

Support recovery with Stochastic Gates: theory and application for linear models

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Abstract

We analyze the problem of simultaneous estimation and support recovery of the coefficient vector (β^*) in a linear data model with independent and identically distributed Gaussian errors. We study the problem of estimating the model coefficients based on a recently proposed non-convex regularizer, namely the stochastic gates (STG) [YLNK20]. Considering Gaussian design matrices, we show that under reasonable conditions on dimension and sparsity of β^* , the STG-based estimator converges to the true data generating coefficient vector and also detects its support-set with high probability. We propose a new projection-based algorithm that improves upon the existing STG estimator and enjoys theoretical guarantees. Our new procedure outperforms many classical estimators for support recovery in synthetic data analysis.

Keywords: Support recovery, sparsity, feature selection, consistency, non-convex penalty, LASSO, SCAD, orthogonal matching pursuit, stochastic gates, compressed sensing

1 Introduction

We study the following question: given observations from a noisy linear model, how can we recover the positions of the non-zero entries of the unknown model parameter β^* (also known as the *sparsity pattern* or *support-set* [Wai09])? The analysis of the above problem, often referred to as sparse recovery, has seen many uses across fields ranging from theoretical computer science to applied mathematics to digital signal processing. Examples include compressed sensing [Don06], image denoising [EA06, ZY14], manifold learning [GIK10, LSS⁺20] etc. One popular solution for sparse recovery is the Least Absolute Shrinkage and Selection Operator (LASSO) [Tib96, Wai09], which has several extensions, such as [DDFG10, CWB08, WY10]. Recently many authors [SSR⁺19, LS21a, LS21b] have demonstrated that introducing controlled noise in the optimization process can lead to improved model performance. Greedy methods, such as Orthogonal Matching Pursuit (OMP) [TG07], Randomized OMP [EY09a] and their extensions [EY09b, DTDS12, NT09], are also well studied.

Another interesting avenue of research on this topic involves the analysis of non-convex penalties that approximate the sparsity constraints in the objective function. Examples of such

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penalties include the well-known smoothly clipped absolute deviation (SCAD) [FL01, FFW09, XH09, PL09]. Even though estimators based on conventional convex penalties (e.g., LASSO) come with computational benefits, it is shown in many applications that non-convex penalties can yield significantly improved performances (see [MFH11, WCLQ18] for detailed discussions). In recent years many new non-convex penalties have surfaced in the study of sparse Neural Networks [YLNK20, JGP16, MMT16, LWK17]. Estimators based on these new penalties show promising performances in both real and synthetic data analysis. However, theoretical results are sometimes difficult to obtain due to the complex nature of the models and penalties.

Nevertheless, it is interesting to see whether these new penalties provide good theoretical guarantees in the more specific settings of linear models. For the current paper, we are interested in analyzing one such penalized estimator: the stochastic gates (STG) proposed in [YLNK20]. We explore its theoretical aspects in a linear model setup. We show that the STG estimators are consistent for estimating the actual parameter vector even when the dimension of the problem increases with sample size. We also study the STG algorithm, which was previously constructed for feature selection in general non-linear models [YLNK20, Algorithm 1], and improve it for application to linear models by constructing high probability optimal choices for specific parameter updates. The new STG algorithm in linear model setup provides competitive performances compared with other classical methods of support recovery.

The rest of the paper is organized as follows. In Section 1.1 we define our notations and describe the optimization problem. In Section 1.2 we describe the results and new STG algorithm for linear models (termed as Projected STG). The proofs of our results are provided in Section 2. Finally, we end our discussion with simulation studies in Section 3.

1.1 Problem Setting

Let $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]^\top$ be a set of N input vectors of dimension D and suppose that data is generated via the linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}^* + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_N), \quad (1)$$

where \mathbf{I}_N is an identity matrix of dimension N , $\mathcal{N}(0, \sigma^2 \mathbf{I}_N)$ denotes a multivariate Gaussian distribution with mean 0 and covariance $\sigma^2 \mathbf{I}_N$, and σ is assumed to be known. For any vector \mathbf{v} , let $\|\mathbf{v}\|_0$, $\|\mathbf{v}\|_2$ denote the sparsity (i.e., the number of nonzero entries) of \mathbf{v} and the Euclidean norm of \mathbf{v} , respectively. When it is known beforehand that the support-set of $\boldsymbol{\beta}^*$ has at most K elements the optimization problem with squared error loss translates to finding

$$\operatorname{argmin}_{\boldsymbol{\beta}} \frac{\|\mathbf{X}\boldsymbol{\beta} - \mathbf{y}\|_2^2}{N} \quad \text{such that } \|\boldsymbol{\beta}\|_0 \leq K. \quad (2)$$

Due to intractability of the above problem (as it involves discrete search over exponential number of possible parameter vectors, see [Nat95, GJ79] for more details) it is general practice to instead solve some penalized objective that approximates the sparsity constrained problem. The idea of penalization via *gates* uses separate random variables that work as filters on the parameters. Consider the re-parameterization of $\boldsymbol{\beta}$ via random variables $\mathbf{z} = \{z_d\}_{d=1}^D$ which we refer to as gates

$$\beta_d = \theta_d z_d, \quad \theta_d \neq 0, \quad z_d \in [0, 1].$$

As $\|\boldsymbol{\beta}\|_0 = \|\mathbf{z}\|_0$, one considers the following regularized least square formulation of (2) (here $\mathbb{E}_{\mathbf{z}}$ denotes expectation with respect to distribution of \mathbf{z})

$$\mathbb{E}_{\mathbf{z}} \left[\frac{\|\mathbf{X}(\boldsymbol{\theta} \odot \mathbf{z}) - \mathbf{y}\|_2^2}{N} + \lambda_N \|\mathbf{z}\|_0 \right], \quad (3)$$

where \odot denotes the coordinate wise product (also known as the Hadamard product, see [Hor90] for historical uses) and $\lambda_N = \lambda_N(K)$ is some regularization parameter depending on N, K . The optimization of above risk function is done over $\boldsymbol{\theta}$ and the parameters controlling the distribution of \mathbf{z} . Even though Bernoulli distribution seems natural choice for modelling \mathbf{z} , minimization over discrete distributions is difficult and it is natural to consider continuous relaxation of the Bernoulli distribution. Examples of such relaxations include Concrete distribution [JGP16, MMT16], Hard-Concrete distribution [LWK17] etc. In recent work [YLNK20] discussed that the previous two distributions induce high variance in the corresponding Bernoulli approximations and proposed the alternative STG, a differentiable relaxation of Bernoulli gates, given by $\mathbf{z} = \mathbf{z}(\boldsymbol{\mu}) = \{z_d(\mu_d)\}_{d=1}^D$ with

$$z_d(\mu_d) = \max(0, \min(1, \mu_d + \delta_d)), \quad \delta_d \sim \mathcal{N}(0, \tau^2), \quad (4)$$

where $\tau > 0$ is fixed throughout training. The objective in (3) simplifies to

$$\text{Risk}(\boldsymbol{\theta}, \boldsymbol{\mu}; \lambda_N, \tau) = \frac{\mathbb{E}_{\mathbf{z}} [\|\mathbf{y} - \mathbf{X}(\boldsymbol{\theta} \odot \mathbf{z}(\boldsymbol{\mu}))\|_2^2]}{N} + \lambda_N \sum_{d=1}^D \Phi\left(\frac{\mu_d}{\tau}\right) \quad (5)$$

where Φ is the standard normal cumulative distribution function. We minimize the above Risk with respect to $\boldsymbol{\theta}, \boldsymbol{\mu}$.

1.2 Results

The results in this paper also apply to high-dimensional settings where $D = D(N), K = K(N)$ are allowed to grow with N . Let $\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\mu}}$ be a minimizer of (5). We provide guarantees for our final estimator $\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\theta}} \odot \mathbf{z}(\hat{\boldsymbol{\mu}})$ for the settings of Gaussian design matrices. For the setup of fixed design matrix \mathbf{X} , the proofs require conditions on the eigenvalues of $\mathbf{X}^\top \mathbf{X}$, which is outside the scope of this paper. The analysis for fixed setup is not too different from that of the random case; see [HX07] for similar analysis in case of SCAD penalty.

Theorem 1 (Consistency). *Suppose that σ, τ are bounded, $\lim_{N \rightarrow \infty} \frac{D}{N} + K\lambda_N = 0$ and the rows of design matrix \mathbf{X} satisfy $\mathbf{x}_i \stackrel{iid}{\sim} \mathcal{N}(\mathbf{0}, \mathbf{I}_D), i = 1, \dots, N$. Then for any $c > 0$*

$$\lim_{N \rightarrow \infty} \mathbb{P} \left[\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2^2 > c \right] = 0.$$

Theorem 2 (Support recovery). *Suppose that $\boldsymbol{\beta}^*$ has K non-zero entries and let $\max_{i: \beta_i^* \neq 0} |\beta_i^*| > \eta > 0$ for some absolute constant η . Then under the conditions in Theorem 1, the indices of $\hat{\boldsymbol{\beta}}$ with K -largest magnitudes (tie broken arbitrarily) recover the exact support of $\boldsymbol{\beta}^*$ with probability tending to 1.*

Turning to computational aspects we note that the usual algorithm for obtaining minimizer of $\text{Risk}(\boldsymbol{\theta}, \boldsymbol{\mu}; \lambda_N, \tau)$ [YLNK20, Algorithm 1] updates $(\boldsymbol{\theta}, \boldsymbol{\mu})$ via simultaneous gradient descent on the parameters until convergence. Their algorithm was formulated for analyzing general non-linear models. For the special case of linear models, it turns out that at each stage of such updates, instead of changing $\boldsymbol{\theta}$ with a certain gradient step, we can directly find the optimum choice via solving a simple quadratic objective. Additionally, with high probability the optimal choice has a closed-form that is similar to the classical projection-based estimator of $\boldsymbol{\beta}^*$ given by $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$.

Theorem 3. Given fixed $\boldsymbol{\mu}, \mathbf{X}$, the minimizer $\hat{\boldsymbol{\theta}}$ of (5) also minimizes

$$\boldsymbol{\theta}^\top (\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_z [\mathbf{z}(\boldsymbol{\mu}) \mathbf{z}(\boldsymbol{\mu})^\top]) \boldsymbol{\theta} - 2\boldsymbol{\theta}^\top ((\mathbf{X}^\top \mathbf{y}) \odot \mathbb{E}_z [\mathbf{z}(\boldsymbol{\mu})]) .$$

If $\lim_{N \rightarrow \infty} \frac{D}{N} = 0$ then $\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_z [\mathbf{z}(\boldsymbol{\mu}) \mathbf{z}(\boldsymbol{\mu})^\top]$ is invertible with probability tending to 1 and the above quadratic has unique minimizer

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_z [\mathbf{z}(\boldsymbol{\mu}) \mathbf{z}(\boldsymbol{\mu})^\top])^{-1} ((\mathbf{X}^\top \mathbf{y}) \odot \mathbb{E}_z [\mathbf{z}(\boldsymbol{\mu})]) .$$

Our new algorithm uses this improved update method.

Algorithm 1 Projected STG

Input: $\mathbf{X} \in \mathbb{R}^{N \times D}$, $\mathbf{y} \in \mathbb{R}^N$, K, λ_N , number of epochs R , learning rate γ , sample sizes for approximations L . Initialize model parameter $\mu_d = 0.5$ for $d = 1, \dots, D$

Output: Trained parameters $\boldsymbol{\theta}, \boldsymbol{\mu}$ and estimated support-set

- 1: Compute $\mathbf{Q} = \mathbb{E}_z [\mathbf{z}(\boldsymbol{\mu}) \mathbf{z}(\boldsymbol{\mu})^\top]$, $\mathbf{q} = \mathbb{E}_z [\mathbf{z}(\boldsymbol{\mu})]$ numerically
 - 2: Update $\boldsymbol{\theta} := [\mathbf{X}^\top \mathbf{X} \odot \mathbf{Q}]^{-1} [(\mathbf{X}^\top \mathbf{y}) \odot \mathbf{q}]$
 - 3: **for** $\ell = 1, \dots, L$ **do**
 - 4: **for** $d = 1, \dots, D$ **do**
 - 5: Sample $\delta_d^{(\ell)} \sim \mathcal{N}(0, \tau^2)$
 - 6: Compute $z_d^{(\ell)} = \max(0, \min(1, \mu_d + \delta_d^{(\ell)}))$
 - 7: **end for**
 - 8: **end for**
 - 9: Compute $V = \frac{1}{NL} \sum_{\ell=1}^L \|\mathbf{y} - \mathbf{X}(\boldsymbol{\theta} \odot \mathbf{z}^{(\ell)})\|_2^2 + \lambda_N \sum_{d=1}^D \Phi\left(\frac{\mu_d}{\tau}\right)$
 - 10: Update $\boldsymbol{\mu} := \boldsymbol{\mu} - \gamma \nabla_{\boldsymbol{\mu}} V$
 - 11: Repeat R epochs
 - 12: support-set: coordinates of $\boldsymbol{\theta} \odot \mathbf{z}(\boldsymbol{\mu})$ with K highest magnitudes
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Remark 1. The matrix $\mathbf{X}^\top \mathbf{X} \odot \mathbf{Q}$ in the above algorithm is invertible with high probability as Theorem 3 suggests. Otherwise we update $\boldsymbol{\theta}$ by choosing the optimal candidate from the set of minimizers of the quadratic function in Theorem 3.

2 Proof of results

Proof of Theorem 1. We will construct a set \mathbb{S} such that under the given conditions $\mathbb{P}[\mathbb{S}^c] \rightarrow 0$ and $\mathbb{E} \left[\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2^2 \middle| \mathbb{S} \right] \rightarrow 0$. In view of Markov inequality this will imply for every $c > 0$

$$\begin{aligned} \mathbb{P} \left[\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2^2 > c \right] &= \mathbb{P} \left[\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2^2 > c \middle| \mathbb{S} \right] \mathbb{P}[\mathbb{S}] + \mathbb{P} \left[\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2^2 > c \middle| \mathbb{S}^c \right] \mathbb{P}[\mathbb{S}^c] \\ &\leq \frac{\mathbb{E} \left[\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2^2 \middle| \mathbb{S} \right]}{c} + \mathbb{P}[\mathbb{S}^c] \rightarrow 0, \end{aligned}$$

as N tends to infinity.

Let us assume for simplicity that the first K coordinates of $\boldsymbol{\beta}^*$ contain its support and $\sigma = \tau = 1$. Note that any other such choice can be analyzed similarly. For any symmetric matrix \mathbf{A} , define its spectral norm

$$\|\mathbf{A}\|_{\text{sp}} \triangleq \max\{|\rho| : \rho \text{ is an eigenvalue of } \mathbf{A}\}.$$

Define $\mathbb{B} \triangleq \left\{ \mathbf{X} : \left\| \frac{\mathbf{X}^\top \mathbf{X}}{N} - \mathbf{I} \right\|_{\text{sp}} < \frac{1}{4} \right\}$ and choose $\boldsymbol{\mu}^* = (M\mathbf{1}_K, -M\mathbf{1}_{D-K})$ where $\mathbf{1}_a$ is an “a” length vector of all 1’s and M is some arbitrary large number to be chosen later. Then the complement of set \mathbb{B} acquires negligible mass under Gaussian setting, as the following lemma suggests. Concentration bounds similar to this are classical, we provide a proof in Section 2 for completeness.

Lemma 4. *For a Gaussian design matrix \mathbf{X} as in Theorem 1 and any $t > 0, \frac{1}{2} > \xi > 0$*

$$\mathbb{P} \left[\left\| \frac{\mathbf{X}^\top \mathbf{X}}{N} - \mathbf{I} \right\|_{\text{sp}} \geq t \right] \leq 2 \left(\frac{3}{\xi} \right)^D e^{-\frac{Nt^2(1-2\xi)^2}{8}}.$$

In view of above we note the following:

- substituting $t = \xi = \frac{1}{4}$ in Lemma 4 we have $\mathbb{P}[\mathbf{X} \notin \mathbb{B}] \leq 2(12^D)e^{-\frac{N}{c_0}}$ with $c_0 = 512$.
- from Mill’s ratio bound on $\Phi(-M) = 1 - \Phi(M)$ [Gor41]

$$\mathbb{P}[\mathbf{z}(\boldsymbol{\mu}^*) \neq (1_K, 0_{D-K})] \leq D\Phi(-M) \leq \frac{D}{\sqrt{2\pi}M} e^{-\frac{M^2}{2}}.$$

Letting $M \rightarrow \infty$, the last display implies whenever $\frac{D}{N} \rightarrow 0$

$$\mathbb{P}[\{\mathbf{X} \notin \mathbb{B}\} \cup \{\mathbf{z}(\boldsymbol{\mu}^*) \neq (1_K, 0_{D-K})\}] \leq 2 \left(12^{-\frac{D}{N}} e^{\frac{1}{c_0}} \right)^{-N} + \frac{De^{-\frac{M^2}{2}}}{\sqrt{2\pi}M} \rightarrow 0. \quad (6)$$

For the rest of the proof we restrict the design matrix \mathbf{X} on the set \mathbb{B} and fix $\mathbf{z}(\boldsymbol{\mu}^*) = (1_K, 0_{D-K})$. Note that for every $\mathbf{X} \in \mathbb{B}$ the matrix $\mathbf{X}^\top \mathbf{X}$ is invertible [Hal17, Page 52]. Hence using optimality of $\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\mu}}$ and the fact $\boldsymbol{\beta}^* \odot \mathbf{z}(\boldsymbol{\mu}^*) = \boldsymbol{\beta}^*$ we get for each fixed realization of $\mathbf{y}, \boldsymbol{\epsilon}$

$$\begin{aligned} 0 &\geq N \left\{ \text{Risk}(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\mu}}; \lambda_N, 1) - \text{Risk}(\boldsymbol{\beta}^*, \boldsymbol{\mu}^*; \lambda_N, 1) \right\} \\ &\geq \mathbb{E}_{\mathbf{z}} \left[\|\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}\|_2^2 \right] - \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}^*\|_2^2 + N\lambda_N \left(\sum_{d=1}^D \{\Phi(\hat{\boldsymbol{\mu}}) - \Phi(\boldsymbol{\mu}^*)\} \right) \\ &\geq \mathbb{E}_{\mathbf{z}} \left[\|\mathbf{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^*)\|_2^2 - 2\boldsymbol{\epsilon}^\top \mathbf{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^*) \right] - N\lambda_N (K + (D-K)\Phi(-M)) \\ &\geq \mathbb{E}_{\mathbf{z}} \left[\|(\mathbf{X}^\top \mathbf{X})^{\frac{1}{2}}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^*)\|_2^2 - 2\boldsymbol{\epsilon}^\top \mathbf{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^*) \right] - NK\lambda_N - N\frac{\lambda_N De^{-\frac{M^2}{2}}}{\sqrt{2\pi}M} \\ &\geq \mathbb{E}_{\mathbf{z}} \left[\|(\mathbf{X}^\top \mathbf{X})^{\frac{1}{2}}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^*) - (\mathbf{X}^\top \mathbf{X})^{-\frac{1}{2}} \mathbf{X}^\top \boldsymbol{\epsilon}\|_2^2 \right] - \boldsymbol{\epsilon}^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon} - NK\lambda_N - N\frac{\lambda_N De^{-\frac{M^2}{2}}}{\sqrt{2\pi}M}, \end{aligned}$$

and hence using $\|\mathbf{a} + \mathbf{b}\|_2^2 \leq 2(\|\mathbf{a}\|_2^2 + \|\mathbf{b}\|_2^2)$ we get

$$\mathbb{E}_{\mathbf{z}} \|(\mathbf{X}^\top \mathbf{X})^{\frac{1}{2}}(\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}})\|_2^2 \leq 4\boldsymbol{\epsilon}^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon} + NK\lambda_N + N\frac{\lambda_N De^{-\frac{M^2}{2}}}{\sqrt{2\pi}M}. \quad (7)$$

Denote by $\rho_1 > \rho_N > 0$ the extreme eigenvalues of the positive definite matrix $N^{-1}\mathbf{X}^\top \mathbf{X}$. Note that for any matrix \mathbf{A} , ρ is an eigenvalue if and only if $\rho - 1$ is an eigenvalue of $\mathbf{A} - \mathbf{I}$. In view

of this we use $|\sqrt{x} - 1| < |x - 1|$ with $x = \rho_1, \rho_N$ to get

$$\begin{aligned}
\|(\mathbf{X}^\top \mathbf{X})^{\frac{1}{2}}(\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}})\|_2 &\geq \sqrt{N}\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2 - \|((\mathbf{X}^\top \mathbf{X})^{\frac{1}{2}} - \sqrt{N}\mathbf{I})(\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}})\|_2 \\
&\geq \sqrt{N}\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2 \left(1 - \left\|(\mathbf{X}^\top \mathbf{X})^{\frac{1}{2}} - \sqrt{N}\mathbf{I}\right\|_{\text{sp}}\right) \\
&= \sqrt{N}\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2 \left(1 - \max\left\{|\rho_1^{\frac{1}{2}} - 1|, |\rho_N^{\frac{1}{2}} - 1|\right\}\right) \\
&\geq \sqrt{N}\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2 (1 - \max\{|\rho_1 - 1|, |\rho_N - 1|\}) \\
&= \sqrt{N}\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2 \left(1 - \|\mathbf{X}^\top \mathbf{X} - N\mathbf{I}\|_{\text{sp}}\right) \geq \frac{3\sqrt{N}}{4}\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2. \quad (8)
\end{aligned}$$

Using linearity of expectation, $\mathbb{E}_\epsilon[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top] = \mathbf{I}_n$, and commutativity of Trace operator we get that for every $\mathbf{X} \in \mathbb{B}$

$$\begin{aligned}
\mathbb{E}_\epsilon[\boldsymbol{\epsilon}^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon}] &= \mathbb{E}_\epsilon[\text{Trace}(\boldsymbol{\epsilon}^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon})] \\
&= \mathbb{E}_\epsilon[\text{Trace}(\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top)] \\
&= \text{Trace}(\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbb{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top]) = \text{Trace}(\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top) = D.
\end{aligned}$$

In view of (7) and (8) this implies on the set $\mathbb{S} = \{\mathbf{X} \in \mathbb{B}, \mathbf{z}(\boldsymbol{\mu}^*) = (1_K, 0_{D-K})\}$

$$\mathbb{E}[\|\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}}\|_2^2 | \mathbb{S}] \leq \frac{16}{9} \left(\frac{4D}{N} + K\lambda_N + \frac{\lambda_N D e^{-\frac{M^2}{2}}}{\sqrt{2\pi M}} \right).$$

As M is arbitrary, combining the last display with (6) and our assumption $\frac{D}{N} + K\lambda_N \rightarrow 0$, we get the desired result. \square

Proof of Theorem 2. Suppose that the locations of K -largest $\hat{\beta}_i$'s (magnitude wise) do not match the support of β^* . Then there exist two indices i, i' in $\{1, \dots, D\}$ such that $|\hat{\beta}_i| \geq |\hat{\beta}_{i'}|$ (incorporating scenario of ties) and $\beta_i^* = 0, \beta_{i'}^* \neq 0$ (and hence $|\beta_{i'}^*| > \eta$). Then it follows that

- if $|\hat{\beta}_i| \geq \eta/2$ we have $|\hat{\beta}_i - \beta_i^*| > \eta/2$
- if $|\hat{\beta}_i| < \eta/2$ then $\eta/2 > |\hat{\beta}_i|$ and so $|\hat{\beta}_{i'} - \beta_{i'}^*| > \eta/2$.

Combining these we get that unsuccessful recovery implies $\eta/2 \leq \|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^*\|_2$, which occurs with negligible probability by Theorem 1. \square

Proof of Theorem 3. Fix $\boldsymbol{\mu}, \mathbf{X}$ and denote $\mathbf{z}(\boldsymbol{\mu})$ by \mathbf{z} for simplicity. Then the optimal $\boldsymbol{\theta}$ for (5) is given by minimizer of $\mathbb{E}_\mathbf{z}[\|\mathbf{X}(\boldsymbol{\theta} \odot \mathbf{z}) - \mathbf{y}\|_2^2]$ and hence equivalently the minimizer of $\mathbb{E}_\mathbf{z}[(\boldsymbol{\theta}^\top \odot \mathbf{z}^\top)(\mathbf{X}^\top \mathbf{X})(\boldsymbol{\theta} \odot \mathbf{z})] - 2(\boldsymbol{\theta}^\top \odot \mathbb{E}_\mathbf{z}[\mathbf{z}^\top])(\mathbf{X}^\top \mathbf{y})$. We note the followings.

- For any two matrices \mathbf{A}, \mathbf{B} we have $\text{Trace}[\mathbf{AB}] = \text{Trace}[\mathbf{BA}]$ whenever the dimensions agree. In addition if \mathbf{C} is a symmetric matrix then for any i we get $[(\mathbf{A} \odot \mathbf{C})\mathbf{B}]_{ii} = \sum_j \mathbf{A}_{ij} \mathbf{C}_{ij} \mathbf{B}_{ji} = \sum_j \mathbf{A}_{ij} \mathbf{C}_{ji} \mathbf{B}_{ji} = [\mathbf{A}(\mathbf{C} \odot \mathbf{B})]_{ii}$. In view this using linearity of expectation we get

$$\begin{aligned}
\mathbb{E}_\mathbf{z}[(\boldsymbol{\theta}^\top \odot \mathbf{z}^\top)(\mathbf{X}^\top \mathbf{X})(\boldsymbol{\theta} \odot \mathbf{z})] &= \mathbb{E}_\mathbf{z}[\text{Trace}[(\boldsymbol{\theta}^\top \odot \mathbf{z}^\top)(\mathbf{X}^\top \mathbf{X})(\boldsymbol{\theta} \odot \mathbf{z})]] \\
&= \mathbb{E}_\mathbf{z}[\text{Trace}[(\boldsymbol{\theta} \odot \mathbf{z})(\boldsymbol{\theta}^\top \odot \mathbf{z}^\top)(\mathbf{X}^\top \mathbf{X})]] \\
&= \mathbb{E}_\mathbf{z}[\text{Trace}[(\boldsymbol{\theta}\boldsymbol{\theta}^\top \odot \mathbf{z}\mathbf{z}^\top)(\mathbf{X}^\top \mathbf{X})]] \\
&= \text{Trace}[(\boldsymbol{\theta}\boldsymbol{\theta}^\top \odot \mathbb{E}_\mathbf{z}[\mathbf{z}\mathbf{z}^\top])(\mathbf{X}^\top \mathbf{X})] \\
&= \text{Trace}[(\boldsymbol{\theta}\boldsymbol{\theta}^\top)(\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_\mathbf{z}[\mathbf{z}\mathbf{z}^\top])] \\
&= \boldsymbol{\theta}^\top (\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_\mathbf{z}[\mathbf{z}\mathbf{z}^\top]) \boldsymbol{\theta}.
\end{aligned}$$

- For any three vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of same length we have $(\mathbf{a}^\top \odot \mathbf{b}^\top) \mathbf{c} = \sum_i a_i b_i c_i = \mathbf{a}^\top (\mathbf{b} \odot \mathbf{c})$, which means

$$(\boldsymbol{\theta}^\top \odot \mathbb{E}_z[\mathbf{z}^\top]) (\mathbf{X}^\top \mathbf{y}) = \boldsymbol{\theta}^\top ((\mathbf{X}^\top \mathbf{y}) \odot \mathbb{E}_z[\mathbf{z}]).$$

Combining above we conclude that our problem reduces to minimizing

$$\boldsymbol{\theta}^\top (\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_z[\mathbf{z} \mathbf{z}^\top]) \boldsymbol{\theta} - 2\boldsymbol{\theta}^\top ((\mathbf{X}^\top \mathbf{y}) \odot \mathbb{E}_z[\mathbf{z}]) \quad (9)$$

as needed to be shown. Now assume that $\frac{D}{N} \rightarrow 0$. Then it follows from Lemma 4 that $\mathbf{X}^\top \mathbf{X}$ is invertible with probability tending to 1 and hence $\mathbf{X}^\top \mathbf{X}$ is positive definite with high probability as well. Note that $\mathbb{E}_z[\mathbf{z} \mathbf{z}^\top]$ is also positive definite as given any $\mathbf{u} \neq 0$ we have

$$\mathbf{u}^\top \mathbb{E}_z[\mathbf{z} \mathbf{z}^\top] \mathbf{u} = \sum_{d=1}^D u_d^2 \text{Var}(z_d) + (\mathbf{u}^\top \mathbb{E}_z[\mathbf{z}])^2 > 0.$$

Then using Schur's Theorem [Sty73, Theorem 3.1] we get that $\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_z[\mathbf{z} \mathbf{z}^\top]$ is positive definite. For any positive definite matrix \mathbf{A} and vector \mathbf{b} we have

$$\boldsymbol{\theta}^\top \mathbf{A} \boldsymbol{\theta} - 2\boldsymbol{\theta}^\top \mathbf{b} = \|\mathbf{A}^{\frac{1}{2}} \boldsymbol{\theta} - \mathbf{A}^{-\frac{1}{2}} \mathbf{b}\|_2^2 - \|\mathbf{A}^{-\frac{1}{2}} \mathbf{b}\|_2^2,$$

which implies $\boldsymbol{\theta}^\top \mathbf{A} \boldsymbol{\theta} - 2\boldsymbol{\theta}^\top \mathbf{b}$ has unique minimizer $\hat{\boldsymbol{\theta}} = \mathbf{A}^{-1} \mathbf{b}$. Then it follows that (9) has the unique minimizer given by $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top \mathbf{X} \odot \mathbb{E}_z[\mathbf{z} \mathbf{z}^\top])^{-1} ((\mathbf{X}^\top \mathbf{y}) \odot \mathbb{E}_z[\mathbf{z}])$. \square

Proof of Lemma 4. Denote $\mathbf{A} = \frac{\mathbf{X}^\top \mathbf{X}}{N} - \mathbf{I}$ and suppose that it admits spectral decomposition $\mathbf{A} = \sum_{i=1}^D \alpha_i \mathbf{u}_i \mathbf{u}_i^\top$ for eigenvalues $\alpha_1, \dots, \alpha_D$, in decreasing order, and orthonormal eigenvectors $\{\mathbf{u}_i\}_{i=1}^D$. Using the fact $\left\{ \{c_i\}_{i=1}^D : c_i \geq 0, \sum_{i=1}^D c_i = 1 \right\} = \left\{ \{(\mathbf{u}_i^\top \mathbf{w})^2\}_{i=1}^D : \mathbf{w} \in \mathbb{R}^D, \|\mathbf{w}\|_2 = 1 \right\}$, we get

$$\begin{aligned} \|\mathbf{A}\|_{\text{sp}} &= \max \{|\alpha_1|, |\alpha_D|\} \\ &= \sup \left\{ \left| \sum_{i=1}^D \alpha_i c_i \right| : \{c_i\}_{i=1}^D \geq 0, \sum_{i=1}^D c_i = 1 \right\} = \sup_{\|\mathbf{w}\|_2=1} \left| \sum_{i=1}^D \alpha_i (\mathbf{u}_i^\top \mathbf{w})^2 \right| = \sup_{\|\mathbf{w}\|_2=1} |\mathbf{w}^\top \mathbf{A} \mathbf{w}|. \end{aligned} \quad (10)$$

Fix $0 < \xi < \frac{1}{2}$ and let M_ξ be the ξ -packing number of the unit sphere $S^{D-1} = \{\mathbf{w} \in \mathbb{R}^D : \|\mathbf{w}\|_2 = 1\}$, i.e. the largest number for which there exist points $\mathbf{v}_1, \dots, \mathbf{v}_{M_\xi} \in S^{D-1}$ with $\|\mathbf{v}_i - \mathbf{v}_j\|_2 > \xi$ for all $i \neq j$. Thus for any $\mathbf{w} \in S^{D-1}$ we can choose $1 \leq i \leq M_\xi$ with $\|\mathbf{w} - \mathbf{v}_i\|_2 \leq \xi$, which implies

$$\begin{aligned} |\mathbf{w}^\top \mathbf{A} \mathbf{w}| &\leq |(\mathbf{w} - \mathbf{v}_i)^\top \mathbf{A} \mathbf{w}| + |\mathbf{v}_i^\top \mathbf{A} (\mathbf{w} - \mathbf{v}_i)| + |\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i| \\ &\stackrel{(a)}{\leq} \|\mathbf{w} - \mathbf{v}_i\|_2 (\|\mathbf{A} \mathbf{w}\|_2 + \|\mathbf{A} \mathbf{v}_i\|_2) + |\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i| \\ &\leq \xi \left(\sqrt{\mathbf{w}^\top \mathbf{A}^2 \mathbf{w}} + \sqrt{\mathbf{v}_i^\top \mathbf{A}^2 \mathbf{v}_i} \right) + |\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i| \\ &\stackrel{(b)}{\leq} 2\xi \sqrt{\|\mathbf{A}^2\|_{\text{sp}}} + |\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i| \stackrel{(c)}{\leq} 2\xi \|\mathbf{A}\|_{\text{sp}} + |\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i| \end{aligned}$$

where (a) followed by using Cauchy-Schwarz inequality, (b) followed using (10) and (c) followed using definition of spectral norm as eigenvalues of \mathbf{A}^2 are squares of eigenvalues of \mathbf{A} . Taking

supremum over \mathbf{w} in last display, in view of (10) we get $\|\mathbf{A}\|_{\text{sp}} \leq \frac{1}{1-2\xi} \sup_{1 \leq i \leq M_\xi} |\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i|$. By union bound, for any $t > 0$

$$\mathbb{P} \left[\|\mathbf{A}\|_{\text{sp}} > t \right] \leq \sum_{i=1}^{M_\xi} \mathbb{P} \left[|\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i| > (1 - 2\xi)t \right]. \quad (11)$$

As $\{\mathbf{x}_j^\top \mathbf{v}_i\}_{j=1}^N \stackrel{iid}{\sim} \mathcal{N}(0, 1)$ for every unit vector \mathbf{v}_i , we get that $N(\mathbf{v}_i^\top \mathbf{A} \mathbf{v}_i + 1) = \sum_{j=1}^N (\mathbf{x}_j^\top \mathbf{v}_i)^2$ has χ^2 -distribution with N degrees of freedom. For all $1 \leq i \leq M_\xi$ using concentration bound for random variables following χ^2 distribution with N degrees of freedom [Wai19, Example 2.11] and bound on packing number $M_\xi \leq (3/\xi)^D$ (see e.g. [Pol90, Lemma 4.1], [Ver18, Section 4.2]) we continue (11) to get

$$\mathbb{P} \left[\|\mathbf{A}\|_{\text{sp}} > t \right] \leq 2M_\xi e^{-\frac{Nt^2(1-2\xi)^2}{8}} \leq 2(3/\xi)^D e^{-\frac{Nt^2(1-2\xi)^2}{8}}$$

as required. \square

3 Simulation studies

We evaluate the performance guarantees of our algorithm based on the probability of *exact support recovery*, i.e., when the algorithm correctly identifies all non-zero entries of β^* . Once the support is identified, estimating coefficients becomes much less challenging as the number of unknowns becomes relatively smaller. This quantity is estimated over a batch of runs of the algorithm by computing the ratio of the number of exact recovery events to the number of total runs. We consider comparing our method Projected STG (Proj-STG) against LASSO [Tib96], OMP [TG07], Randomized OMP (Rand-OMP) [EY09a] and SCAD [FL01]. The success rate of our method is compared against the algorithms mentioned above in two empirical studies – (a) as the number of data points N grows large, and (b) as the sparsity level K grows large. One should expect that in (a), the target probabilities will grow monotonically to 1 as N grows large, a direct consequence of Theorem 2 when non-zero coordinates of β^* are bounded away from 0. In (b), the success rate should decrease as K takes larger values (keeping everything else fixed) which signifies difficulty recovering sporadic null coordinates when the signal is strong. As we will see below, our simulations identify these behaviors as well.

In both simulations, we fixed $D = 64$ and varied either N or K . For each run, we re-sampled the dataset in the following way. We generated the design matrix $\mathbf{X} \in \mathbb{R}^{N \times D}$ by drawing each of X_{ij} ’s independently from a standard Gaussian distribution. To then generate the signal β^* we first assigned 0 value to $D - K$ randomly chosen coordinates. Next, the nonzero values of β^* were drawn from a symmetric Bernoulli distribution with values 1 or -1 . Finally, the target vector \mathbf{y} is simulated using (1) separately with two different values of $\sigma = 0.5, 1$. We ran 100 simulations of Algorithm 1 with $\tau = 0.5$. We used 20 Monte Carlo samples to approximate the expectations in \mathbf{Q}, \mathbf{q} in Algorithm 1. For updating values of μ , instead of fixed step size (γ in Algorithm 1) we used the Adam optimizer [KB14] which stochastically chooses an improved step size. For LASSO, the regularization parameter is set to $\lambda_{N,0} = \sqrt{\frac{2\sigma^2 \log(D-K) \log(K)}{N}}$ as suggested in [Wai09, Section VII]. For Projected STG, we use the regularization parameter $\lambda_N = C\lambda_{N,0}$, where C is a constant selected using a cross validated grid search in $[0.1, 10]$.

In the first simulation, we fixed $K = \lceil 0.40D^{0.75} \rceil = 10$ (as suggested in [Wai09, Section I(B)]) and varied N within the interval $[10, 100]$. Fig. 1 presents the estimated probabilities of exact support recovery, along with corresponding 90 percent confidence bands (computed via

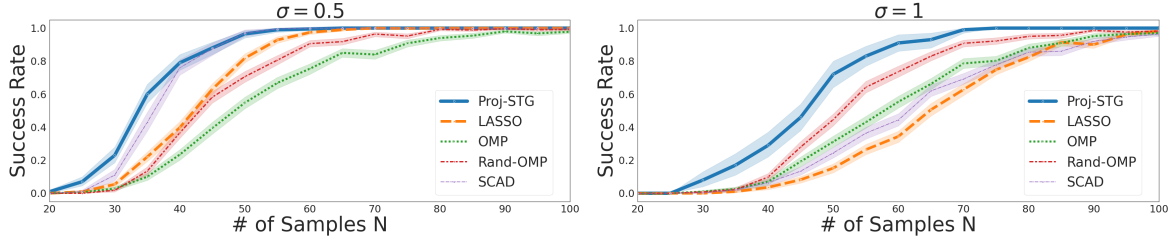


Figure 1: Probability of success in support recovery vs. number of samples.

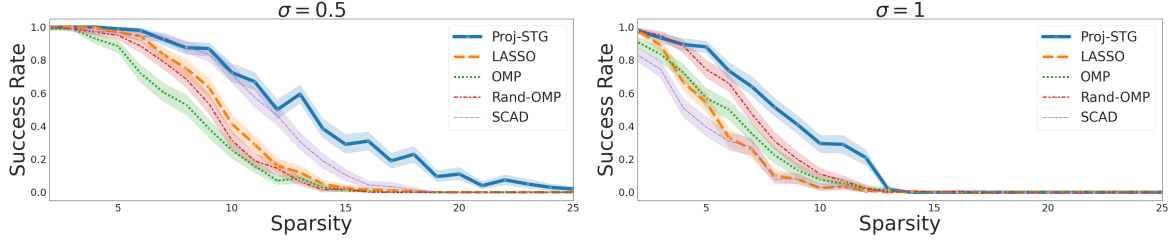


Figure 2: Probability of success in support recovery vs. sparsity level K .

bootstrap), for Projected STG, LASSO, OMP, Rand-OMP, and SCAD. Given any estimate $\hat{\beta}$ we choose K of its coordinates with the largest magnitudes and use it as our estimated support. As demonstrated in this figure, the Projected STG requires fewer samples for perfect support recovery than the alternatives. Moreover, as suggested by these results, our method’s outcomes substantially improve when σ is large (i.e., the signal-to-noise ratio is small).

Next, we investigated the impact of varying the sparsity K on the success rate of the estimators. We retained the same experimental setup as the previous experiment and fixed the number of observations $N = 40$ such that the system is underdetermined (recall that $D = 64$). We varied K within $[1, 25]$. Fig. 2 presents the probability of success along with 90 percent confidence bands (computed via bootstrap). The figure suggests that the proposed model’s outcomes can substantially improve when the sparsity level is high (large values of K).

We also studied how the number of Monte Carlo estimates in our algorithm affects the performance. It was found that for $\sigma = 0.5$, the performances of our algorithm become indistinguishable when the number of estimates is not too small (≥ 8).

Our code has been uploaded at https://github.com/lihenryhfl/projection_stg.

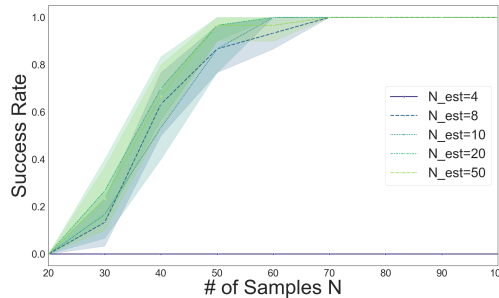


Figure 3: Probability of success vs. number of samples, for Projected STG where we vary the number of Monte Carlo estimators (“N_est”) used for \mathbf{Q} and \mathbf{q} in step 1 of Algorithm 1.

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