

Support Recovery for Orthogonal Matching Pursuit

Upper and Lower bounds

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Sparse Regression

$$\bar{\mathbf{x}} = \arg \min_{\|\mathbf{x}\|_0 \leq s^*} f(\mathbf{x}) \quad (1.1)$$

$\mathbf{x} \in \mathbb{R}^d$ and $s^* \ll d$.

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 $f(\mathbf{x}) = \|\mathbf{Ax} - \mathbf{y}\|_2^2$, SLR's objective is to find

$$\bar{\mathbf{x}} = \arg \min_{\|\mathbf{x}\|_0 \leq s^*} \|\mathbf{Ax} - \mathbf{y}\|_2^2 \quad (2.1)$$

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

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Assumptions of interest

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

- **Incoherence** -

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

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

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

$$\|\mathbf{A}_S^T \mathbf{A}_S - \mathbf{I}\|_2 \leq \delta_{|S|} \quad (\delta_s \leq M(s-1) \quad \forall s \geq 2)$$

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

- **Null space property** -

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

$$\implies \{\mathbf{v} \in \mathbb{R}^d \mid \mathbf{A}\mathbf{v} = 0\} \cap \{\mathbf{v} \in \mathbb{R}^d \mid \|\mathbf{v}_{S^c}\|_1 \leq \|\mathbf{v}_S\|_1\} = \{0\}$$

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

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

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Goals of SLR

SLR can be modelled as

$$\mathbf{y} = \mathbf{A}\bar{\mathbf{x}} + \boldsymbol{\eta} \quad (2.2)$$

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

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

Model with deterministic conditions on $\boldsymbol{\eta}$ can also be analyzed.

Goals of SLR

- **Bounding Generalization error** - Upper bound $G(\mathbf{x}) := \frac{1}{n} \|\mathbf{A}(\mathbf{x} - \bar{\mathbf{x}})\|_2^2$ where the rows of \mathbf{A} are i.i.d.
- **Support Recovery** - Recover the true features of \mathbf{A} , i.e., find a $\mathbf{S} \supseteq \mathbf{S}^*$.

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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 $S_0 = \emptyset$ & $\mathbf{x}_0 = \mathbf{0}$.

\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 $\mathbf{A}_{S_{k-1}^c}$), find the column with maximum absolute inner product with \mathbf{r}_{k-1} .

$$[|(\mathbf{A}_{i_1, S_{k-1}^c} \mathbf{r}_{k-1})| \quad |(\mathbf{A}_{i_2, S_{k-1}^c} \mathbf{r}_{k-1})| \quad \dots \quad |(\mathbf{A}_{i_j, S_{k-1}^c} \mathbf{r}_{k-1})| \quad \dots \quad |(\mathbf{A}_{i_{n-k+1}, S_{k-1}^c} \mathbf{r}_{k-1})|]$$

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

- Include i_j into the set: $S_k = S_{k-1} \cup \{i_j\}$.
- Fully optimize on S_k : $\mathbf{x}_k = \arg \min_{\text{supp}(\mathbf{x}) \subseteq S_k} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2$ (Simple least squares).
- Update residual: $\mathbf{r}_k = \mathbf{y} - \mathbf{A}\mathbf{x}_k$.

Orthogonal Matching Pursuit for SLR

Set initial support set $S_0 = \phi$ & $\mathbf{x}_0 = \mathbf{0}$.

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Orthogonal Matching Pursuit for SLR

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

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

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

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

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

$\mathbf{x}_k \leftarrow \arg \min_{\text{supp}(\mathbf{x}) \subseteq \mathbf{S}_k} \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2^2$

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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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$\mathbf{x}_k := \arg \min_{\text{supp}(\mathbf{x}) \subseteq \mathbf{S}_k} f(\mathbf{x})$

end

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

Key quantities

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

$$\rho_s^- \|\mathbf{x} - \mathbf{z}\|_2^2 \leq \|\mathbf{Ax} - \mathbf{Az}\|_2^2 \leq \rho_s^+ \|\mathbf{x} - \mathbf{z}\|_2^2 \quad (4.1)$$

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

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

$$\tilde{\kappa}_s = \frac{\rho_1^+}{\rho_s^-} \quad (4.2)$$

- 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

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

- 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

$$\sup_{\|\bar{\mathbf{x}}\|_0 \leq s^*} \frac{1}{n} \mathbb{E} \left[\|\mathbf{A}(\hat{\mathbf{x}}_{\text{poly}} - \bar{\mathbf{x}})\|_2^2 \right] \gtrsim \frac{\sigma^2 s^{*1-\delta} \tilde{\kappa}_{s^*}}{n} \quad \forall \delta > 0 \quad (4.5)$$

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 $\tilde{\kappa}$ 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 $s \gtrsim s^* \tilde{\kappa}_{s+s^*} \log \kappa_{s+s^*}$ 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 $\tilde{\kappa}$ on $|\bar{x}_{\min}|$ (Shen'17).
- If S is the support set of the s^{th} OMP iterate \hat{x}_s , and if $S^* \setminus S \neq \emptyset$, 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 $s \gtrsim s^* \tilde{\kappa}_{s+s^*} \log \kappa_{s+s^*}$ iterations s.t. $S^* \setminus S \neq \emptyset$ and $|\bar{x}_{\min}| \gtrsim \frac{\sigma \gamma \sqrt{\rho_1^+}}{\rho_{s+s^*}^-}$ then with high probability

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

γ is similar to standard incoherence condition.

Support Recovery upper bound

Since $\|\mathbf{Ax} - \mathbf{y}\|_2^2 \geq 0 \forall \mathbf{x} \in \mathbb{R}^d$, 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 $s \gtrsim s^* \tilde{\kappa}_{s+s^*} \log \kappa_{s+s^*}$ iterations, s.t.

$|\bar{x}_{\min}| \gtrsim \frac{\sigma \gamma \sqrt{\rho_1^+}}{\rho_{s+s^*}^-}$, then with high probability

$$1 \quad \mathbf{S}^* \subseteq \text{supp}(\hat{\mathbf{x}}_s)$$

$$2 \quad \|\hat{\mathbf{x}}_s - \bar{\mathbf{x}}\|_\infty \lesssim \sigma \sqrt{\frac{\log s}{\rho_s^-}}$$

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- 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 $\sqrt{\tilde{\kappa}}$ 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 $\bar{\mathbf{x}}$

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

- Construct $\mathbf{M}^{(\epsilon)} \in \mathbb{R}^{n \times d}$ parameterized by ϵ
 - $\mathbf{M}_{1:s^*}^{(\epsilon)}$ are random s^* orthogonal column vectors s.t. $\|\mathbf{M}_i^{(\epsilon)}\|_2^2 = n \ \forall i \in [s^*]$.
 - $\mathbf{M}_i^{(\epsilon)} = \sqrt{1-\epsilon} \left[\frac{1}{\sqrt{s^*}} \sum_{j=1}^{s^*} \mathbf{M}_j^{(\epsilon)} \right] + \sqrt{\epsilon} \mathbf{g}_i \ \forall i \notin [s^*]$ where \mathbf{g}_i 's are orthogonal to each other and $\mathbf{M}_{1:s^*}^{(\epsilon)}$ with $\|\mathbf{g}_i\|_2^2 = n$.

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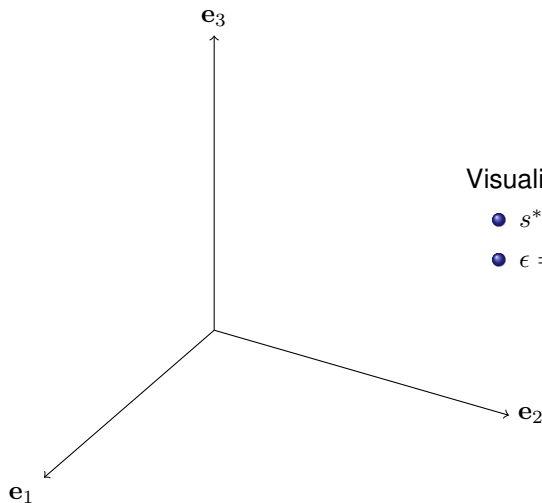
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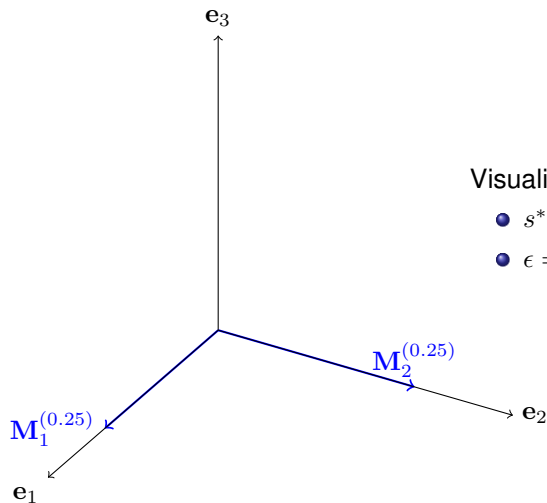
Lower bound instance construction



Visualizing in $d = 3$ with

- $s^* = 2$
- $\epsilon = 0.25$

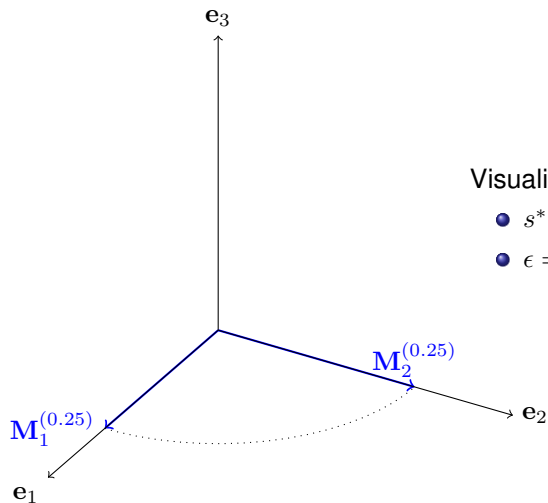
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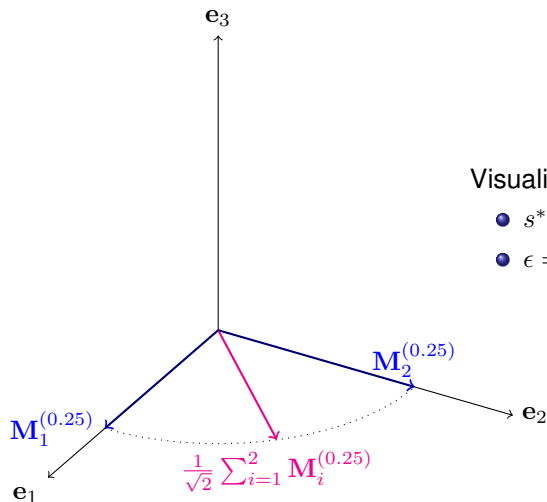
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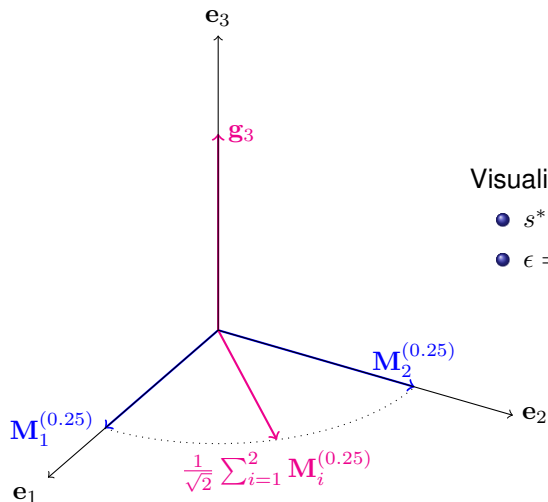
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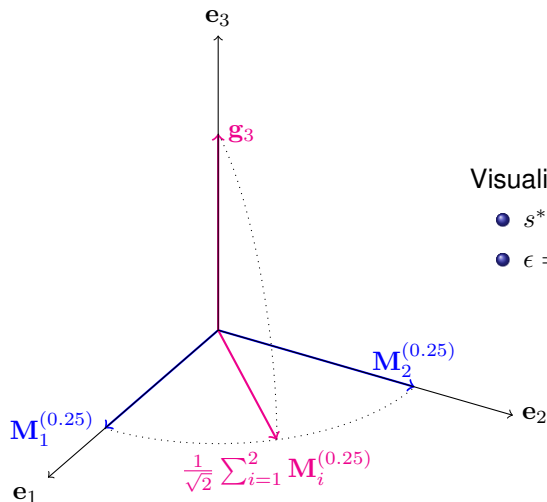
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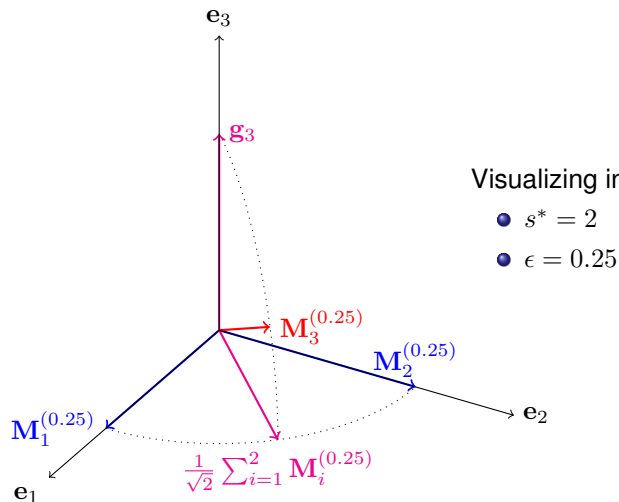
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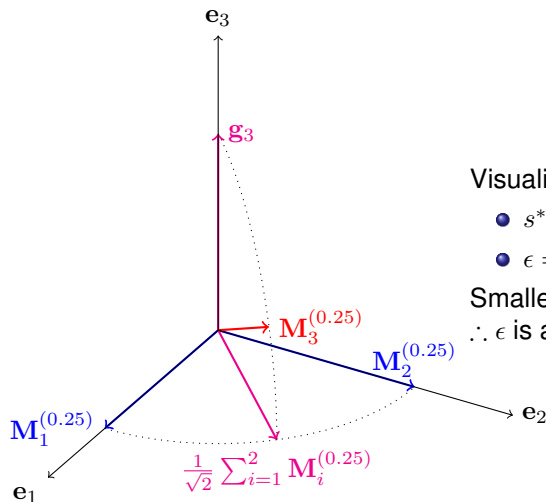
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Smaller $\epsilon \implies$ more correlation.

$\therefore \epsilon$ is a proxy for $\tilde{\kappa}_s$.

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

- $\tilde{\kappa}_s(\mathbf{M}^{(\epsilon)}) \lesssim \frac{s}{s^*}$ and $\gamma \leq \sqrt{\frac{3}{2}}$
- $\mathbf{S}^* \cap \text{supp}(\hat{\mathbf{x}}_s) = \emptyset$

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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 $\boldsymbol{\eta} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_{n \times n})$, then

- $\tilde{\kappa}_s(\mathbf{M}^{(\epsilon)}) \lesssim \frac{s}{s^*}$ and $\gamma \leq \frac{1}{2}$
- with high probability $\frac{1}{n} \|\mathbf{A} \hat{\mathbf{x}}_s - \mathbf{A} \bar{\mathbf{x}}\|_2^2 \gtrsim \frac{1}{n} \sigma^2 \tilde{\kappa}_{s+s^*} s^*$
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$\implies s \gtrsim \tilde{\kappa}_s s^*$ iterations are indeed necessary.

Addition of noise can only help.

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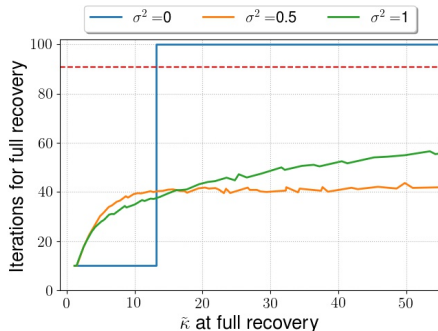
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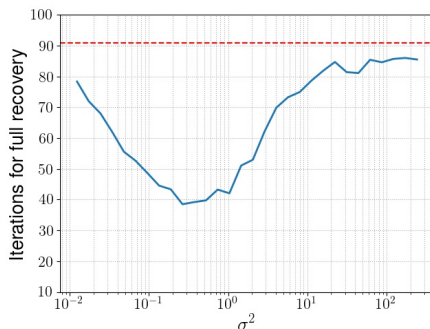
Simulations

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 ($\tilde{\kappa}_{s+s^*}$) of design matrix and the variance of noise (σ^2).