda(e_i'x) : x \in \mathbb{R}^p \to \mathbb{R}^1, i = 1, \ldots, p,$$ where the column vector $e_i$ is the $i$th orthonormal basis in $\mathbb{R}^p$. Then, it follow from (A.9) and (A.10) that $$e_i'1_{\{|x_i| > \lambda\}} \in \nabla N F_i(x). \quad (A.11)$$

By using (A.7) and (A.11) we have $T_\lambda(x) = (F_1(x), \ldots, F_p(x))'$ is Newton differentiable and $\text{diag}(b) \in \nabla N T_\lambda(x)$. This completes the proof of Lemma 7.1.

B Proofs

Proof of Proposition 3.1.

Proof. This is a standard result in convex optimization, we include a proof her e for completeness. Obviously $L_\lambda(\cdot)$ is bounded below by 0, thus, has infimum denoted by $L^*$. Let $\{\beta^k\}_k$ be a sequence such that $L_\lambda(\beta^k) \to L^*$. Then $\{\beta^k\}_k$ is bounded due to

$$L_\lambda(\beta) \to +\infty \quad \text{as} \quad \|\beta\|_1 \to +\infty. \quad (A.12)$$

Hence $\{\beta^k\}_k$ has a subsequence still denoted by $\{\beta^k\}_k$ that converge to some $\beta_\lambda$. Then the continuity of $L_\lambda(\cdot)$ implies $\beta_\lambda \in M_\lambda$, i.e., $M_\lambda$ is nonempty. The boundedness of $M_\lambda$ follows from (A.12) and the closeness follows from the continuity of $L_\lambda(\cdot)$, i.e., $M_\lambda$ is compact. The convexity of $M_\lambda$ follows from the convexity of $L_\lambda(\cdot)$. This completes the proof of Proposition 3.1.

Proof of Proposition 3.2

Proof. By the same argument in the proof of Proposition 3.1, there exists a minimizer of $J_{\lambda,\alpha}(\cdot)$. We denote this minimizer by $\beta_{\lambda,\alpha}$. It follow from the strict convexity of $J_{\lambda,\alpha}(\cdot)$ that $\beta_{\lambda,\alpha}$ is unique. Let $\hat{\beta}_\lambda$ be the one in $M_\lambda$ with the minimum Euclidean. We have

$$L_\lambda(\hat{\beta}_\lambda) + \frac{\alpha}{2n} \|\beta_{\lambda,\alpha}\|_2^2 \leq L_\lambda(\beta_{\lambda,\alpha}) + \frac{\alpha}{2n} \|\beta_{\lambda,\alpha}\|_2^2 = J_{\lambda,\alpha}(\beta_{\lambda,\alpha}) \leq J_{\lambda,\alpha}(\hat{\beta}_\lambda) = L_\lambda(\hat{\beta}_\lambda) + \frac{\alpha}{2n} \|\beta_\lambda\|_2^2, \quad (A.13)$$

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where the first inequality use the the property that $\hat{\beta}_\lambda$ is a minimizer of $L_\lambda(\cdot)$, and the second inequality use the the property that $\hat{\beta}_{\lambda,\alpha}$ is a minimizer of $J_{\lambda,\alpha}(\cdot)$. Then it follows from (A.13) that
\[
\|\hat{\beta}_{\lambda,\alpha}\|_2^2 \leq \|\hat{\beta}_\lambda\|_2^2. \tag{A.14}
\]
This implies $\{\hat{\beta}_{\lambda,\alpha}\}_\alpha$ is bounded and thus there exist a subsequence of $\{\hat{\beta}_{\lambda,\alpha}\}_\alpha$ denoted by $\{\tilde{\beta}_{\lambda,\alpha}\}_\alpha$ that converge to some $\beta_*$ as $\alpha \to 0^+$. Let $\alpha \to 0^+$ in (A.13) and (A.14) we get
\[L_\lambda(\beta_*) \leq L_\lambda(\hat{\beta}_\lambda)\]
and
\[\|\beta_*\|_2 \leq \|\hat{\beta}_\lambda\|_2.\]
The above two inequality imply $\beta_*$ is a minimizer of $L_\lambda(\cdot)$ with minimum 2-norm. Thus, $\beta_* = \hat{\beta}_\lambda$ due to the uniqueness of such a minimizer. Hence $\tilde{\beta}_{\lambda,\alpha}$ converges to $\beta_\lambda$. The same argument shows that any subsequence of $\{\hat{\beta}_{\lambda,\alpha}\}_\alpha$ has a further subsequence converging to $\beta_\lambda$. This implies that the whole sequence $\{\hat{\beta}_{\lambda,\alpha}\}_\alpha$ converges to $\hat{\beta}_\lambda$. This completes the proof of Proposition 3.2.

**Proof of Proposition 3.3.**

*Proof.* We first assume $\hat{\beta}_{\lambda,\alpha} \in \mathbb{R}^p$ is a minimizer of (1.3). Then it follows from (A.1)-(A.3) that
\[
0 \in X'(X\hat{\beta}_{\lambda,\alpha} - y)/n + \alpha \hat{\beta}_{\lambda,\alpha} + \lambda \partial \|\cdot\|_1(\hat{\beta}_{\lambda,\alpha}).
\]
Therefore, there exists $\tilde{d}_{\lambda,\alpha} \in \lambda \|\cdot\|_1(\hat{\beta}_{\lambda,\alpha})$ such that
\[
0 = X'(X\hat{\beta}_{\lambda,\alpha} - y)/n + \alpha \hat{\beta}_{\lambda,\alpha} + \tilde{d}_{\lambda,\alpha},
\]
i.e. the first equation of (2.1) holds by noticing $G = X'X + \alpha I$ and $\tilde{y} = X'y$. Furthermore, it follow from (A.4) that
\[
\tilde{d}_{\lambda,\alpha} \in \lambda \|\cdot\|_1(\hat{\beta}_{\lambda,\alpha})
\]
is equivalent to
\[
\hat{\beta}_{\lambda,\alpha} = \text{Prox}_{\lambda \|\cdot\|_1}(\tilde{\beta}_{\lambda,\alpha} + \tilde{d}_{\lambda,\alpha}).
\]
By using (A.5), we have
\[
\hat{\beta}_{\lambda,\alpha} = T_\lambda(\hat{\beta}_{\lambda,\alpha} + \tilde{d}_{\lambda,\alpha}),
\]
which is the second equation of (2.1).

Conversely, if (2.1) are satisfied for some $\hat{\beta}_{\lambda,\alpha} \in \mathbb{R}^p$, $\tilde{d}_{\lambda,\alpha} \in \mathbb{R}^p$. By using (A.4) and (A.5) again, we deduce
\[
\tilde{d}_{\lambda,\alpha} \in \lambda \|\cdot\|_1(\hat{\beta}_{\lambda,\alpha})
\]
from the second equation of (2.1). Substituting this into the first equation of (2.1) we have
\[
0 \in (G\hat{\beta}_{\lambda,\alpha} - \tilde{y})/n + \lambda \|\cdot\|_1(\hat{\beta}_{\lambda,\alpha}),
\]
which implies that $\hat{\beta}_{\lambda,\alpha}$ is a minimizer of (1.3) by Fermat’s rule (A.3).

The proof for (1.2) can be derived similarly. This completes the proof of Proposition 3.3.

\[\square\]

**Proof of Theorem 3.1.**

**Proof.** It follows from Lemma 7.1 and (A.8)-(A.9) that $F_1(z)$ is Newton differentiable. Furthermore, by using Lemma 7.1 and the definition of $A$ and $B$, we have

\[
\begin{bmatrix}
-I_{AA} & 0 & 0 & 0 \\
0 & I_{BB} & 0 & 0
\end{bmatrix} \in \nabla_N F_1(z) \tag{A.15}
\]

Obviously, $F_2(z)$ is continuously differentiable with

\[
\nabla F_2(z) = \begin{bmatrix}
nI_{AA} & X_A'X_B & G_{AA} & 0 \\
0 & G_{BB} & X_B'X_A & nI_{BB}
\end{bmatrix}. \tag{A.16}
\]

Then it follows from (A.15)-(A.16) and (A.7) that $F$ is Newton differentiable with $H \in \nabla_N F(z)$.

Let

\[
H_1 = \begin{bmatrix}
-I_{AA} & 0 \\
0 & I_{BB}
\end{bmatrix}, H_2 = \begin{bmatrix}
nI_{AA} & X_A'X_B \\
0 & G_{BB}
\end{bmatrix}, H_3 = \begin{bmatrix}
G_{AA} & 0 \\
X_B'X_A & nI_{BB}
\end{bmatrix}.
\]

Obviously, $H_i, i = 1, 2, 3$ is invertible and

\[
H^{-1} = \begin{bmatrix}
H_1^{-1} & 0 \\
-H_3^{-1}H_2H_1^{-1} & H_3^{-1}
\end{bmatrix}.
\]

Let $g = (g_1', g_2')'$ be an arbitrary vector in $\mathbb{R}^{2p}$. Then

\[
\|H^{-1}g\|_2^2 = \| \begin{bmatrix} H_1^{-1} & 0 \\
-H_3^{-1}H_2H_1^{-1} & H_3^{-1}
\end{bmatrix} \begin{bmatrix} g_1 \\
g_2
\end{bmatrix} \|_2^2
\]

\[
= \|H_1^{-1}g_1\|_2^2 + \| -H_3^{-1}H_2H_1^{-1}g_1 + H_3^{-1}g_2\|_2^2
\]

\[
\leq \|H_1^{-1}\|_2\|g_1\|_2^2 + \|H_3^{-1}\|_2^2(\|H_2\|\|H_1^{-1}\|\|g_1\|_2 + \|g_2\|_2)^2
\]

\[
\leq (\|H_1^{-1}\| + \|H_3^{-1}\|(1 + \|H_2\|\|H_1^{-1}\|))\|g\|_2^2
\]

which shows

\[
\|H^{-1}\| \leq \|H_1^{-1}\| + \|H_3^{-1}\|(1 + \|H_2\|\|H_1^{-1}\|). \tag{A.17}
\]

The similar argument shows

\[
\|H_2\| \leq n + \alpha + 2 \|X\|^2, \tag{A.18}
\]
and
\[ \|H^{-1}\| \leq \frac{1}{n} + \left(1 + \|X\|^2\right)/\alpha. \]
(A.19)

Combining (A.18)-(A.19) with (A.17) and observing
\[ \|H^{-1}\| = 1 \]
we get
\[ \|H^{-1}\| < 1 + 2(n + 1 + \alpha + \|X\|^2)/\alpha. \]
This completes the proof of Theorem 3.1. \(\square\)

**Proof of Theorem 3.2.**

**Proof.** Let \(z_\alpha = (\hat{\beta}_\alpha', \hat{d}_\alpha')'\) be a root of \(F(z)\). Let \(z^k\) be sufficiently close to \(z_\alpha\). By using the definition of Newton derivative and \(H_k \in \nabla_N F(z^k)\), we have
\[ \|H_k(z^k - z_\alpha) - F(z^k) + F(z_\alpha)\|_2 \leq \varepsilon\|z^k - z_\alpha\|_2, \]
(A.20)

where \(\varepsilon \to 0\) as \(z^k \to z_\alpha\). Then,
\[
\begin{align*}
\|z^{k+1} - z_\alpha\|_2 &= \|z^k - H_k^{-1}F(z^k) - z_\alpha\|_2 \\
&= \|z^k - H_k^{-1}F(z^k) - z_\alpha + H_k^{-1}F(z_\alpha)\|_2 \\
&\leq \|H_k^{-1}\| \|H_k(z^k - z_\alpha) - F(z^k) + F(z_\alpha)\|_2 \\
&\leq \varepsilon(1 + 2(n + 1 + \alpha + \|X\|^2)/\alpha)\|z^k - z_\alpha\|_2,
\end{align*}
\]

where the first equality uses (3.2) - (3.3), the second equality is some algebra, and the last inequality uses (A.20) and the uniform boundedness of \(H_k^{-1}\) proved in Theorem 3.1. Then we get the sequence \(z^k\) generated by Algorithm 3 converge to \(z_\alpha\) locally superlinearly. The definition of \(F(z)\) implies its root \(z_\alpha = (\hat{\beta}_\alpha', \hat{d}_\alpha')'\) satisfies the KKT conditions (2.1). Thus, it follows from Proposition 3.3 that \(\hat{\beta}_\alpha\) is the unique minimizer of (1.3). Therefore, Theorem 3.2 holds by the equivalence between Algorithm 1 and Algorithm 3. This completes the proof of Theorem 3.2. \(\square\)

**Proof of Theorem 3.3.**

**Proof.** First, we have
\[
\begin{align*}
\hat{\beta}_i + \hat{d}_i - \beta_0^i - d^0_i &= |eta_0^i + d^0_i - \hat{\beta}_i - \hat{d}_i| \\
&\leq \|\hat{\beta} - \beta^0\|_\infty + \|\hat{d} - d^0\|_\infty \\
&\leq C \\
&\leq \hat{\beta}_i + \hat{d}_i - \lambda, \quad \forall i \in \{j \in \tilde{A} : \hat{\beta}_j + \hat{d}_j > \lambda\}
\end{align*}
\]

where the last inequality uses the definition that \(C = \min_{i \in \tilde{A}} |\hat{\beta}_i + \hat{d}_i - \lambda|\). This implies that \(\hat{\beta}_i + \hat{d}_i > \lambda \implies \beta_0^i + d^0_i > \lambda\) (similarly, we can show \(\hat{\beta}_i + \hat{d}_i < -\lambda \implies \beta_0^i + d^0_i < -\lambda\),
i.e., \( A = \{ i : |\tilde{\beta}_i + \tilde{d}_i| > \lambda \} \subseteq A_0 = \{ i : |\beta_i^0 + d_i^0| > \lambda \} \). Meanwhile, by the same argument we can show that \( |\tilde{\beta}_i + \tilde{d}_i| < \lambda \iff |\beta_i^0 + d_i^0| < \lambda \), i.e., \( A_0 \subseteq \bar{A} = \{ i : |\tilde{\beta}_i + \tilde{d}_i| \geq \lambda \} \).

Then by the second equation of (2.1) and the definition of soft threshold operator we get \( \vec{d}_A = \lambda \text{sgn}(\vec{d}_A + \vec{\beta}_A) \) which implies \( d_{A_0} = \lambda \text{sgn}(d_{A_0} + \beta_{A_0}) \). This together with the first equation of (2.1) and (2.11) implies

\[
X'_{A_0} X_{A_0} \beta_{A_0} + n d_{A_0} = X'_{A_0} y = X'_{A_0} X_{A_0} \beta_{A_0} + n d_{A_0}.
\]

Then we get \( X'_{A_0} X_{A_0} (\hat{\beta}_{A_0} - \beta_{A_0}) = 0 \), therefore, \( \hat{\beta}_{A_0} = \beta_{A_0} \) follows from the above equation and the assumption that rank(\( X_A \)) = \( |A| \). Let \( B^0 = (A_0)^c \), by (2.9) and the fact \( A \subset A_0 \) we deduce that \( \beta_{B^0} = 0 = \beta_{B_0} \). Hence, \( \hat{\beta} = \beta^1 \). This completes the proof of Theorem 3.3.

In order to prove Lemma 4.1, we need the following two lemmas. Lemma 7.2 collects some property on mutual coherence and Lemma 7.3 states that the effect of the noise \( \eta \) can be controlled with high probability.

**Lemma 7.2.** Let \( A, B \) be disjoint subsets of \( S = 1, 2, ..., p \), with \( |A| = a \), \( |B| = b \). Let \( \nu \) be the mutual coherence of \( X \). Then we have

\[
\|X'_{B} X_{A} u\|_{\infty} \leq n a \nu \|u\|_{\infty}, \quad \forall u \in \mathbb{R}^{|A|}, \tag{A.21}
\]

\[
\|X_{A}\| = \|X'_{A}\| \leq \sqrt{n(1 + (a - 1)\nu)}. \tag{A.22}
\]

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

\[
\|(X'_{A} X_{A}) u\|_{\infty} \geq n(1 - (a - 1)\nu) \|u\|_{\infty}, \tag{A.23}
\]

\[
\|(X'_{A} X_{A})^{-1} u\|_{\infty} \leq \frac{\|u\|_{\infty}}{n(1 - (a - 1)\nu)}, \tag{A.24}
\]

\[
\|(X'_{A} X_{A} - nI) u\|_{\infty} \leq n(1 + (a - 1)\nu) \|u\|_{\infty}. \tag{A.25}
\]

**Proof.** Let \( G = X'X/n \). \( \forall i \in B, |\sum_{j=1}^{a} G_{i,j} u_j| \leq \mu a \|u\|_{\infty} \), which implies (A.21). For any \( i \in A \), by using Gerschgorin’s disk theorem, \( \|G_{A,i} - G_{i,i}\| \leq \sum_{i \neq j=1}^{a} |G_{i,j}| \leq (a - 1)\mu \), i.e., (A.21) holds. Let \( i \in A \) such that \( \|u\|_{\infty} = |u_i| \). (A.23) follows from that \( |\sum_{j=1}^{a} G_{i,j} u_j| \geq |u_i| - \sum_{i \neq j=1}^{a} |G_{i,j}| |u_j| \geq \|u\|_{\infty} - \mu(a - 1)\|u\|_{\infty} \). (A.24) follows directly from (A.23). And (A.25) can be showed similarly as the (A.23). This complete the proof of Lemma 7.2.

**Lemma 7.3.** Suppose (A3) holds. We have

\[
P\left(\|X'\eta\|_{\infty}/n \leq \lambda_n\right) \geq 1 - \frac{1}{2\sqrt{\pi \log(p)}} \tag{A.26}
\]

**Proof.** This inequality follows from standard probabilities calculations.

Recall that \( \lambda_n = \sigma \sqrt{2 \log(p)/n}, \delta_n = 3\lambda_n, \gamma = 8/13, \lambda_0 = \|X'y/n\|_{\infty} \) and \( \lambda_t = \lambda_0 \gamma^t \), \( t = 0, 1, ... \).

**Proof of Lemma 4.1.**
Proof. We first show that under the assumption of Lemma 4.1,

\[ \lambda_1 > 10 \delta_u \]  

(A.27) holds with probability at least \( 1 - \frac{1}{2 \sqrt{\pi \log(p)}} \). In fact,

\[
\begin{align*}
\lambda_1 &= \lambda_0 \gamma \\
&= \frac{8}{13} \|[X'y/n]_\infty = \frac{8}{13} \|[X'(X\beta^\dagger + \eta)/n]_\infty \\
&\geq \frac{8}{13} (\|[X'_{A_1}X_{A_1}^\dagger/n]_\infty - \|[X'\eta/n]_\infty) \\
&\geq \frac{8}{13} ((1 - (T - 1)\nu)\|[\beta^\dagger]_\infty - \lambda_u) \text{ W. H. P.} \\
&> \frac{8}{13} \left( \frac{3}{4} 26 \delta_u - \frac{\delta_u}{3} \right) \\
&> 10 \delta_u
\end{align*}
\]

where the first inequality is the triangle inequality, the second inequality uses Lemma (A.23)-(A.26), and the third one follows uses assumption (A1)-(A2). Here in the third line, "W. H. P." stands for with high probability, that is, with probability at least \( 1 - 1/(2 \sqrt{\pi \log(p)}) \). Then it follow from (A.27) and the definition of \( \lambda_i \) that there exist an integer \( N \in [1, \log_\gamma(10 \delta_u \lambda_0)) \) such that

\[ \lambda_N > 10 \delta_u \geq \lambda_{N+1} \]  

(A.28) holds with high probability. It follows from assumption (A2) and (A.28) that \( \lambda_{N+1} = \lambda_N 8/13 \leq 10 \delta_u \leq |\beta^\dagger|_{\min} 10/26 \), which implies that with high probability \( |\beta^\dagger|_{\min} > 8 \lambda_N /5 \) holds. This complete the proof of Lemma 4.1.

The main idea behind the proof of Theorem 4.1 is that under assumption (A1)-(A3) the active generated by SNAP is contained in the underlying target support and increase in some sense with high probability. To show this we need the following two Lemmas. Lemma 7.4 gives one step error estimations of SNA (Algorithm 1) and Lemma 7.4 shows that some monotone property of the active set.

**Lemma 7.4.** Suppose assumption (A1) holds. Let \( A^k, B^k, \beta^{k+1}, d^{k+1} \) are generated by Sna(\( \beta^0, d^0, \lambda, X, K \)) with \( \lambda > \lambda = \frac{9 \lambda}{10} + \delta_u \). Denote \( E^k = A^\dagger \setminus A^k \) and \( i_k = \{ i \in B^k : |\beta^i| = \|[\beta^i]_\infty \} \). If \( A^k \subset A^\dagger \), then with probability at least \( 1 - \frac{1}{2 \sqrt{\pi \log(p)}} \) we have

\[
\begin{align*}
|\beta^{k+1} + d^{k+1} - \beta^k|_\infty < \frac{1}{3} |\beta^i_k| + \frac{\lambda}{30}, \quad &\text{(A.29)} \\
|\beta^{k+1} + d^{k+1} - \beta^i_k| > |\beta^i_k| - \frac{1}{3} |\beta^i_k| - \frac{\lambda}{30}, &\forall i \in A^k, \quad &\text{(A.30)} \\
|d^{k+1}| < \frac{1}{3} |\beta^i_k| + \frac{\lambda}{30}, \quad &\text{(A.31)} \\
|d^{k+1}| > \frac{2}{3} |\beta^i_k| - \frac{\lambda}{30}. \quad &\text{(A.32)}
\end{align*}
\]
Proof. Since \( \beta^{k+1}, d^{k+1} \) are generated by SNA with \( \lambda > \overline{\lambda} = \frac{9\lambda}{10} + \delta_u, A^k \subset A^\dagger, E^k = A^\dagger \setminus A^k \) and \( y = X_A \beta^\dagger_A + \eta \) we have

\[
\beta^{k+1}_{A^k} = (X'_{A^k} X_{A^k})^{-1}(X'_{A^k} (X_A \beta^\dagger_A + X_{E^k} \beta^\dagger_{E^k} + \eta) - nd^{k+1})
\]

and

\[
\|\beta^{k+1}_{A^k} + d^{k+1}_{A^k} - \beta^\dagger_{A^k}\|_{\infty} \leq \|(X'_{A^k} X_{A^k})^{-1}(X'_{A^k} (X_A \beta^\dagger_A + X_{E^k} \beta^\dagger_{E^k} + \eta) - nd^{k+1})\|_{\infty}
\]

where the first inequality uses (A.33) and the triangle inequality, the second inequality uses (A.21), (A.24) and (A.24), the third inequality uses (A.26), the last inequality uses assumption (A1). Thus, (A.29) holds. Then, (A.30) follows from (A.29) and the triangle inequality. \( \forall i \in B^k, \)

\[
|d^{k+1}_{i_k}| = |X'_i (X_A \beta^\dagger_A - \beta_{A^k}^{k+1} - d_{A^k}^{k+1}) + X_{A^k} d_{A^k}^{k+1} + X_{E^k} \beta_{E^k}^{\dagger}|/n|
\]

where the first equality uses (A.33), the first inequality is the triangle inequality, the second inequality is due to (A.21) and (A.26), and the third inequality uses (A.29), i.e., (A.31) holds. Observing \( i_k \in E^k \) and (A.33) we get

\[
|d^{k+1}_{i_k}| = |X'_i (X_A \beta^\dagger_A - \beta_{A^k}^{k+1} - d_{A^k}^{k+1}) + X_{A^k} d_{A^k}^{k+1} + X_{E^k \setminus i_k} \beta_{E^k \setminus i_k}^{\dagger} + \eta)/n|
\]

where the first inequality is the triangle inequality, the second inequality is due to Lemma (A.21) and (A.26), and the third one uses A.29, i.e., (A.32) holds. This complete the proof of Lemma 7.4. \( \square \)
For a given $\tau > 0$, we define $S_{\lambda, \tau} = \{ i : |\beta_i^\dagger| \geq \lambda \tau \}$.

**Lemma 7.5.** Suppose assumption (A1) hold. Let $\kappa = \frac{\lambda}{3}$ and $\tau = \kappa$ or $\kappa + 1$. Denote $E^k = A^1 \setminus A^k$ and $i_k = \{ i \in B^k : |\beta_i^\dagger| = \|\beta_i^\dagger\|_\infty \}$. If $S_{\lambda, \tau} \subset A^k \subset A^\dagger$ then $S_{\lambda, \tau} \subset A^{k+1} \subset A^\dagger$. Meanwhile, if $S_{\lambda, \kappa+1} \subset A^k \subset A^\dagger$ and $S_{\lambda, \kappa} \not\subset A^k$ then $|\beta_i^\dagger| > |\beta_i^\dagger|$.

**Proof.** Assume $S_{\lambda, \tau} \subset A^k \subset A^\dagger$. Since $E^k = A^1 \setminus A^k$ and $i_k \in E^k$, we get $i_k \not\in A^k$ which implies $|\beta_i^\dagger| < \lambda \tau$. $\forall i \in S_{\lambda, \tau} \subset A^k$. By using (A.30) we have

$$|\beta_i^{k+1} + d_i^{k+1}| > |\beta_i^\dagger| - \frac{1}{3} |\beta_i^\dagger| - \frac{\lambda}{30} > \lambda \tau - \frac{1}{3} \lambda \tau - \frac{\lambda}{30} > \lambda,$$

which implies $i \in A^{k+1}$, i.e., $S_{\lambda, \kappa} \subset A^{k+1}$ holds. $\forall i \in (A^\dagger)^c \subset B^k$. By using (A.31) we get

$$|\beta_i^{k+1} + d_i^{k+1}| = |d_i^{k+1}| < \frac{1}{3} |\beta_i^\dagger| + \frac{\lambda}{30} < \frac{\lambda}{\kappa + 1}, \quad \tau = \kappa + 1,$$

(A.34)

i.e., $i \not\in A^{k+1}$ which implies $A^{k+1} \subset A^\dagger$. Next we turn to the second assertion. Assume $S_{\lambda, \kappa+1} \subset A^k \subset A^\dagger$, $S_{\lambda, \kappa} \not\subset A^k$. It suffice to show all the elements of $|\beta_i|$ that larger than $|\beta_i^\dagger|$ move into $A^{k+1}$. It follows from the definition of $S_{\lambda, \kappa}$, $S_{\lambda, \kappa+1}$ and $i_k \in E^k = A^1 \setminus A^k$ that $i_k \in S_{\lambda, \kappa} \setminus S_{\lambda, \kappa+1}$, i.e., $|\beta_i^\dagger| \in [\lambda \kappa, \lambda (\kappa + 1))$. By using (A.32) we have

$$|\beta_i^{k+1} + d_i^{k+1}| = |d_i^{k+1}| > \frac{2}{3} |\beta_i^\dagger| - \frac{1}{3} \lambda \kappa > \frac{2}{3} \lambda \kappa - \frac{1}{3} \lambda > \lambda,$$

which implies $i_k \in A^{k+1}$. Let $i \in A^k$ satisfy $|\beta_i| \geq |\beta_i^\dagger|$. Then it follows from (A.30) that

$$|\beta_i^{k+1} + d_i^{k+1}| > |\beta_i| - \frac{1}{3} |\beta_i^\dagger| - \frac{\lambda}{30}$$

$$> \frac{2}{3} |\beta_i^\dagger| - \frac{1}{3} \lambda$$

$$> \frac{2}{3} \lambda \kappa - \frac{1}{3} \lambda > \lambda,$$

which implies $i \in A^{k+1}$. This complete the proof of Lemma 7.5. $\square$

**Proof of Theorem 4.1.**

**Proof.** Let $\lambda_t = \frac{a}{2^t} \lambda_t + \delta_t$. By using Lemma 4.1 and the definition of $\lambda_t$ and we get $\lambda_t > \lambda_t, t = 0, 1, \ldots, N$. At the $t_{th}$ knot of Snap($\lambda_t, \gamma, N, K$), suppose it takes Algorithm $\text{Sna}(\beta^0, d^0, \lambda_t, \lambda_t, K)$ iterations to get the solution $(\hat{\beta}(\lambda_t), \hat{d}(\lambda_t))$, where $(\beta^0, d^0) = (\hat{\beta}(\lambda_{t-1}), \hat{d}(\lambda_{t-1}))$ and $k_t \leq K$ by the definition of SNAP. We denote the approximate primal dual solution pair and active set generated in $\text{Sna}(\hat{\beta}(\lambda_{t-1}), \hat{d}(\lambda_{t-1}), \lambda_t, \lambda_t, K)$ by $(\beta^k_t, d^k_t)$ and $A^k_t$, respectively, $k = 0, 1, \ldots, k_t$. By the construction of SNAP we have $(\beta^k_t, d^k_t) = (\hat{\beta}(\lambda_t), \hat{d}(\lambda_t))$, i.e, the solution at the $t_{th}$ stage is the initial value for the $t+1$ stage which implies

$$A_{t}^k \subseteq A_{t+1}^k.$$  

(A.35)
We claim that
\[ S_{\lambda_{t+1}, \kappa+1} \subseteq A_{t+1}^{0} \subseteq A^{\dagger}, \ t = 0, 1, \ldots, N. \] (A.36)

\[ S_{\lambda_{t}, \kappa} \subseteq A_{t}^{k_t} \subseteq A^{\dagger}, \ t = 0, 1, \ldots, N. \] (A.37)

We prove the above two claims by mathematical induction. First we show that \( \emptyset = S_{\lambda_{0}, \kappa+1} \subseteq A_{0}^{0} \subseteq A^{\dagger} \). Let \( |\beta_{i}^{\dagger}| = \| \beta_{i}^{\dagger} \|_{\infty} \).

\[(\kappa + 1)\lambda_{0} = \frac{13}{5} \| X' y / n \|_{\infty} = \frac{13}{5} \| X' (X \beta^{\dagger} + \eta) / n \|_{\infty} \]
\[ \geq \frac{13}{5} (\| X_{A}^{\dagger} X_{A}^{\dagger} \beta_{A_{t}}/n \|_{\infty} - \| X' \eta / n \|_{\infty}) \]
\[ \geq \frac{13}{5} ((1 - (T - 1)\nu) |\beta_{i}^{\dagger}| - \lambda_{u}), \ W.H.P \]
\[ > \frac{3}{4} |\beta_{i}^{\dagger}| - \lambda_{u} \] (A.38)

where the first inequality is the triangle equation and the second inequality uses (A.23) and (A.26), the third inequality uses assumption (A1), and the last inequality is derive from assumption (A2). This implies \( \emptyset = S_{\lambda_{0}, \kappa+1} \). By the construction of \( Snap(\lambda_{0}, \gamma, N, K) \) we get \( A_{0}^{0} = \{ j : |X' j y / n| > \lambda_{0} = \| X' y / n \|_{\infty} \} = \emptyset \). Therefore, (A.36) holds when \( t = 0 \).

Now we suppose (A.36) holds for some \( t \geq 0 \). Then by the first assertion of Lemma 7.5 we get
\[ S_{\lambda_{t}, \kappa+1} \subseteq A_{t}^{k_t} \subseteq A^{\dagger}, \ k = 0, 1, \ldots, k_t. \] (A.39)

By the stopping rule of \( Sna(\beta^{0}, d^0, \lambda_{t}, \lambda_{t}, K) \) it holds either \( A_{t}^{k_t} = A_{t}^{k_{t-1}} \) or \( k_{t} = K \geq T \) when it stops. In both cases, by using (A.39) and the second assertion of Lemma 7.5 we get
\[ S_{\lambda_{t+1}, \kappa+1} \subseteq A_{t+1}^{0} \subseteq A^{\dagger}, \] i.e., (A.37) holds for this given \( t \). Observing the relation \( S_{\lambda_{t+1}, \kappa+1} = S_{\lambda_{t}, \kappa} \) and (A.34)-(A.35) we get \( S_{\lambda_{t+1}, \kappa+1} \subseteq A_{t+1}^{0} \subseteq A^{\dagger} \), i.e., (A.36) holds for \( t + 1 \). Therefore, (A.36) - (A.37) are verified by mathematical induction on \( t \). That is all the active set generated in SNAP is contained in \( A^{\dagger} \). Therefore, by Lemma 4.1 we get
\[ A^{\dagger} \subseteq S_{\lambda_{N}, \kappa} \subseteq A_{N}^{k_N} \subseteq A^{\dagger}, \] i.e.,
\[ \text{supp}(\hat{\beta}(\lambda_{N})) = A^{\dagger}. \] (A.40)
Then,
\[
\|\beta^i - \hat{\beta}(\lambda_N)\|_\infty = \|\beta^i_{A^1} - (X'_{A^1}X_{A^1})^{-1}(\tilde{y}_{A^1} - n\tilde{d}(\lambda_N)A^1)\|_\infty \\
= \|\beta^i_{A^1} - (X'_{A^1}X_{A^1})^{-1}(X'_{A^1}(X_{A^1}\beta^i_{A^1} + \eta) - n\tilde{d}(\lambda_N)A^1)\|_\infty \\
\leq \left\{ X_{A^1}\eta \right\}_\infty + n(\lambda_N - \overline{\lambda}_N) \\
\leq \frac{\lambda_u + \frac{\lambda_N}{10} - 3\lambda_u}{1 - \frac{1}{4}} \text{ W.H.P.}
\]
where the first inequality uses (A.24), the second inequality uses (A.26), and last inequality uses Lemma 4.1, i.e., (4.2) holds. The sign consistency (4.1) follows directly from (A.40), (4.2) and assumption (A2). This complete the proof of Theorem 4.1. □

**C Details in Algorithm 3**

We now describe in detail the quantities in the kth iteration in Algorithm 3. This paves the way for showing that Algorithm 1 is a specialization of Algorithm 3. At \(z^k = (\beta^{k'}, d^{k'})\), we define \(A_k\) and \(B_k\) by (2.8). By a similar reordering of \((\beta^{k'}, d^{k'})\), \(F_1(z^k)\) and \(F_2(z^k)\) as concerning the Newton derivative of \(F\) in Theorem 3.1, and using the definition of \(T_\lambda(\cdot)\), we get

\[
\begin{align*}
z^k = & \left( \begin{array}c d^k_{A_k} \\ \beta^k_{A_k} \\ \beta^k_{B_k} \\ d^k_{B_k} \end{array} \right), \\
F(z^k) = & \begin{bmatrix} -d^k_{A_k} + \lambda \text{sgn}(\beta^k_{A_k} + d^k_{A_k}) \\
\beta^k_{B_k} \\
G_{A_kA_k} \beta^k_{A_k} + G_{A_kB_k} \beta^k_{B_k} + nd^k_{A_k} - \tilde{y}^k_{A_k} \\
G_{B_kA_k} \beta^k_{A_k} + G_{B_kB_k} \beta^k_{B_k} + nd^k_{B_k} - \tilde{y}^k_{B_k} \end{bmatrix}.
\end{align*}
\] (A.41)

Then, by using Theorem 3.1 and noting that \(G_{B_kA_k} = X'_{B_k}X_{A_k}, G_{A_kB_k} = X'_{A_k}X_{B_k}\) we have \(H_k \in \nabla_N F(z^k)\), where

\[
H_k = \begin{bmatrix} -I_{A_kA_k} & 0 & 0 & 0 \\
0 & I_{B_kB_k} & 0 & 0 \\
nI_{A_kA_k} & X'_{A_k}X_{B_k} & G_{A_kA_k} & 0 \\
0 & G_{B_kB_k} & X'_{B_k}X_{A_k} & nI_{B_kB_k} \end{bmatrix}.
\] (A.42)

Algorithm 3 is well defined if we choose \(H_k\) in the form of (A.42), since \(H_k\) is invertible as shown in Theorem 3.1.

In Section 2.1 we derived Algorithm 1 in an intuitive way. We now verify that Algorithm 1 is indeed Algorithm 3 in a form that can be easily and efficiently implemented.
computationally. Let

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

and substitute (A.41) and (A.42) into (3.2) we get

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

(A.43)

$$\beta_{B_k}^k + D_{B_k}^\beta = 0,$$

(A.44)

$$G_{A_k A_k}(\beta_{A_k}^k + D_{A_k}^\beta) = \tilde{y}_{A_k} - n(d_{A_k}^k + D_{A_k}^d) - X'_{A_k} X_{B_k}(\beta_{B_k}^k + D_{B_k}^\beta),$$

(A.45)

$$n(d_{B_k}^k + D_{B_k}^d) = \tilde{y}_{B_k} - X'_{B_k} X_{A_k}(\beta_{A_k}^k + D_{A_k}^\beta) - G_{B_k B_k}(\beta_{B_k}^k + D_{B_k}^\beta).$$

(A.46)

Observing the relationship (by (3.3)),

$$\begin{pmatrix} d_{A_k}^{k+1} \\ \beta_{B_k}^{k+1} \\ \beta_{A_k}^{k+1} \\ d_{B_k}^{k+1} \end{pmatrix} = \begin{pmatrix} d_{A_k}^k + D_{A_k}^d \\ \beta_{B_k}^k + D_{B_k}^\beta \\ \beta_{A_k}^k + D_{A_k}^\beta \\ d_{B_k}^k + D_{B_k}^d \end{pmatrix},$$

and substituting (A.43) - (A.44) into (A.45)-(A.46), we obtain (2.9) - (2.12), which are the computational steps in Algorithm 1.

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