Support Recovery for Orthogonal Matching Pursuit
Upper and Lower bounds

Raghav Somani, Chirag Gupta, Prateek Jain and Praneeth Netrapalli

September 24, 2018

Sparse Regression

$$\bar{\mathbf{x}} = \underset{\|\mathbf{x}\|_0 \leq s^*}{\arg\min} f(\mathbf{x}) \tag{1.1}$$

$\mathbf{x} \in \mathbb{R}^d$ and $s^* << d$.
ℓ_0 norm counts the number of non-zero elements.

Applications

- Resource constrained Machine Learning
- High dimensional Statistics
- Bioinformatics

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Sparse Linear Regression (SLR)

- Sparse *Linear* Regression is a representative problem. Results typically extend easily to general case.
- With $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2$, SLR's objective is to find

$$\bar{\mathbf{x}} = \operatorname*{arg\,min}_{\|\mathbf{x}\|_0 \leq s^*} \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2 \tag{2.1}$$

where $\mathbf{A} \in \mathbb{R}^{n \times d}, \mathbf{x} \in \mathbb{R}^d$ and $\mathbf{y} = \mathbb{R}^n$.

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Assumptions of interest

Despite being NP hard, SLR is tractable under certain assumptions.

- **Incoherence** -

  If $\Sigma = A^\top A$, then $\max_{i \neq j} |\Sigma_{ij}| \leq M$

  If $M \leq \frac{1}{2s^* - 1}$ and $y = A\bar{x} \implies \bar{x}$ is unique sparsest solution, and OMP can recover $\bar{x}$ in s^* steps.

- **Restricted Isometry Property (RIP)** -

  $\left\| A_S^\top A_S - I \right\|_2 \leq \delta_{|S|}$ $(\delta_s \leq M(s-1) \quad \forall s \geq 2)$

  $\implies (1 - \delta_s) \|v\|_2^2 \leq \|Av\|_2^2 \leq (1 + \delta_s) \|v\|_2^2 \quad \forall v \text{ s.t. } \|v\|_0 \leq s.$

- **Null space property** -

  $\forall S \in [d] \text{ s.t. } |S| \leq s, \text{ if } v \in \text{Null}(A) \setminus \{0\}, \text{ then } \|v_S\|_1 \leq \|v_{S^c}\|_1$

  $\implies \{v \in \mathbb{R}^d \mid Av = 0\} \cap \{v \in \mathbb{R}^n \mid \|v_{S^c}\|_1 \leq \|v_S\|_1\} = 0$

- **Restricted Strong Convexity (RSC)** -

  $\|Ax - Az\|_2^2 \geq \rho_s^- \|x - z\|_2^2 \ \forall x, z \in \mathbb{R}^d \text{ s.t. } \|x - z\|_0 \leq s$

Incoherence $\implies$ RIP $\implies$ Null space property $\implies$ RSC

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SLR can be modelled as

$$\mathbf{y} = \mathbf{A}\bar{\mathbf{x}} + \boldsymbol{\eta} \tag{2.2}$$

where $\boldsymbol{\eta} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_{n \times n})$, $\operatorname{supp}(\bar{\mathbf{x}}) = \mathbf{S}^*$ and $|\mathbf{S}^*| = s^*$.

$$\implies \mathbf{y} = \mathbf{A}_{\mathbf{S}^*}\bar{\mathbf{x}}_{\mathbf{S}^*} + \boldsymbol{\eta} \tag{2.3}$$

Model with deterministic conditions on η can also be analyzed.

Goals of SLR

1. **Bounding Generalization error** - Upper bound $G(\mathbf{x}) := \frac{1}{n} \|\mathbf{A}(\mathbf{x} - \bar{\mathbf{x}})\|_2^2$ where the rows of A are i.i.d.

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Algorithms to solve SLR

The literature mainly studies 3 classes of algorithms

Existing SLR algorithms

- ℓ_1 minimization based (LASSO based). E.g. - Dantzig selector
- Non-convex penalty based. E.g. - IHT, SCAD penalty, Log-sum penalty
- Greedy methods. E.g. - Orthogonal Matching Pursuit (OMP)

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Orthogonal Matching Pursuit for SLR

Set initial support set $\mathbf{S}_0 = \phi$ & $\mathbf{x}_0 = \mathbf{0}$.

$\therefore$ residual $\mathbf{r}_0 = \mathbf{y} - \mathbf{A}\mathbf{x}_0 = \mathbf{y}$.

At k^{th} iteration ($k \geq 1$)

- From the left-over columns of $\mathbf{A}$ (in $\mathbf{A}_{\mathbf{S}_{k-1}^c}$), find the column with maximum absolute inner product with $\mathbf{r}_{k-1}$.

$$\left[i_j = \arg\max_{i \notin \mathbf{S}_{k-1}} |\langle \mathbf{A}_i, \mathbf{r}_{k-1} \rangle| = \arg\max_{i \notin \mathbf{S}_{k-1}} |\mathbf{A}_i^\top (\mathbf{y} - \mathbf{A}\mathbf{x}_{k-1})| \right]$$

- Include i_j into the set: $\mathbf{S}_k = \mathbf{S}_{k-1} \cup \{i_j\}$.

- Fully optimize on $\mathbf{S}_k$: $\mathbf{x}_k = \arg\min_{\text{supp}(\mathbf{x}) \subseteq \mathbf{S}_k} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2$ (Simple least squares).

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Orthogonal Matching Pursuit for SLR

Set initial support set $\mathbf{S}_0 = \phi$ & $\mathbf{x}_0 = \mathbf{0}$.
$\therefore$ residual $\mathbf{r}_0 = \mathbf{y} - \mathbf{A}\mathbf{x}_0 = \mathbf{y}$.
At k^{th} iteration ($k \geq 1$)

- From the left-over columns of $\mathbf{A}$ (in $\mathbf{A}_{\mathbf{S}_{k-1}^c}$), find the column with maximum absolute inner product with $\mathbf{r}_{k-1}$.

$$\left[\; |\langle \mathbf{A}_{i_1}, \mathbf{r}_{k-1} \rangle| \;\; |\langle \mathbf{A}_{i_2}, \mathbf{r}_{k-1} \rangle| \; \ldots \; \left|\langle \mathbf{A}_{i_j}, \mathbf{r}_{k-1} \rangle\right| \; \ldots \; \left|\langle \mathbf{A}_{i_{d-k+1}}, \mathbf{r}_{k-1} \rangle\right| \;\right]$$

- Include i_j into the set: $\mathbf{S}_k = \mathbf{S}_{k-1} \cup \{i_j\}$.
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Orthogonal Matching Pursuit for SLR

Result: OMP sparse estimate $\hat{\mathbf{x}}_s^{\mathsf{OMP}} = \mathbf{x}_s$

$\mathbf{S}_0 = \phi$, $\mathbf{x}_0 = \mathbf{0}$, $\mathbf{r}_0 = \mathbf{y}$

for $k = 1, 2, \ldots, s$ **do**

$\quad j \leftarrow \underset{i \notin \mathbf{S}_{k-1}}{\arg\max} |\mathbf{A}_i^T \mathbf{r}_{k-1}|$ (Greedy selection)

$\quad \mathbf{S}_k \leftarrow \mathbf{S}_{k-1} \cup \{j\}$

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Algorithm 1: Orthogonal Matching Pursuit (OMP) for SLR

Note that $\mathbf{A}_i^T \mathbf{r}_{k-1} \propto [\nabla f(\mathbf{x}_{k-1})]_i$ for $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2$

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Orthogonal Matching Pursuit for general $f(\mathbf{x})$

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Algorithm 2: OMP for a general function $f(\mathbf{x})$

Key quantities

- Restricted Smoothness (ρ^+) & Restricted Strong Convexity (ρ^-)

$$\rho_s^- \|\mathbf{x} - \mathbf{z}\|_2^2 \leq \|\mathbf{A}\mathbf{x} - \mathbf{A}\mathbf{z}\|_2^2 \leq \rho_s^+ \|\mathbf{x} - \mathbf{z}\|_2^2 \tag{4.1}$$

$\forall\, \mathbf{x}, \mathbf{z} \in \mathbb{R}^d$ s.t. $\|\mathbf{x} - \mathbf{z}\|_0 \leq s$.

- Restricted condition number ($\widetilde{\kappa}_s$)

$$\widetilde{\kappa}_s = \frac{\rho_1^+}{\rho_s^-} \tag{4.2}$$

- We also define

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Lower bounds for Fast rates

- If $\hat{\mathbf{x}}_{\ell_0}$ is the best ℓ_0 estimate in the set of s^*-sparse vectors then one can show

$$\sup_{\|\bar{\mathbf{x}}\|_0 \leq s^*} \frac{1}{n} \mathbb{E}\left[\|\mathbf{A}(\hat{\mathbf{x}}_{\ell_0} - \bar{\mathbf{x}})\|_2^2\right] \lesssim \frac{\sigma^2 s^*}{n} \tag{4.4}$$

- Non-tractable since computing $\hat{\mathbf{x}}_{\ell_0}$ involves searching all $\binom{d}{s^*}$ subsets.
- (Y. Zhang, Wainwright & Jordan'15) $\exists \mathbf{A} \in \mathbb{R}^{n \times d}$ s.t. any poly-time algorithm satisfies

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Consequence - Any estimator $\hat{\mathbf{x}}$ achieving fast rate must either **not be poly-time** or must return $\hat{\mathbf{x}}_{\text{poly}}$ that is **not** s^*-sparse.

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Upper bounds on Generalization error

- Tightest known upper bounds for poly-time algorithms like IHT, OMP and Lasso were at least $\widetilde{\kappa}$ times worse than known lower bounds (Jain'14, T. Zhang'10, Y. Zhang'17).

- (T. Zhang'10) If $\hat{\mathbf{x}}_s$ be the output of OMP after $s \gtrsim s^* \widetilde{\kappa}_{s+s^*} \log \kappa_{s+s^*}$ iterations, then with high probability

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Support Recovery upper bound

- Support recovery results are known for SCAD/MCP penalty based methods under bounded incoherence (Loh'14).
- For greedy algorithms like HTP and PHT, known support recovery results require poor dependence of $\widetilde{\kappa}$ on $|\bar{x}_{\min}|$ (Shen'17).
- If S is the support set of the sth OMP iterate $\hat{x}_s$, and if $S^* \setminus S \neq \phi$, then there is a **large additive decrease** in objective if $|\bar{x}_{\min}|$ is larger than the appropriate noise level.

Large decrease in objective

If $\hat{x}_s$ is the output of OMP after $s \gtrsim s^* \widetilde{\kappa}_{s+s^*} \log \kappa_{s+s^*}$ iterations s.t. $S^* \setminus S \neq \phi$ and $|\bar{x}_{\min}| \gtrsim \frac{\sigma \gamma \sqrt{\rho_1^+}}{\rho_{s+s^*}}$ then with high probability

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where $\left\| \mathbf{A}_{\mathbf{S}^* \setminus \mathbf{S}}^T \mathbf{A}_{\mathbf{S}} \left(\mathbf{A}_{\mathbf{S}}^T \mathbf{A}_{\mathbf{S}} \right)^{-1} \right\|_\infty \leq \gamma$ and $\mathbf{S} = \operatorname{supp}(\hat{\mathbf{x}}_s)$.

γ is similar to standard incoherence condition.

Support Recovery upper bound

- Support recovery results are known for SCAD/MCP penalty based methods under bounded incoherence (Loh'14).
- For greedy algorithms like HTP and PHT, known support recovery results require poor dependence of $\widetilde{\kappa}$ on $|\bar{x}_{\min}|$ (Shen'17).
- If $\mathbf{S}$ is the support set of the sth OMP iterate $\hat{\mathbf{x}}_s$, and if $\mathbf{S}^* \setminus \mathbf{S} \neq \phi$, then there is a **large additive decrease** in objective if $|\bar{x}_{\min}|$ is larger than the appropriate noise level.

Large decrease in objective

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Since $\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2 \geq 0 \; \forall \; \mathbf{x} \in \mathbb{R}^d$, the number of extra iterations cannot be too large.

Support recovery and infinity norm bound

If $\hat{\mathbf{x}}_s$ is the output of OMP after $s \gtrsim s^* \widetilde{\kappa}_{s+s^*} \log \kappa_{s+s^*}$ iterations, s.t. $|\bar{x}_{\min}| \gtrsim \frac{\sigma \gamma \sqrt{\rho_1^+}}{\rho_{s+s^*}^-}$, then with high probability

1. $\mathbf{S}^* \subseteq \mathsf{supp}(\hat{\mathbf{x}}_s)$
2. $\|\hat{\mathbf{x}}_s - \bar{\mathbf{x}}\|_\infty \lesssim \sigma \sqrt{\frac{\log s}{\rho_s}}$

where $\left\| \mathbf{A}_{\mathbf{S}^* \backslash \mathbf{S}}^T \mathbf{A}_{\mathbf{S}} \left(\mathbf{A}_{\mathbf{S}}^T \mathbf{A}_{\mathbf{S}} \right)^{-1} \right\|_\infty \leq \gamma$ and $\mathbf{S} = \mathsf{supp}(\hat{\mathbf{x}}_s)$.

- Condition on $|\bar{x}_{\min}|$ scales as $\frac{1}{\sqrt{n}}$ since both $\rho_{s+s^*}^-$ and ρ_1^+ have a factor of n. Also it is better by at-least $\sqrt{\kappa}$ than that in other recent works.
- γ is allowed to be very large.

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Lower bound instance construction

- (Y. Zhang'15)'s lower bounds were for algorithms that output s^*-sparse solutions which does not apply for OMP when it is run for more than s^* iterations.

- We provide matching lower bounds for Support recovery as well as generalization error for OMP.

- Fool OMP into picking incorrect indexes. Large support size $\implies$ large generalization error.

- Construct an evenly distributed $\bar{x}$

$$\bar{x}_i = \begin{cases} \frac{1}{\sqrt{s^*}} & \text{if } 1 \le i \le s^* \\ 0 & \text{if } i > s^* \end{cases} \implies \text{supp}(\bar{x}) = \{1, 2, \ldots, s^*\}$$

- Construct $\mathrm{M}^{(\epsilon)} \in \mathbb{R}^{n \times d}$ parameterized by ϵ

  - $\mathrm{M}^{(\epsilon)}_{1:s^*}$ are random s^* orthogonal column vectors s.t. $\left\| \mathrm{M}^{(\epsilon)}_i \right\|_2^2 = n \ \forall \ i \in [s^*]$.

  - $\mathrm{M}^{(\epsilon)}_i = \sqrt{1-\epsilon} \left[\frac{1}{\sqrt{s^*}} \sum_{j=1}^{s^*} \mathrm{M}^{(\epsilon)}_j \right] + \sqrt{\epsilon} \mathrm{g}_i \ \forall \ i \notin [s^*]$ where g_i's are orthogonal to each other and $\mathrm{M}^{(\epsilon)}_{1:s^*}$ with $\|\mathrm{g}_i\|_2^2 = n$.

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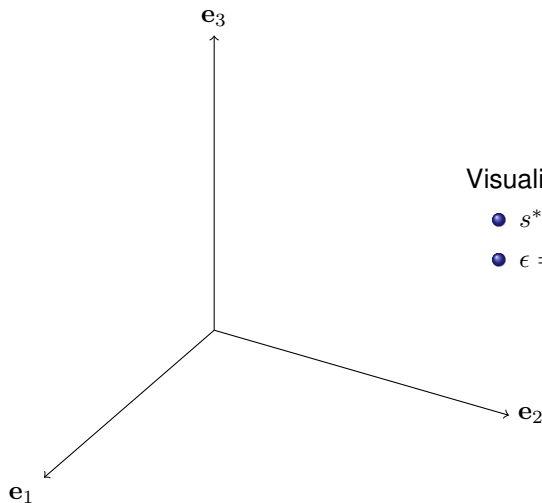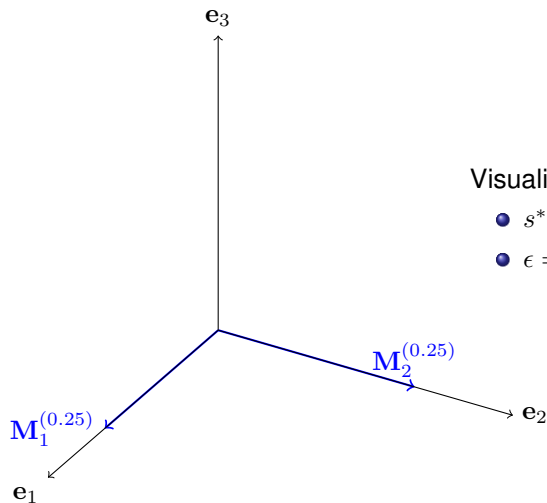
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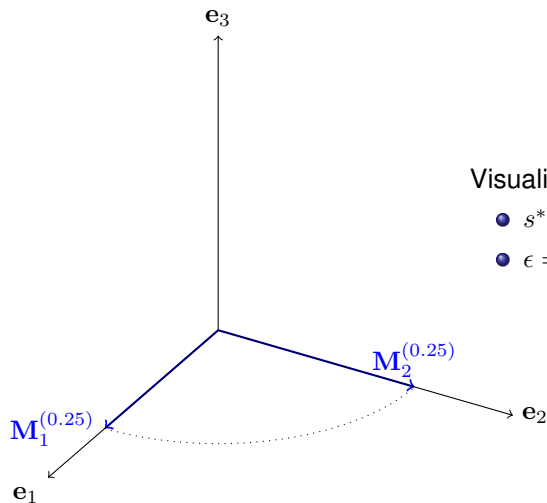
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Visualizing in $d = 3$ with
- $s^* = 2$
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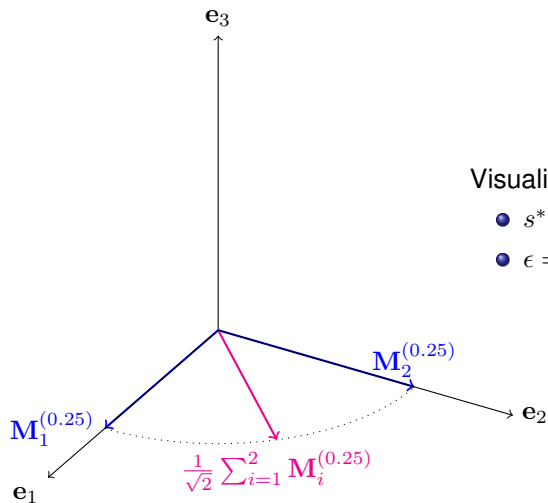
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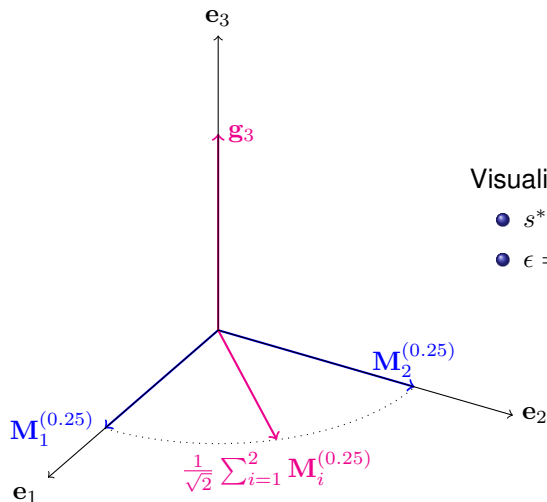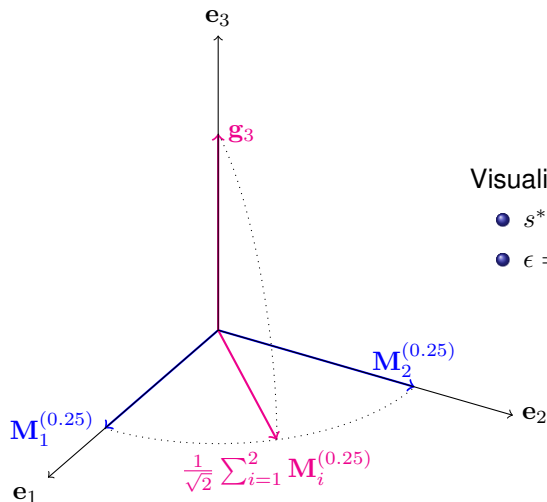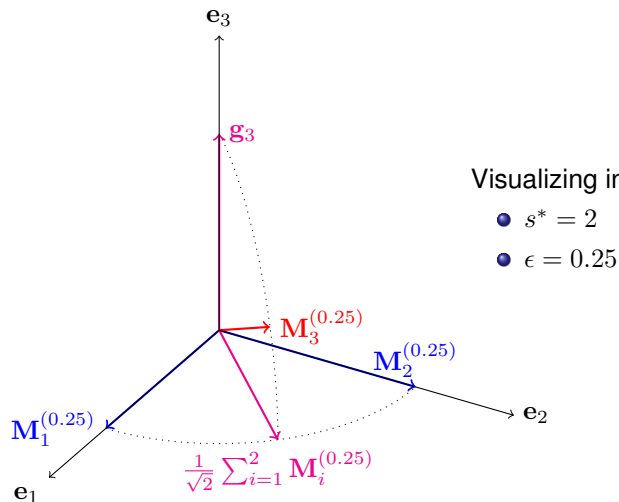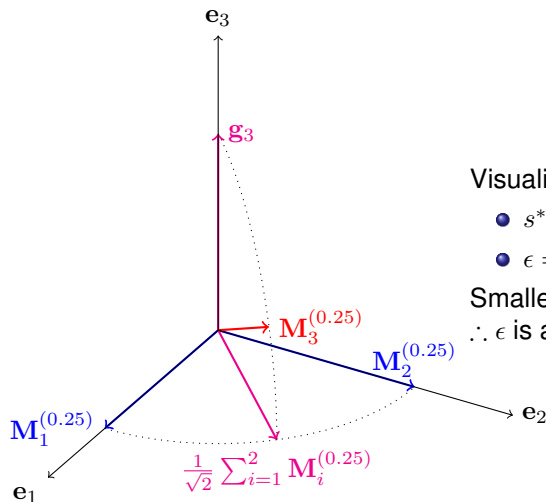
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$\mathbf{e}_3$

$\mathbf{e}_2$

$\mathbf{e}_1$

$\mathbf{M}_1^{(0.25)}$

$\mathbf{M}_2^{(0.25)}$

$\frac{1}{\sqrt{2}} \sum_{i=1}^{2} \mathbf{M}_i^{(0.25)}$

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Smaller $\epsilon \implies$ more correlation.
$\therefore \epsilon$ is a proxy for $\widetilde{\kappa}_s$.

Lower bounds

Noiseless case

For $s^* \leq d \leq n$, $\exists \, \epsilon > 0$ s.t. when OMP is executed on SLR problem with $y = \mathbf{M}^{(\epsilon)}\bar{\mathbf{x}}$ for $s \leq d - s^*$ iterations

- $\widetilde{\kappa}_s(\mathbf{M}^{(\epsilon)}) \lesssim \frac{s}{s^*}$ and $\gamma \leq \sqrt{\frac{2}{3}}$

- $\mathbf{S}^* \cap \mathsf{supp}(\hat{\mathbf{x}}_s) = \phi$

Noisy case

For $s^* \leq s \leq d^{1-\alpha}$ where $\alpha \in (0, 1)$, $\exists \, \epsilon > 0$ s.t. when OMP is executed on SLR problem with $y = \mathbf{M}^{(\epsilon)}\bar{\mathbf{x}} + \boldsymbol{\eta}$ where $\boldsymbol{\eta} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 \mathbf{I}_{n \times n}\right)$, then

- $\widetilde{\kappa}_s(\mathbf{M}^{(\epsilon)}) \lesssim \frac{s}{s^*}$ and $\gamma \leq \frac{1}{2}$

- with high probability $\frac{1}{n} \|\mathbf{A}\hat{\mathbf{x}}_s - \mathbf{A}\bar{\mathbf{x}}\|_2^2 \gtrsim \frac{1}{n}\sigma^2\widetilde{\kappa}_{s+s^*} s^*$

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$\implies s \gtrsim \widetilde{\kappa}_s s^*$ iterations are indeed necessary.
Addition of noise can only help.

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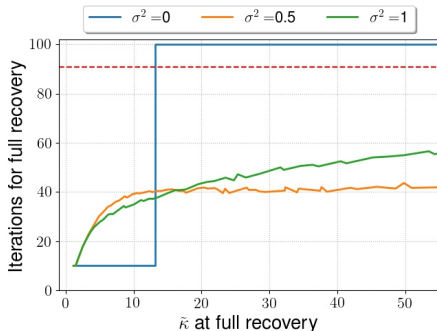- with high probability $\mathbf{S}^* \cap \mathsf{supp}(\hat{\mathbf{x}}_s) = \phi$

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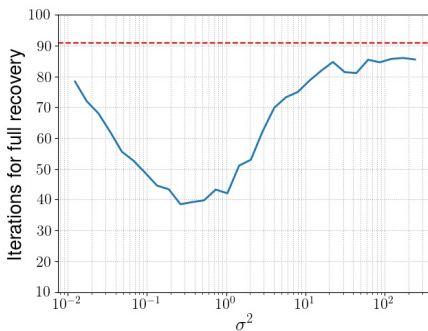Addition of noise can only help.

Simulations

We perform simulations on the lower bound instance class.
$\mathbf{M}^{(\epsilon)} \in \mathbb{R}^{1000 \times 100}$ and $s^* = 10$.

(a) Varying condition number

(b) Varying noise variance

Figure: Number of iterations required for recovering the full support of $\bar{\mathbf{x}}$ with respect to the restricted condition number ($\widetilde{\kappa}_{s+s^*}$) of design matrix and the variance of noise (σ^2).