

Inria



ENS DE LYON

Towards **Compressive Recovery** of **Sparse Precision Matrices**

Titouan Vayer

joint work with

Rémi Gribonval

Paulo Gonçalves

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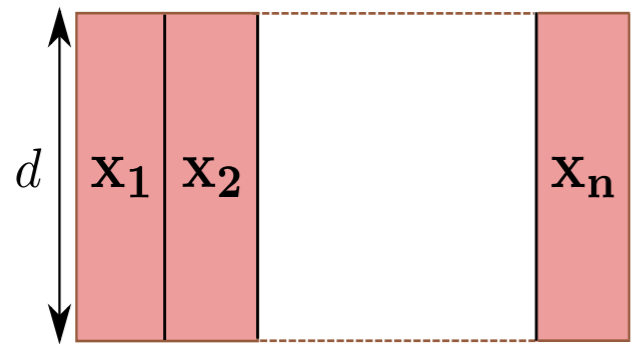
| Overview of the talk

- Part I: **Finding graphs from unstructured data**
- Part II: **The sketching approach**
- Part III: **Algorithmic solution**
- Part IV: **Limits, Open questions, partial answers**

| Graph Learning

■ Input: a dataset

$$\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$$

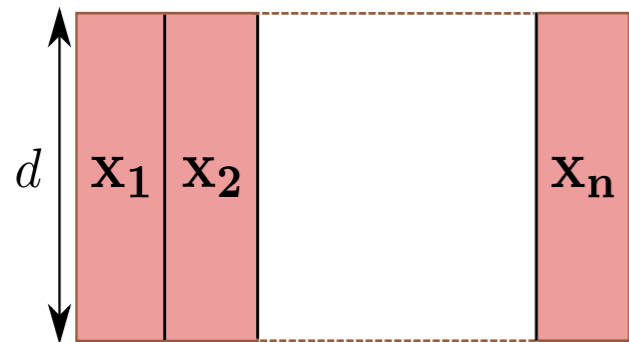


$$\mathbf{x}_i \in \mathbb{R}^d \sim \mu$$

Graph Learning

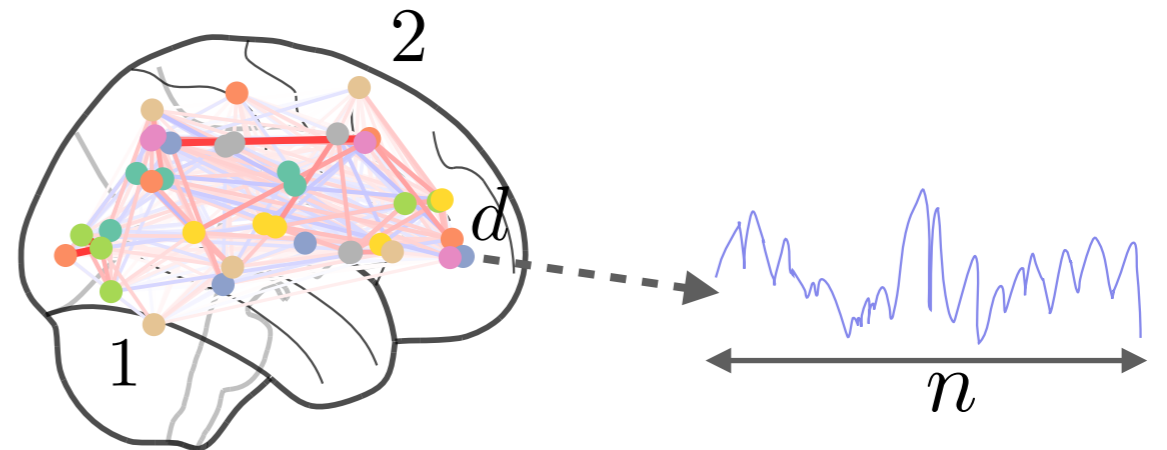
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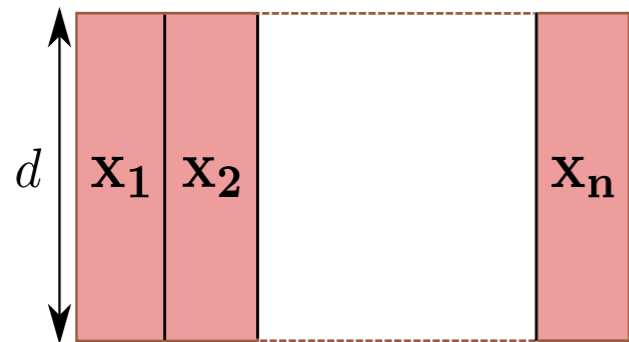
Output: graph of relations between the d variables



Graph Learning

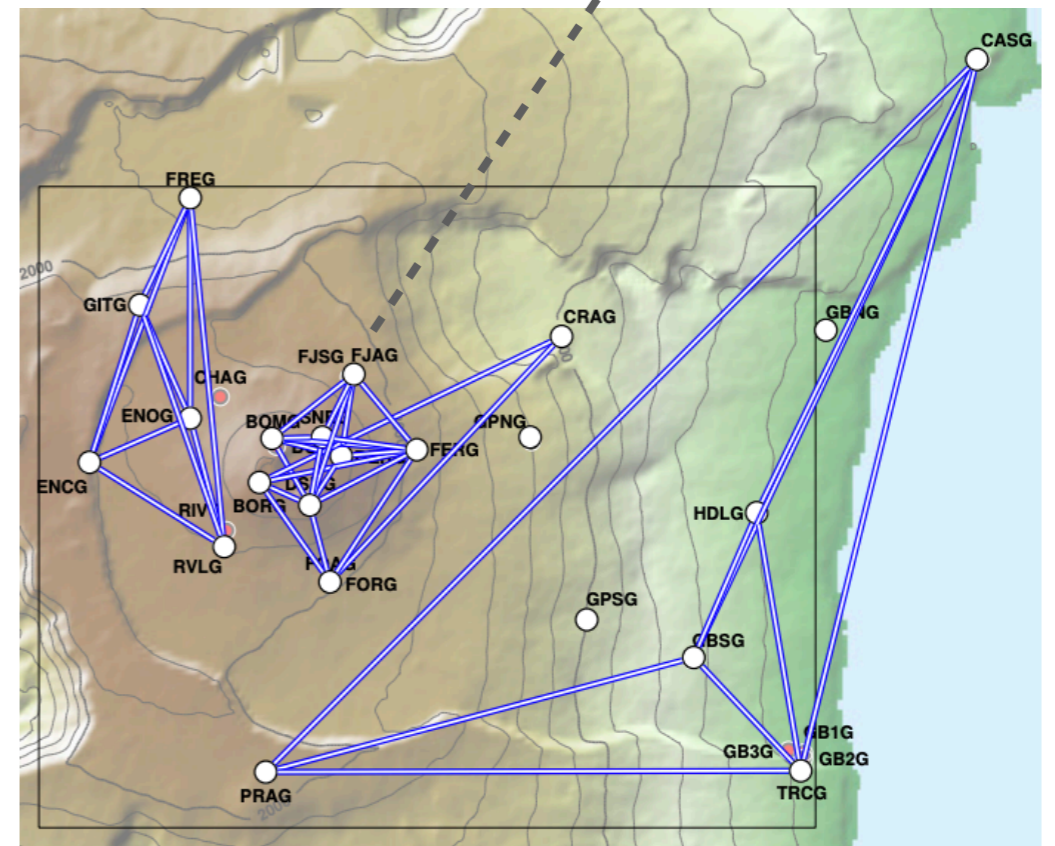
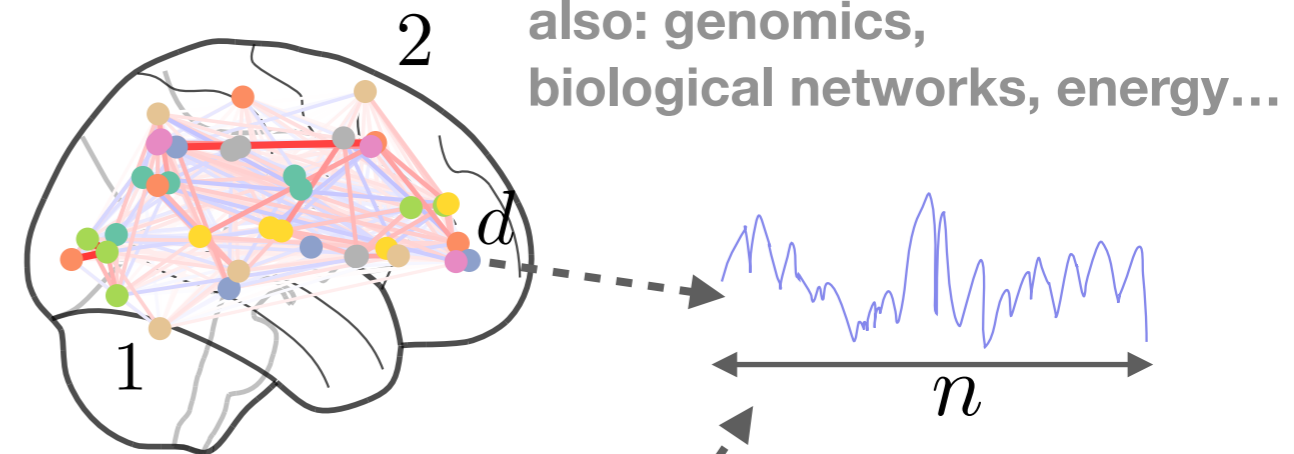
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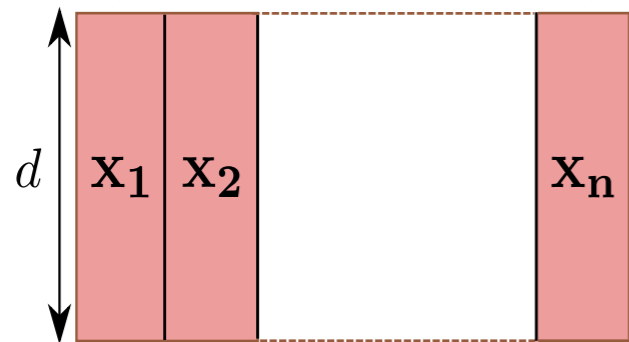
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Graph modeled as a matrix:

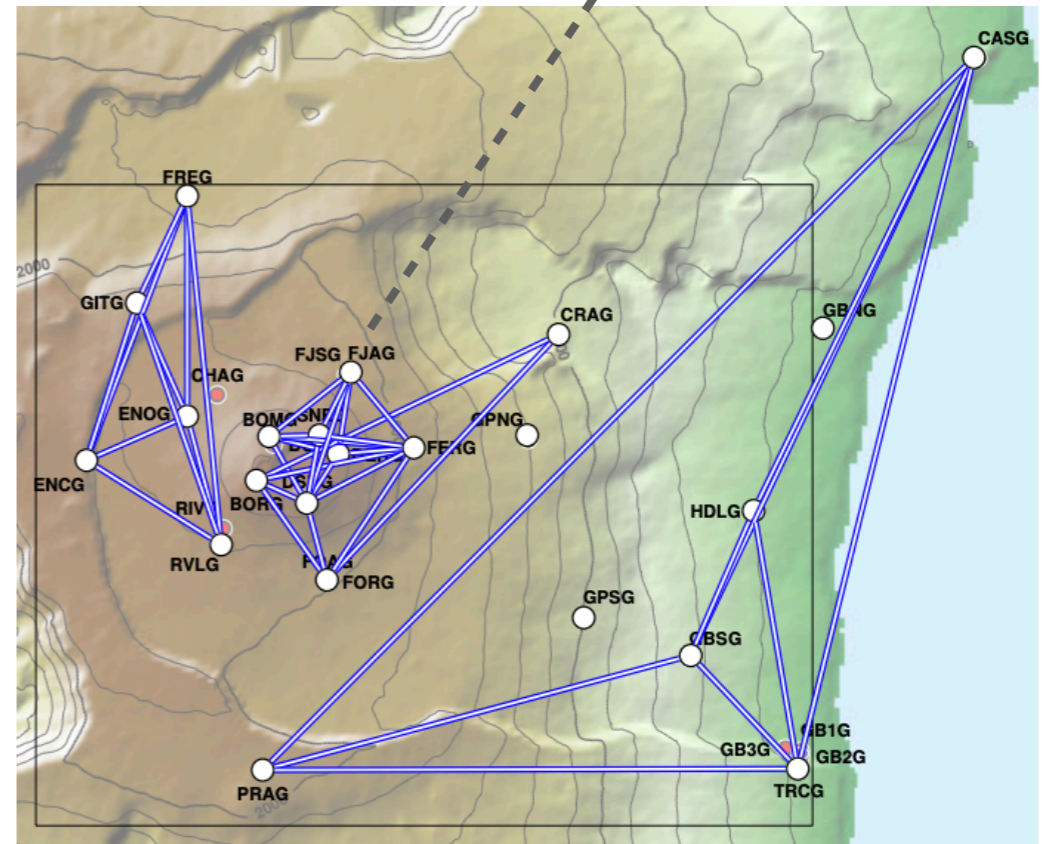
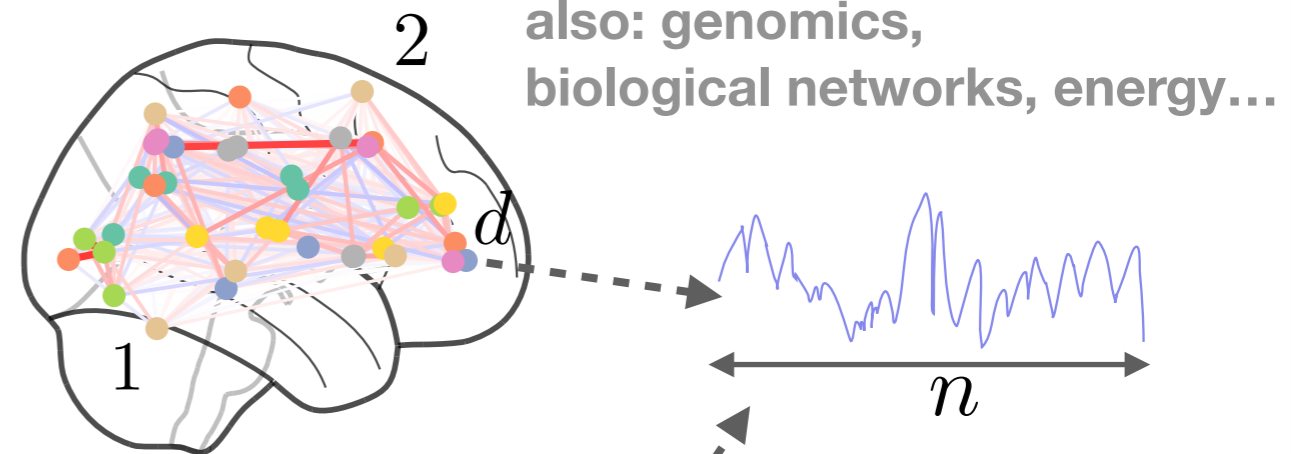
$$\Theta \in \mathbb{R}^{d \times d}$$

Θ_{ij} : **interaction** between variable i and j

| statistical correlations

| statistical dependencies

Output: graph of relations between the d variables



| Graphical LASSO

Side note

- Input: $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$
- $\mathbf{x}_i \in \mathbb{R}^d \sim \mu$
- Output: $\Theta \in \mathbb{R}^{d \times d}$

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■ Gaussian Graphical Model

Gaussian assumption $\mu = \mathcal{N}(0, \Sigma = \Theta^{-1})$

■ $\Theta_{ij} = 0 \iff$ variable i is independent of j conditionally to the others

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Maximum Likelihood estimator

Emp. cov. $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top$

$$\Theta_{\text{MLE}} = \arg \min_{\Theta \succ 0} -\log \det(\Theta) + \langle \hat{\Sigma}, \Theta \rangle_F$$

■ When $\hat{\Sigma}$ is invertible $\Theta_{\text{MLE}} = (\hat{\Sigma})^{-1}$

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May not be true
in high dim $n < d$

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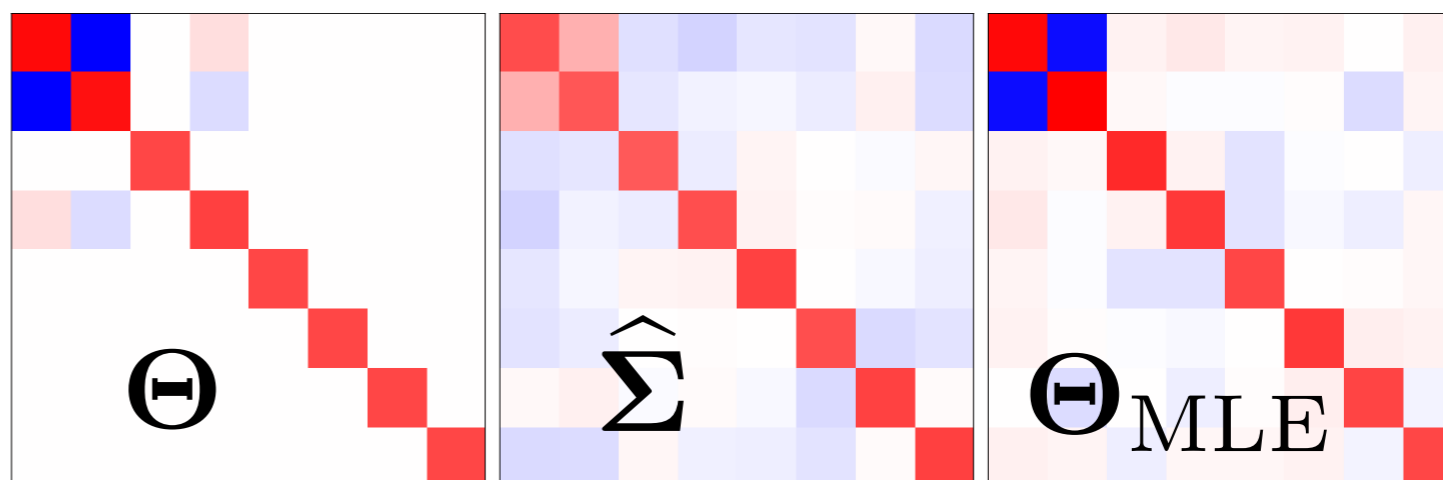
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When $\hat{\Sigma}$ is invertible $\Theta_{\text{MLE}} = (\hat{\Sigma})^{-1} \dashrightarrow$ usually not sparse

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in high dim $n < d$



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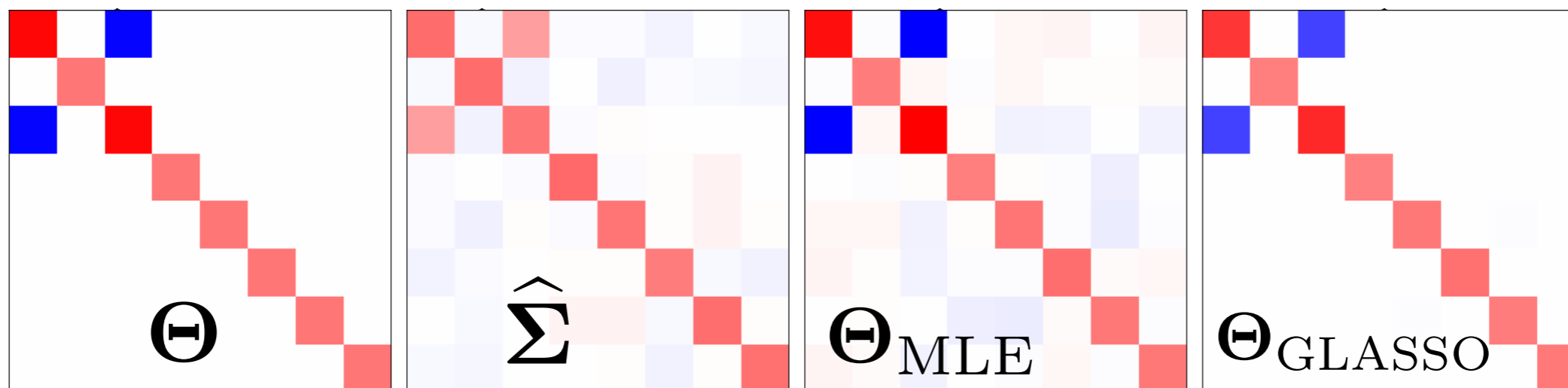
Penalized Maximum Likelihood estimator [Friedman-Hastie-Tibshirani, 2007]

$$\Theta_{\text{GLASSO}} = \arg \min_{\Theta \succ 0} -\log \det(\Theta) + \langle \hat{\Sigma}, \Theta \rangle_F + \lambda \|\Theta\|_{1,\text{off}}$$

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$\|\Theta\|_{1,\text{off}} = \sum_{i < j} |\Theta_{ij}|$ promotes sparsity for the output graph



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■ Optimization: convex problem

Coordinate descent

Involves LASSO steps (on the rows)

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QUIC, Big & QUIC [Hsieh & al, 2013-2014]

SQUIC [Bollhöfer, 2019] + other estimators...

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Many modelisation variants:

$\Theta = \mathcal{L}(\mathcal{G})$ is a Laplacian matrix of a graph
[Kumar, 2020]

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Complexity of GLASSO:

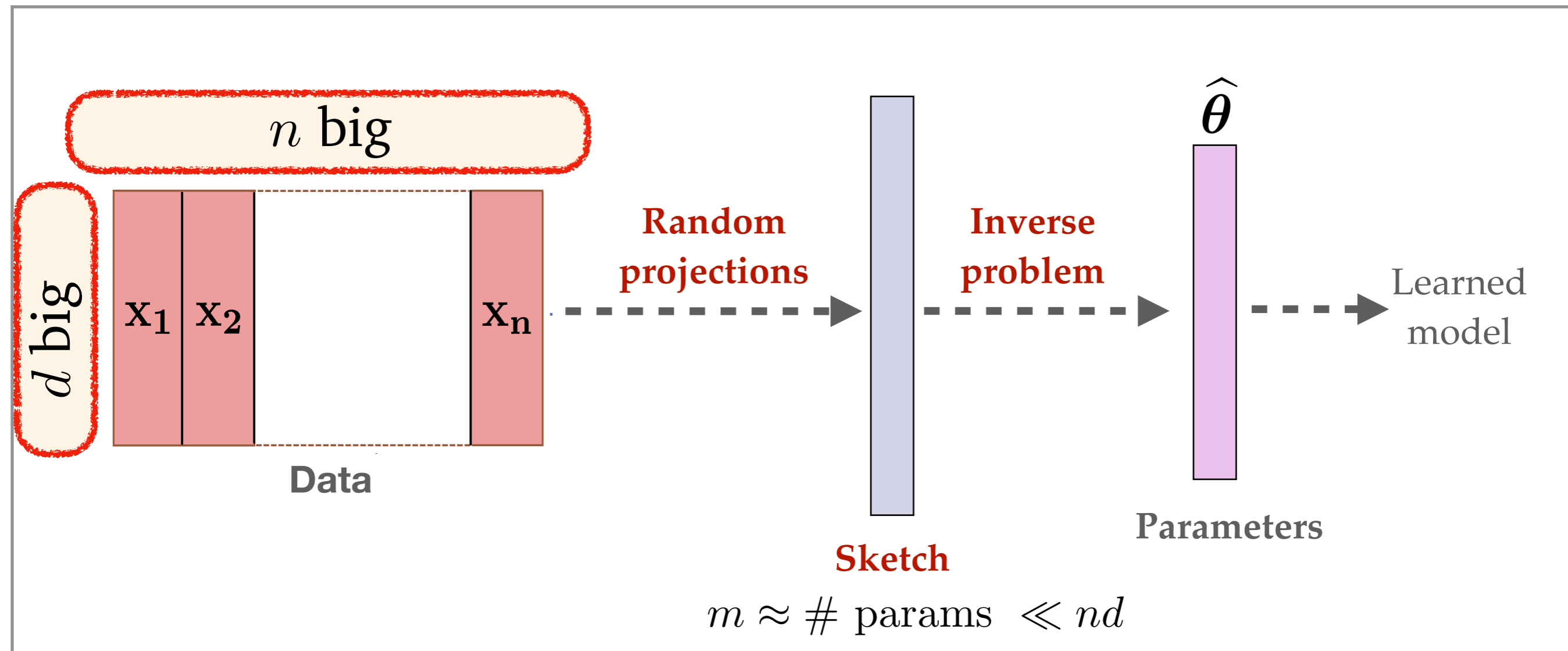
	In memory	In time
$\hat{\Sigma}$	$\mathcal{O}(d^2)$	$\mathcal{O}(d^3)$

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The sketching approach

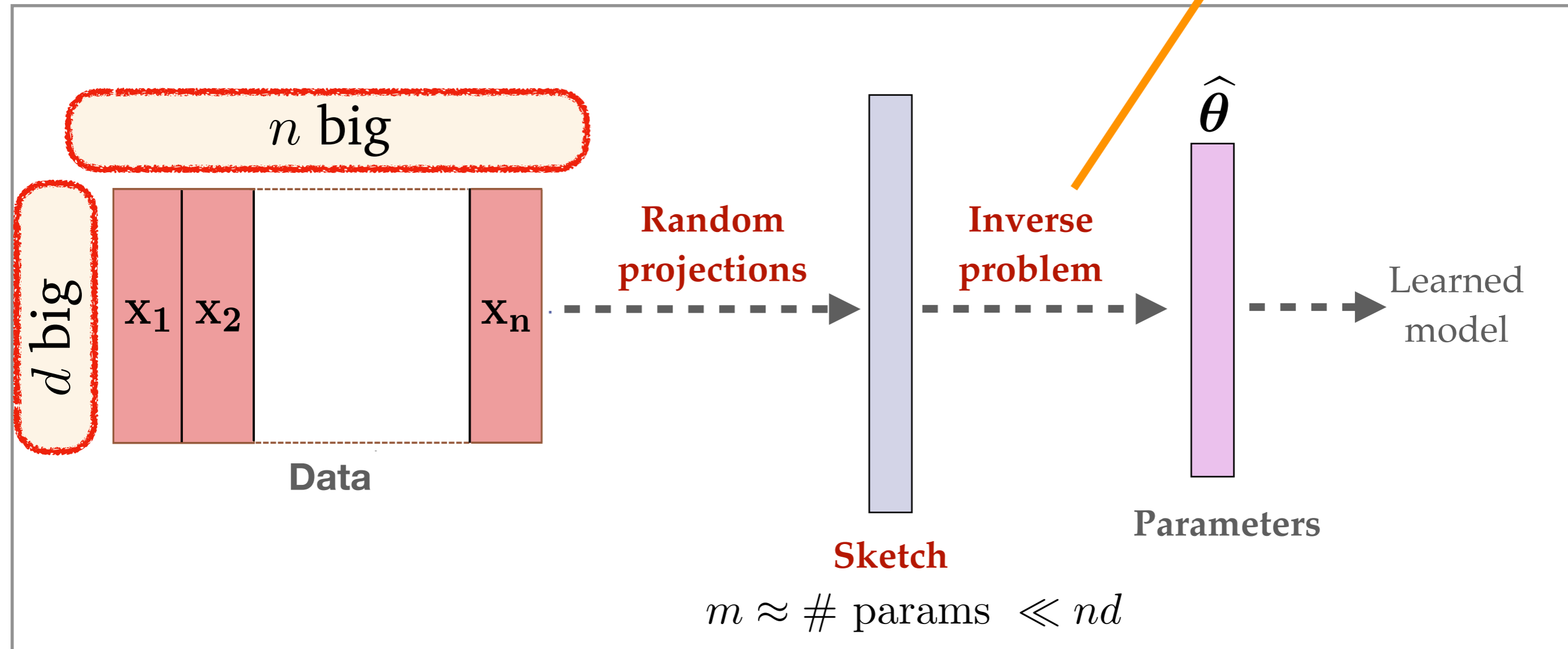
High overview:



The sketching approach

generalizes the principles of **compressed sensing**

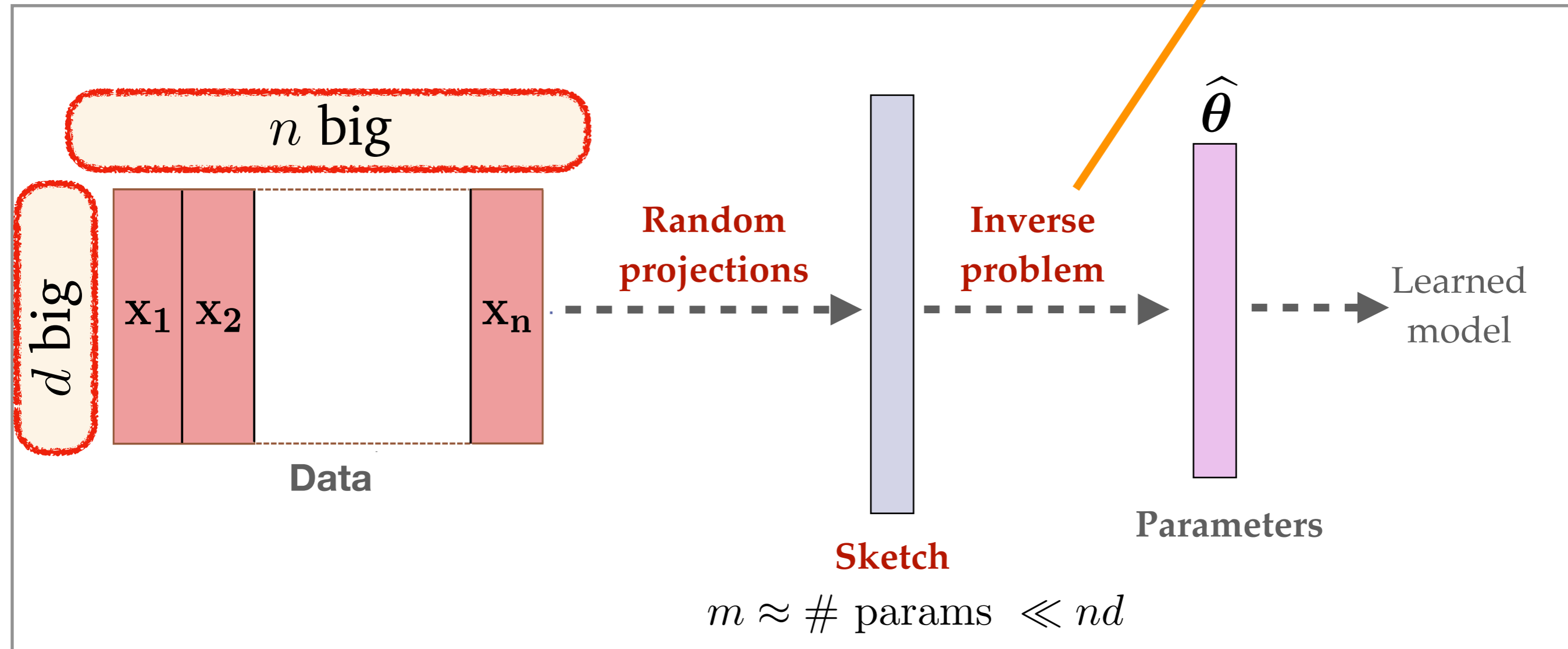
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High overview:



Advantages for **storage and transfer**

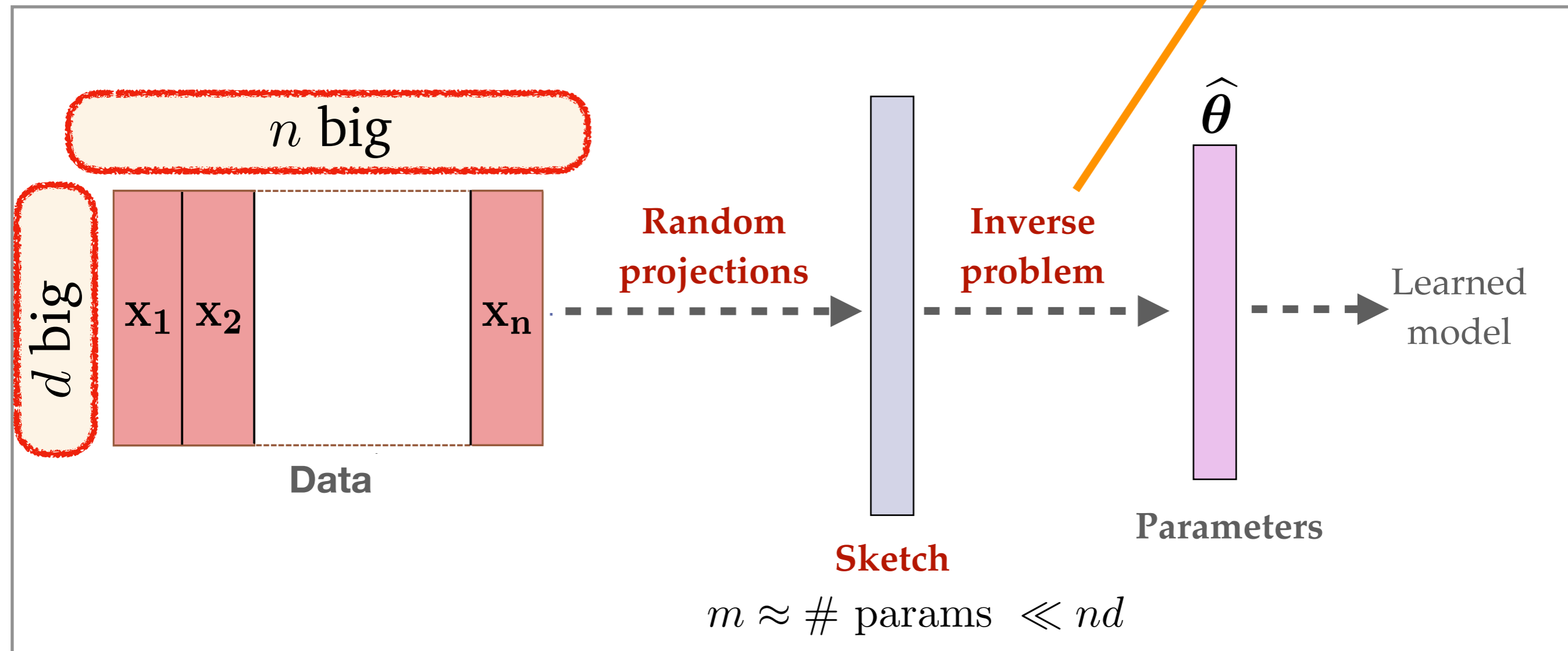
Many statistical problems

How to choose Φ ? -> connection to **optimal transport**

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High overview:



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Many statistical problems

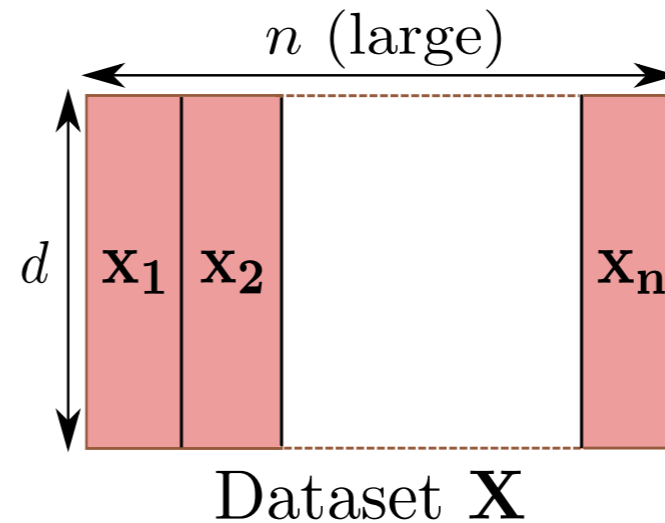
How to choose Φ ? -> connection to **optimal transport**

Rémi Gribonval, Anthony Bourrier, **Nicolas Keriven**, **Antoine Chatalic**, Gilles Puy, Nicolas Tremblay, Yann Traonmilin, Clément Elvira, Patrick Perez, Mike Davies, Gilles Blanchard, Laurent Jacques, **Vincent Schellekens**, Florimond Houssiau, Phil Schniter, Evan Byrne, ...

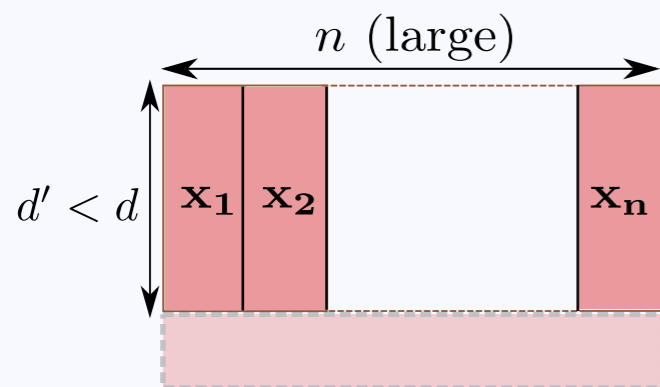
The sketching approach

« Dimension » reduction

« Low-dim » representation of a dataset



Dimension reduction

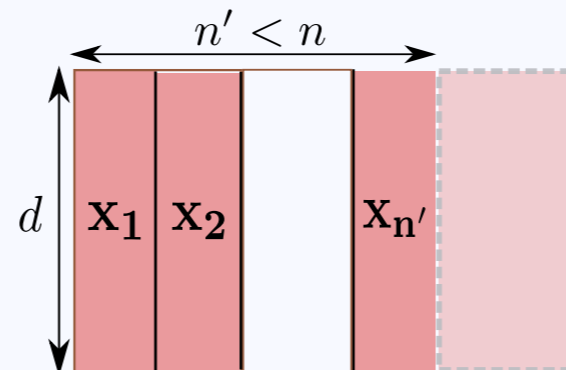


Random projections (JL lemma)

Feature selection

Minimum distortion embedding, PCA

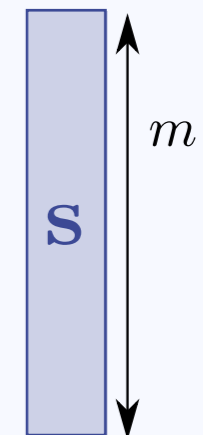
Subsampling



Coresets

Importance sampling

Here: linear « sketch »

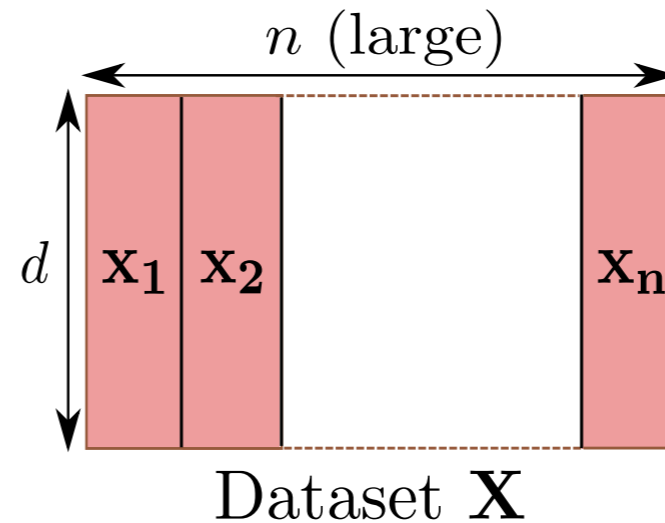


Only one vector

The sketching approach

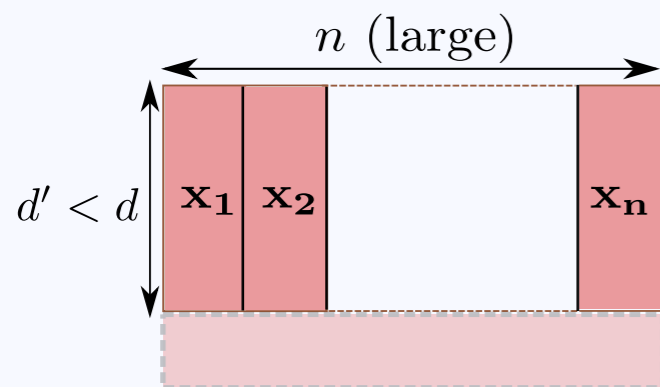
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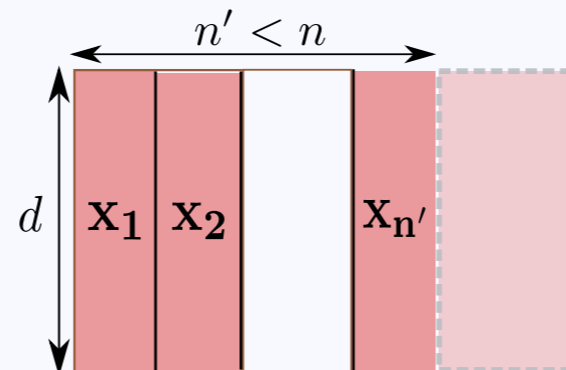
How do we sketch? How do we learn from sketch?

Dimension reduction



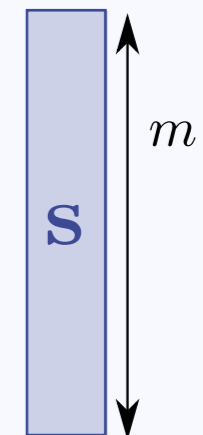
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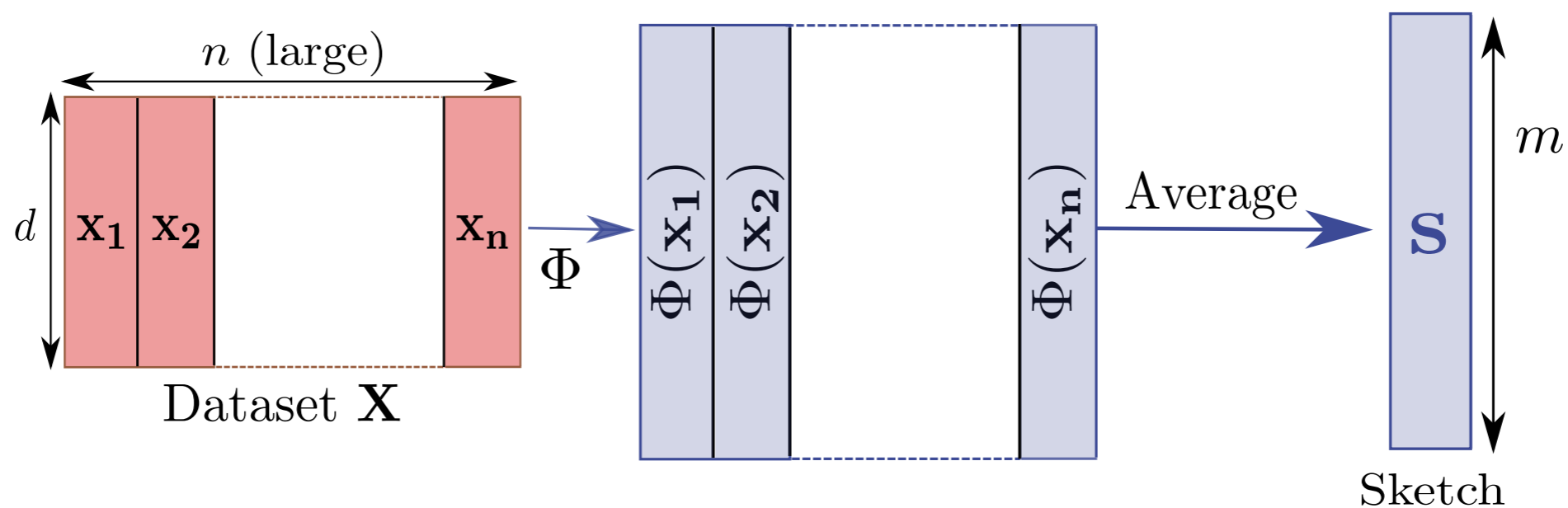
Only one vector

The sketching approach

Obtaining the sketch

A function called **feature operator** $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^m$

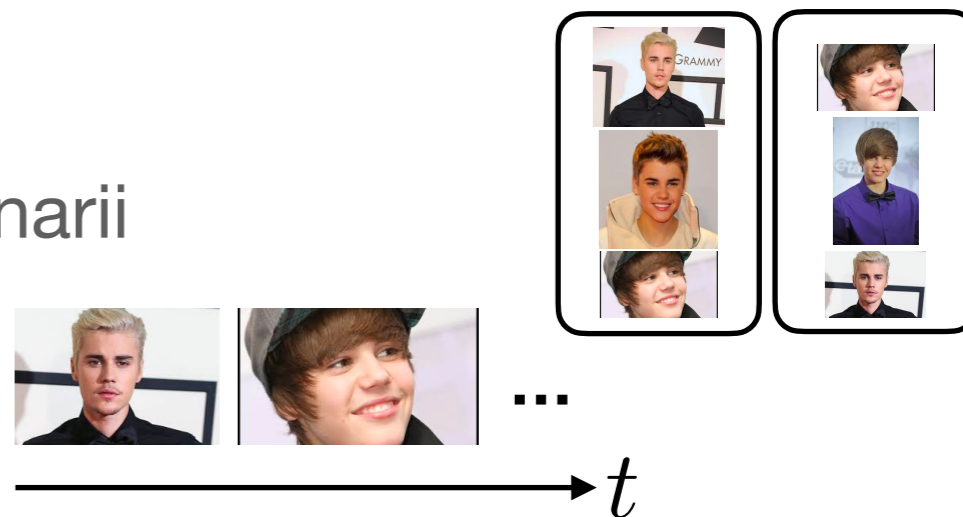
Averaging **n points** $\rightarrow \mathbf{s} := \frac{1}{n} \sum_{i=1}^n \Phi(\mathbf{x}_i)$



Average is a simple idea but ...

Suitable for **distributed / streaming** scenarios

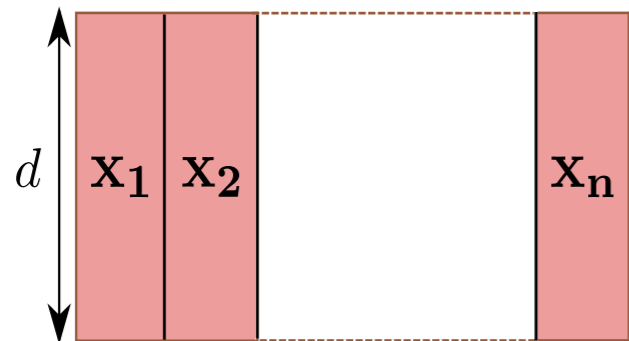
It can be calculated in **parallel**



Goal of this talk

Input: a dataset

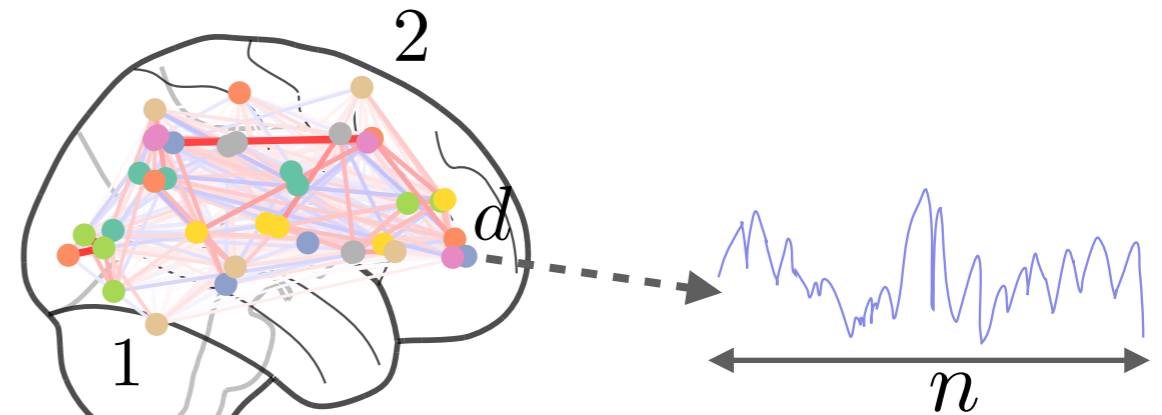
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GLASSO

Output: graph of relations between the d variables $\Theta \in \mathbb{R}^{d \times d}$

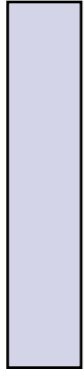


GLASSO

	In memory	In time
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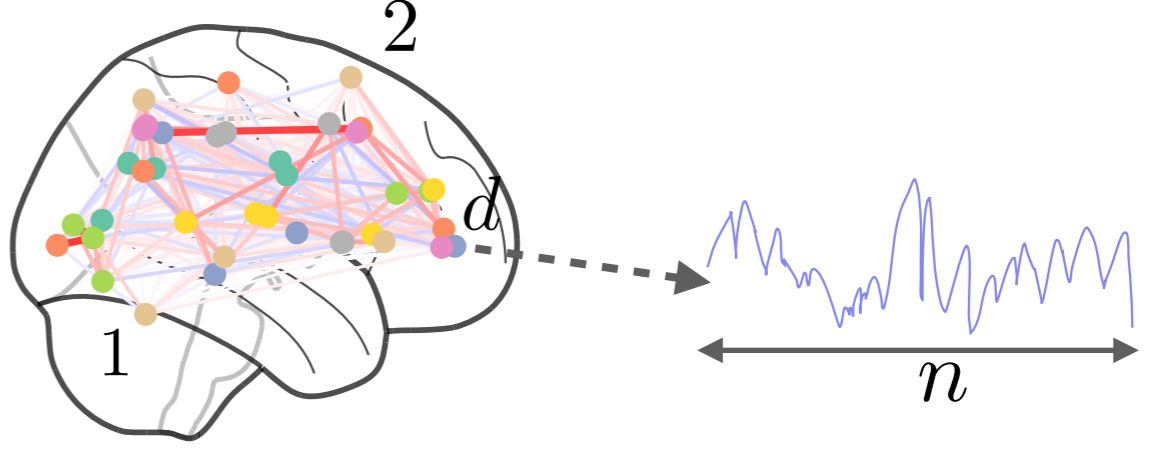
Input: a dataset

$$\mathbf{s} = \text{Sketch}(\mathbf{X}) \in \mathbb{R}^m$$


$m \approx \# \text{ edges}$

Sketch

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GLASSO

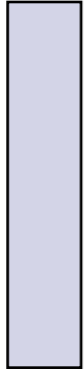
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Sketching

	In memory	In time
\mathbf{s}	$\mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$

Goal of this talk

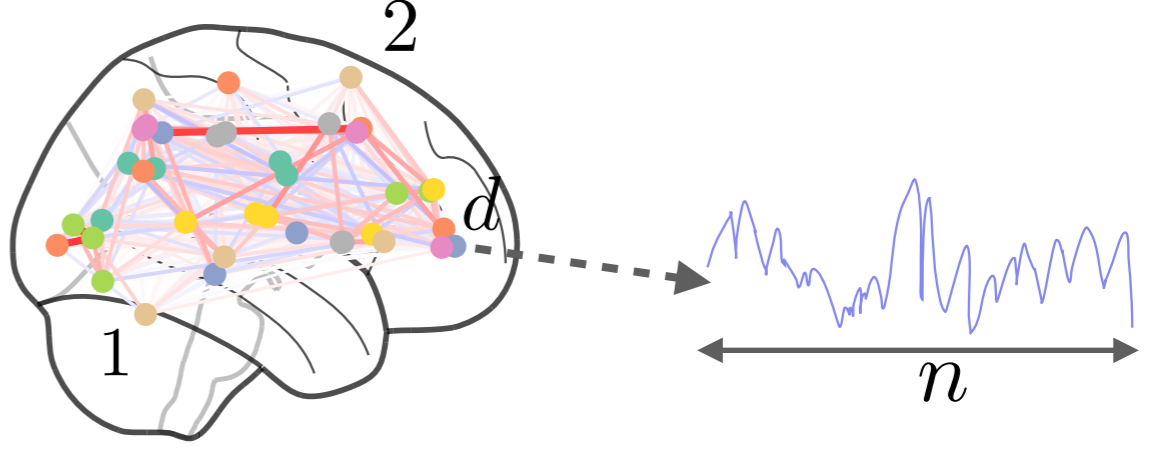
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In memory	In time
$\mathbf{s} \dashrightarrow \mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$

Why should it work ?

- The underlying graph is **sparse**
- Keep only what we need through the sketch

| Towards theoretical compressive recovery

■ The feature operator $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^m$

Towards theoretical compressive recovery

■ The feature operator $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^m$

■ In this talk: quadratic measurements $\mathbf{A}_j \sim \Lambda$ is a random matrix

$$\Phi(\mathbf{x}) = \frac{1}{\sqrt{m}} (\mathbf{x}^\top \mathbf{A}_1 \mathbf{x}, \dots, \mathbf{x}^\top \mathbf{A}_m \mathbf{x})^\top$$

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Gaussian measurements

$$\mathbf{A}_j \underset{i.i.d.}{\sim} \mathcal{N}(0, \mathbf{I}_{d \times d})$$

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Structured rank-one

End of presentation

Rank-one measurements

$$\mathbf{A}_j = \mathbf{a}_j \mathbf{a}_j^\top \quad \mathbf{a}_j \underset{i.i.d.}{\sim} \mathcal{N}(0, \mathbf{I}_d)$$

$$\Phi(\mathbf{x}) = (|\langle \mathbf{a}_j, \mathbf{x} \rangle|^2)_{j \in \llbracket m \rrbracket}$$

■ Inspired by works on low-rank matrix completion

Towards theoretical compressive recovery

■ The feature operator $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^m$

■ In this talk: **quadratic measurements** $\mathbf{A}_j \sim \Lambda$ is a **random matrix**

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■ Inspired by works on low-rank matrix completion

■ Defined a **linear op.** on **symmetric matrices** $\mathcal{A} : S_d \rightarrow \mathbb{R}^m$

$$\mathcal{A}\mathbf{S} = \frac{1}{\sqrt{m}} (\langle \mathbf{A}_j, \mathbf{S} \rangle_F)_{j \in \llbracket m \rrbracket}$$

$$\mathbf{s} = \frac{1}{n} \sum_{i=1}^n \Phi(\mathbf{x}_i) = \mathcal{A} \hat{\Sigma} \in \mathbb{R}^m$$

Emp. cov. 

Towards theoretical compressive recovery

Objective/setting

$$\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n) \quad \mathbf{x}_i \in \mathbb{R}^d \sim \mu \quad \text{with} \quad \mathbb{E}_{\mathbf{x} \sim \mu} [\mathbf{x}\mathbf{x}^\top] = \boldsymbol{\Sigma}_\star = \Theta_\star^{-1}$$

$\Theta_\star \in \mathcal{S}$ in some **low-dim. space** (e.g. sparse p.d matrices = sparse graph)

The objective is to find Θ_\star from the sketch $\mathbf{s} \in \mathbb{R}^m$

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Can be framed as a **compressed sensing problem**

$$\text{Find } \Theta_\star \text{ from } \mathbf{s} = \mathcal{A}\hat{\Sigma} = \mathcal{A}\Sigma_\star + \mathbf{e}$$

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$$\text{Find } \Theta_\star \text{ from } \mathbf{s} = \mathcal{A}\hat{\Sigma} = \mathcal{A}\Sigma_\star + \mathbf{e}$$

Notable difference

We want **the inverse of the matrix**
that is measured

not find Σ_\star given $\mathcal{A}\Sigma_\star + \mathbf{e}$

Towards theoretical compressive recovery



find Σ_{\star} given $\mathcal{A}\Sigma_{\star} + \mathbf{e}$



find Σ_{\star}^{-1} given $\mathcal{A}\Sigma_{\star} + \mathbf{e}$

Towards theoretical compressive recovery

Objective/setting

$$\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n) \quad \mathbf{x}_i \in \mathbb{R}^d \sim \mu \quad \text{with} \quad \mathbb{E}_{\mathbf{x} \sim \mu} [\mathbf{x}\mathbf{x}^\top] = \Sigma_\star = \Theta_\star^{-1}$$

$\Theta_\star \in \mathcal{S}$ in some **low-dim. space** (e.g. sparse p.d matrices = sparse graph)

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Notable difference

We want **the inverse of the matrix**
that is measured
not find Σ_\star given $\mathcal{A}\Sigma_\star + \mathbf{e}$

Ill-posed problem: $m \ll d^2$

Key assumption:

Θ_\star lies in some **low-dim. space**

Towards theoretical compressive recovery

Example of low-dim space

■ \mathcal{S} a subspace of S_d of idealized precision matrices (low-dim)

$$\mathcal{S}_{k,a,b} = \{ \Theta \succ 0 ; \|\Theta\|_0 \leq d + 2k, \text{spec}(\Theta) \subseteq [a, b] \}$$

sym. positive definite matrices

localized spectrum

with at most $2k$ non-zero coeff
outside the diagonal

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■ Sparse precision (= sparse graph) matrices with known spectrum

■ Called **the model set**

| The Restricted Isometric Property

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- Consider a **linear op.** on **symmetric matrices** $\mathcal{A} : \mathcal{S}_d \rightarrow \mathbb{R}^m$
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invRIP

$$\exists \delta \in [0, 1[, \forall \Theta_1, \Theta_2 \in \underline{\mathcal{S}}$$

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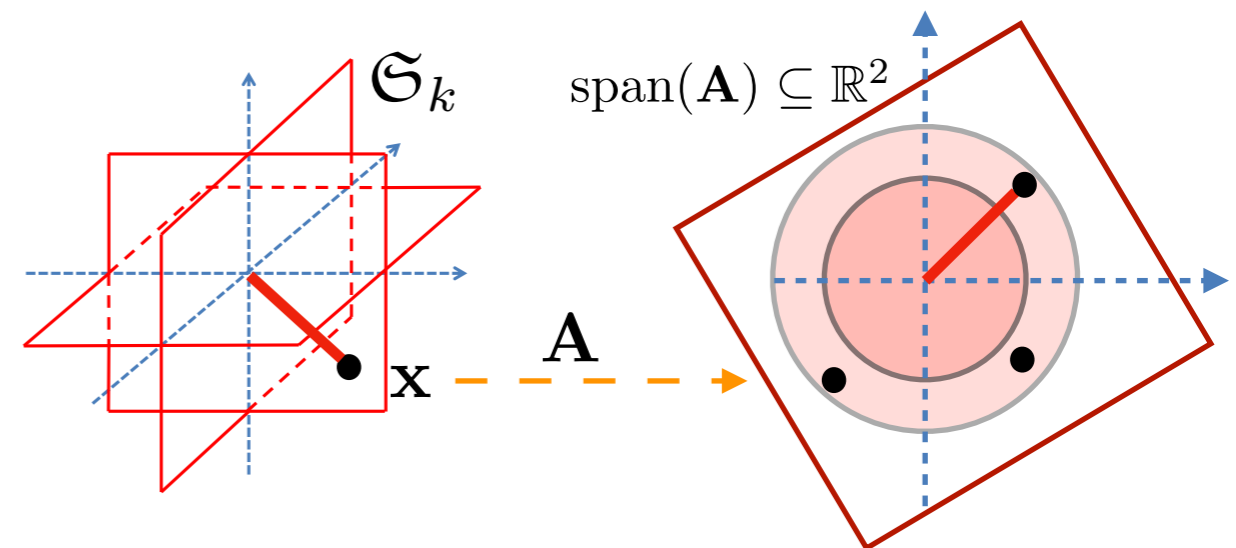
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- The restricted isometric property (**RIP**) [Candes & Tao, 2005]

$$\exists \delta_k \in [0, 1[\quad \forall \mathbf{x} \text{ } k\text{-sparse}$$

$$(1 - \delta_k) \|\mathbf{x}\|_2^2 \leq \|\mathbf{A}\mathbf{x}\|_2^2 \leq (1 + \delta_k) \|\mathbf{x}\|_2^2$$



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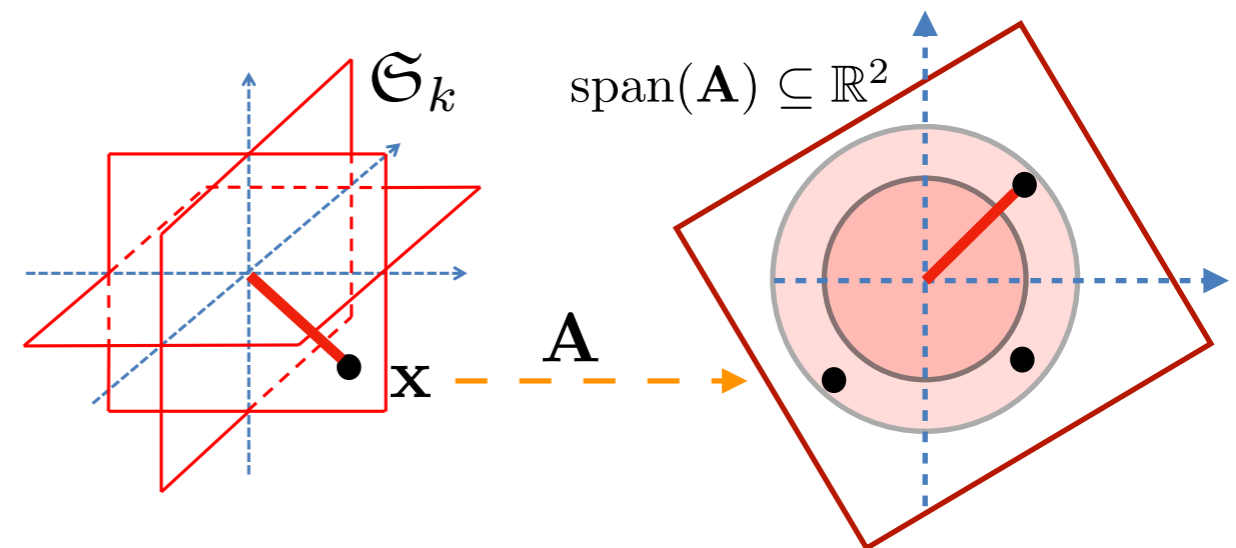
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- E.g. **Gaussian matrices**

$$m \gtrsim \delta^{-2} k \ln\left(e \frac{d}{k}\right)$$

... also Johnson-Lindenstrauss Lemma

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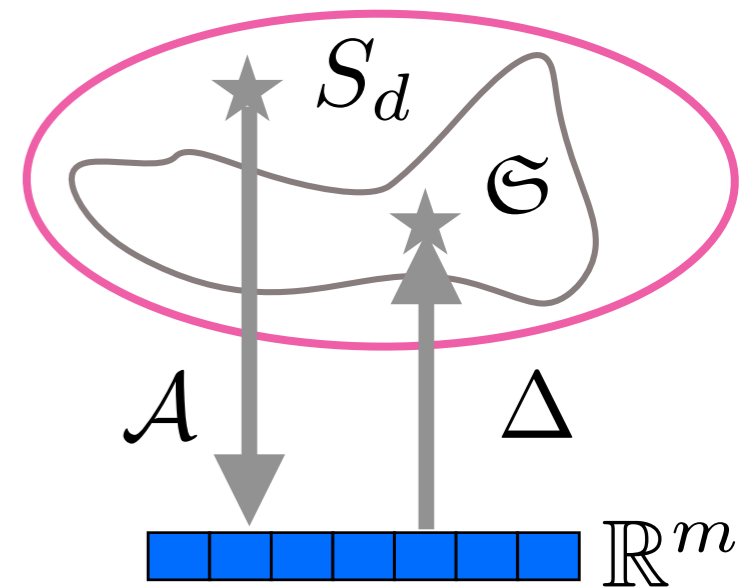
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- Consider a **linear op.** on **symmetric matrices** $A : S_d \rightarrow \mathbb{R}^m$
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■ The optimal decoder

- If $A : S_d \rightarrow \mathbb{R}^m$ satisfies the **invRIP** on \mathcal{S}
- There exists a **optimal decoder** $\Delta : \mathbb{R}^m \rightarrow \mathcal{S}$



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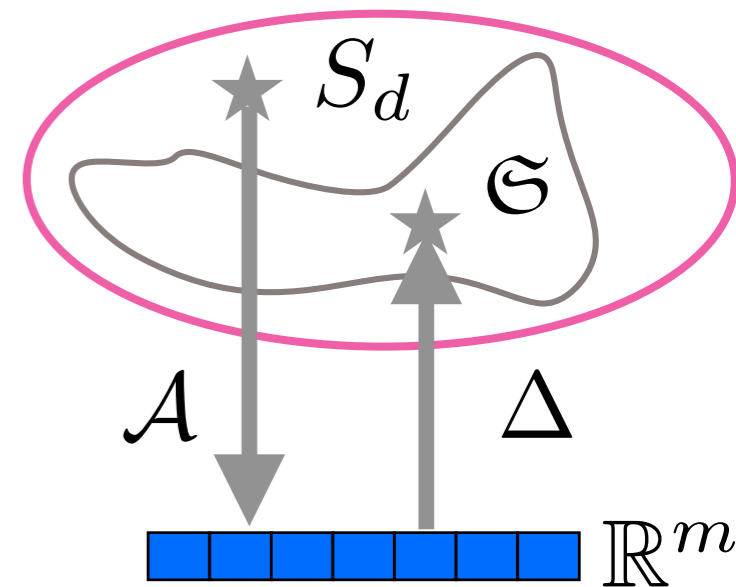
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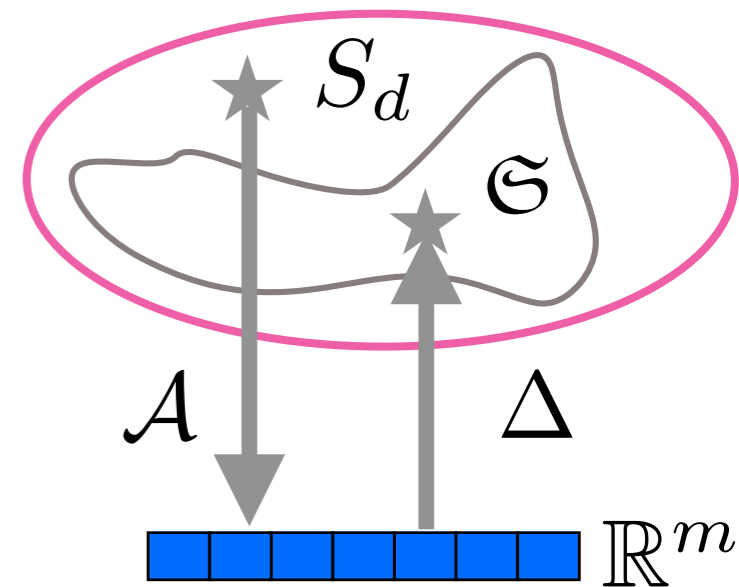
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- + robust to noise !



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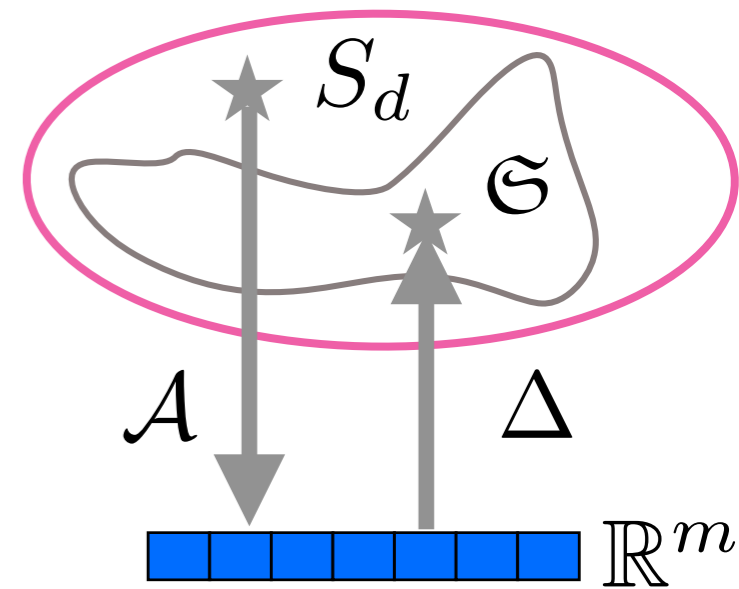
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Happiness and joy

| Proving the Restricted Isometric Property

$\mathcal{AS} = \frac{1}{\sqrt{m}} (\langle \mathbf{A}_j, \mathbf{S} \rangle_F)_{j \in \llbracket m \rrbracket}$ is random - - - \blacktriangleright **invRIP** with high prob.



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Two ingredients

The **pointwise concentration** of \mathcal{A} i.e. $\forall \Theta_1, \Theta_2 \in \underline{\mathcal{S}}$

$$\mathbb{P} \left(\left| \|\mathcal{A}(\Theta_1^{-1} - \Theta_2^{-1})\|_2^2 - \|\Theta_1^{-1} - \Theta_2^{-1}\|_F^2 \right| > t \|\Theta_1^{-1} - \Theta_2^{-1}\|_F^2 \right) \leq C_1(t; m)$$



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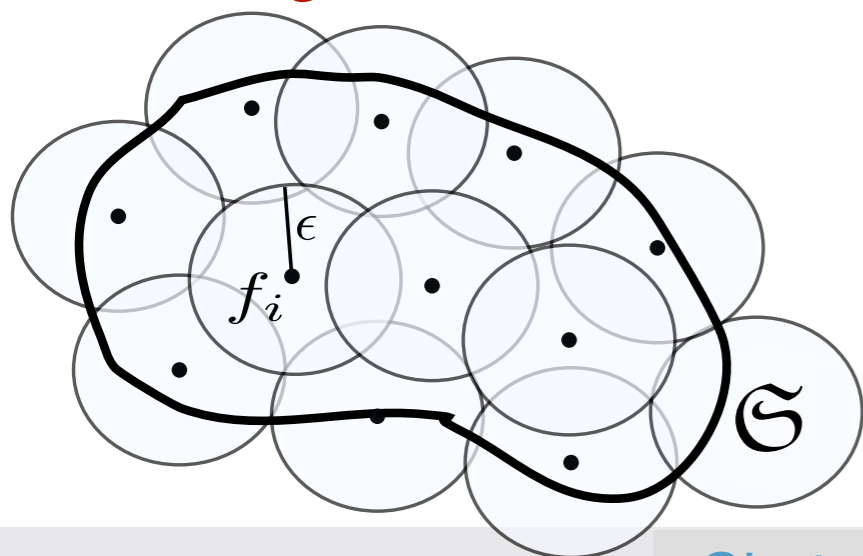
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Covering numbers \dashleftarrow



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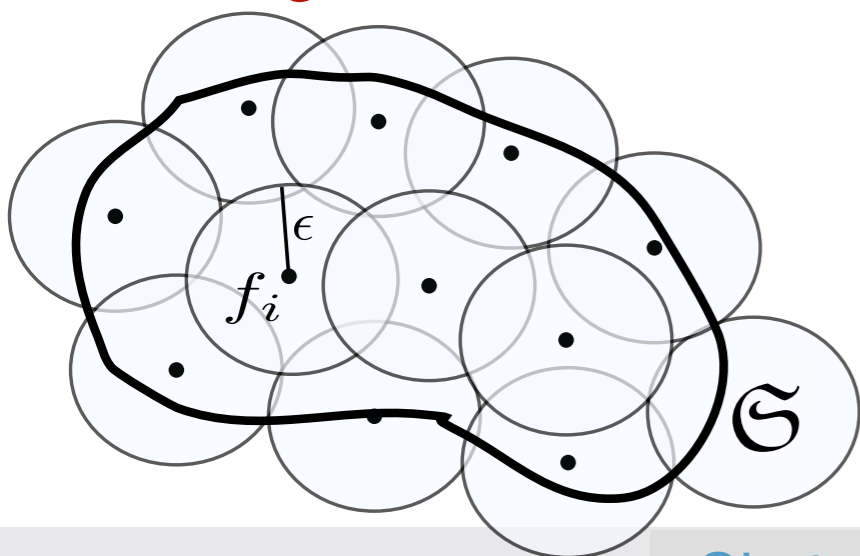
Covering numbers

e.g. k -sparse vectors in dimension d

$$\ln \mathcal{N}(\mathfrak{S}_k, \varepsilon) \leq k \left(\ln(3\varepsilon^{-1}) + \ln\left(e \frac{d}{k}\right) \right)$$

In our case **ok with**:

$$\mathfrak{S}_{k,a,b} = \{ \Theta \succ 0 ; \|\Theta\|_0 \leq d + 2k, \text{spec}(\Theta) \subseteq [a, b] \}$$



Main results

Gaussian measurements

■ Sketch with

$$\mathbf{A}_j \underset{i.i.d.}{\sim} \mathcal{N}(0, \mathbf{I}_{d \times d})$$

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Happiness
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Remarks

■ The number of measurements low compared to d^2

■ Almost optimal up to a logarithmic factor

■ Now all we need is to compute the decoder ...

| Overview of the talk

- Part I: **Finding graphs from unstructured data**
- Part II: **The sketching approach**
- Part III: **Algorithmic solution**
- Part IV: **Limits, Open questions, partial answers**

| Towards practical recovery

■ Recover the precision matrix from the sketch

- We need to compute: $\Delta[\mathbf{s}] \in \arg \min_{\Theta \in \mathcal{S}} \|\mathcal{A}(\Theta^{-1}) - \mathbf{s}\|_2$
- Where: $\mathcal{S}_{k,a,b} = \{\Theta \succ 0 ; \|\Theta\|_0 \leq d + 2k, \text{spec}(\Theta) \subseteq [a, b]\}$
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$$\tilde{\Theta} \in \arg \min_{\substack{\Theta \in S_d(\mathbb{R}) \\ a\mathbf{I}_d \preceq \Theta \preceq b\mathbf{I}_d}} \frac{1}{2} \|\mathcal{A}(\text{inv}(\Theta)) - \mathbf{s}\|_2^2 + \lambda \|\Theta\|_{1,\text{off}}$$

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■ We use Davis & Yin three-operator splitting scheme

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[Davis & Yin, 2017]

Algorithm 1 Three-operator splitting algorithm

- 1: Input: initial guess Θ_{init} and step size $\gamma > 0$.
- 2: Initialize $\mathbf{Z}_0 = \text{prox}_{\gamma h}(\Theta_{\text{init}})$ and $\mathbf{U}_0 = 0$.
- 3: **for** $t \in 0, 1, \dots$, **do**
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- 6: $\mathbf{U}_{t+1} = \mathbf{U}_t + (\Theta_{t+1} - \mathbf{Z}_{t+1})/\gamma$
- 7: **end for**

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■ We know the prox

$$\text{prox}_{\lambda g}(\Theta) = \mathbf{D} + \mathbf{D}^\top + \text{diag}(\Theta)$$

$$\text{where } \begin{cases} D_{ij} = \max\{\Theta_{ij} - \lambda, 0\} & i < j \\ D_{ij} = 0 & i \geq j \end{cases}$$

$$\text{prox}_h(\Theta) = \mathbf{U} \text{diag}(\mathbf{v}) \mathbf{U}^\top$$

$$\text{where } v_i = \min\{\max\{\lambda_i(\Theta), a\}, b\}$$

$\mathcal{O}(d^3)$ complexity

[Davis & Yin, 2017]

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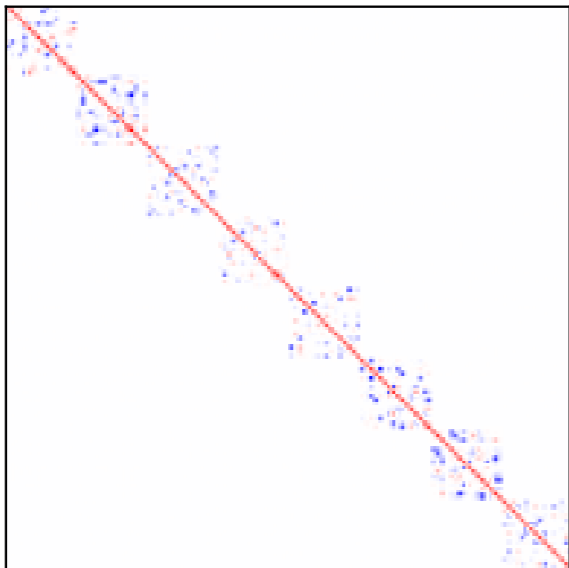
Results

Setting:

- We generate sparse Θ_{\star} according to **some laws**

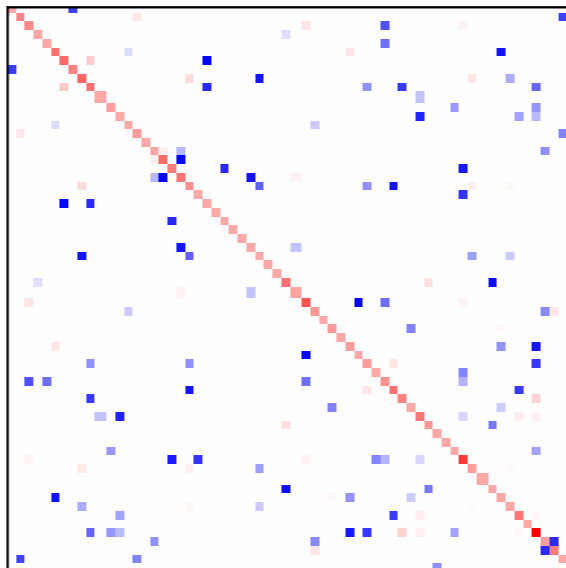
Erdős-Rényi

True precision matrix. $d = 128$



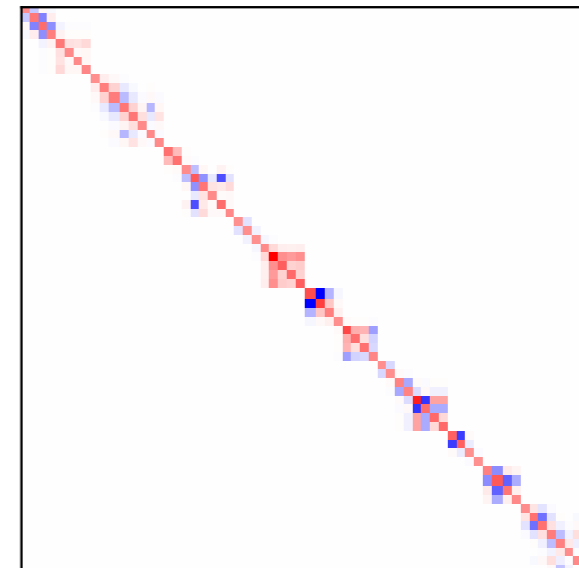
Sklearn

True precision matrix. $d = 64$



Powerlaw

True precision matrix. $d = 64$



- Data $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ $\mathbf{x}_i \sim \mathcal{N}(0, \Theta_{\star}^{-1})$ and **sketch**
- Compare with the approximate decoder $\tilde{\Theta}$

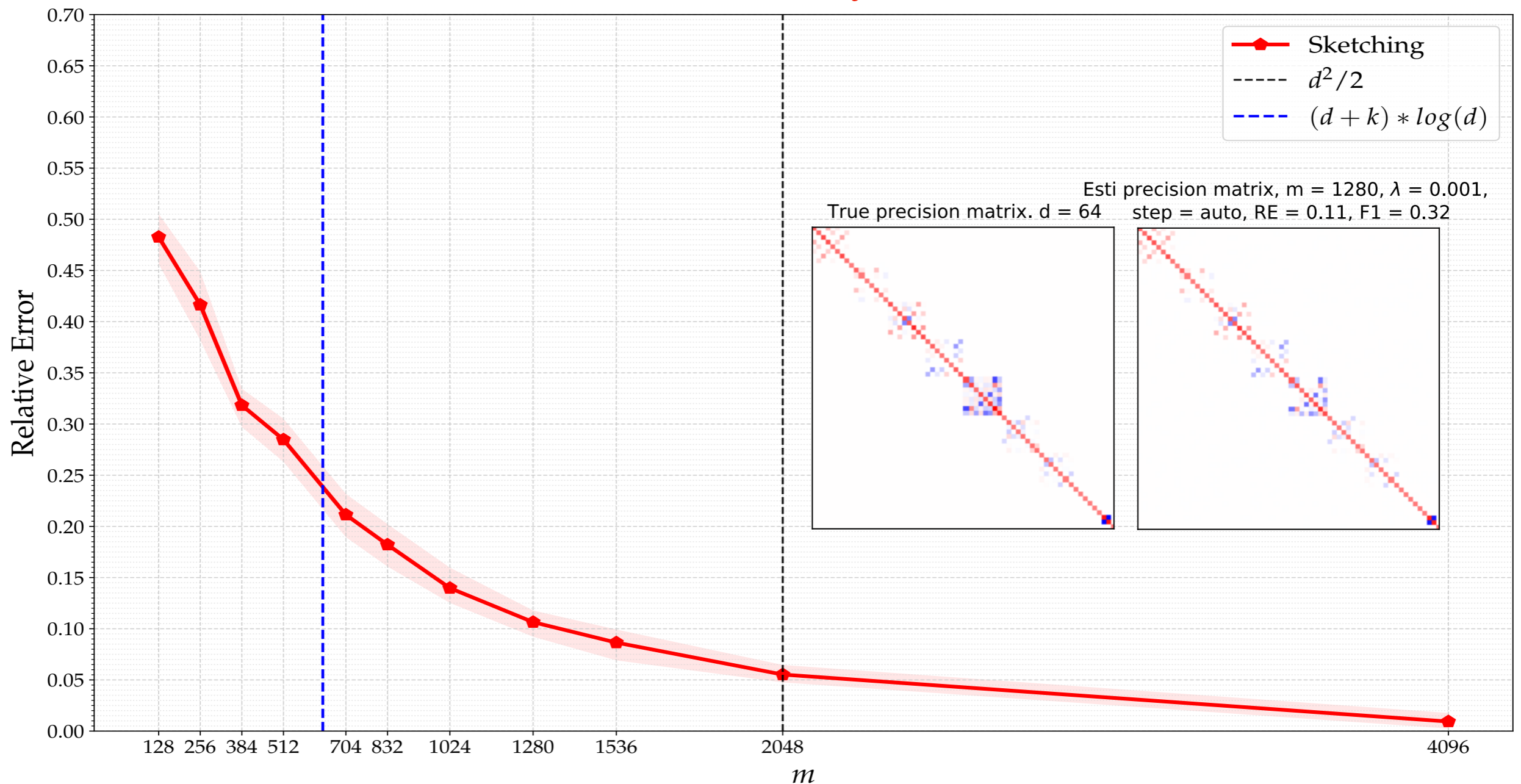
Results

Sketch of the true cov

Sanity-check: $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ $\mathbf{x}_i \sim \mathcal{N}(0, \Theta_\star^{-1})$

$$\mathbf{S} = \mathbf{A}\Sigma_\star$$
$$(n = +\infty)$$

Erdős-Rényi $d = 64$



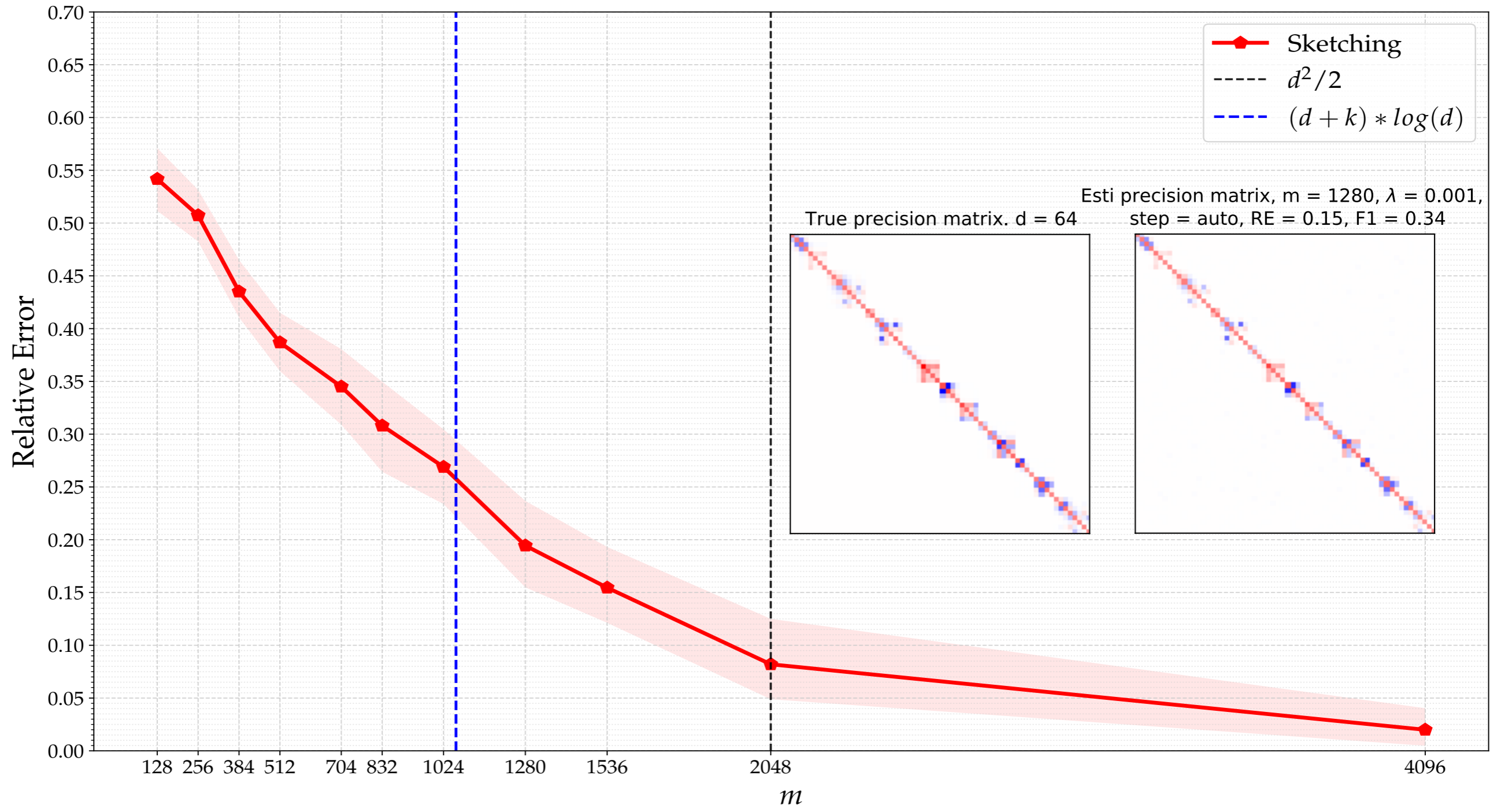
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$$(n = +\infty)$$

Powerlaw $d = 64$



Algorithmic solution

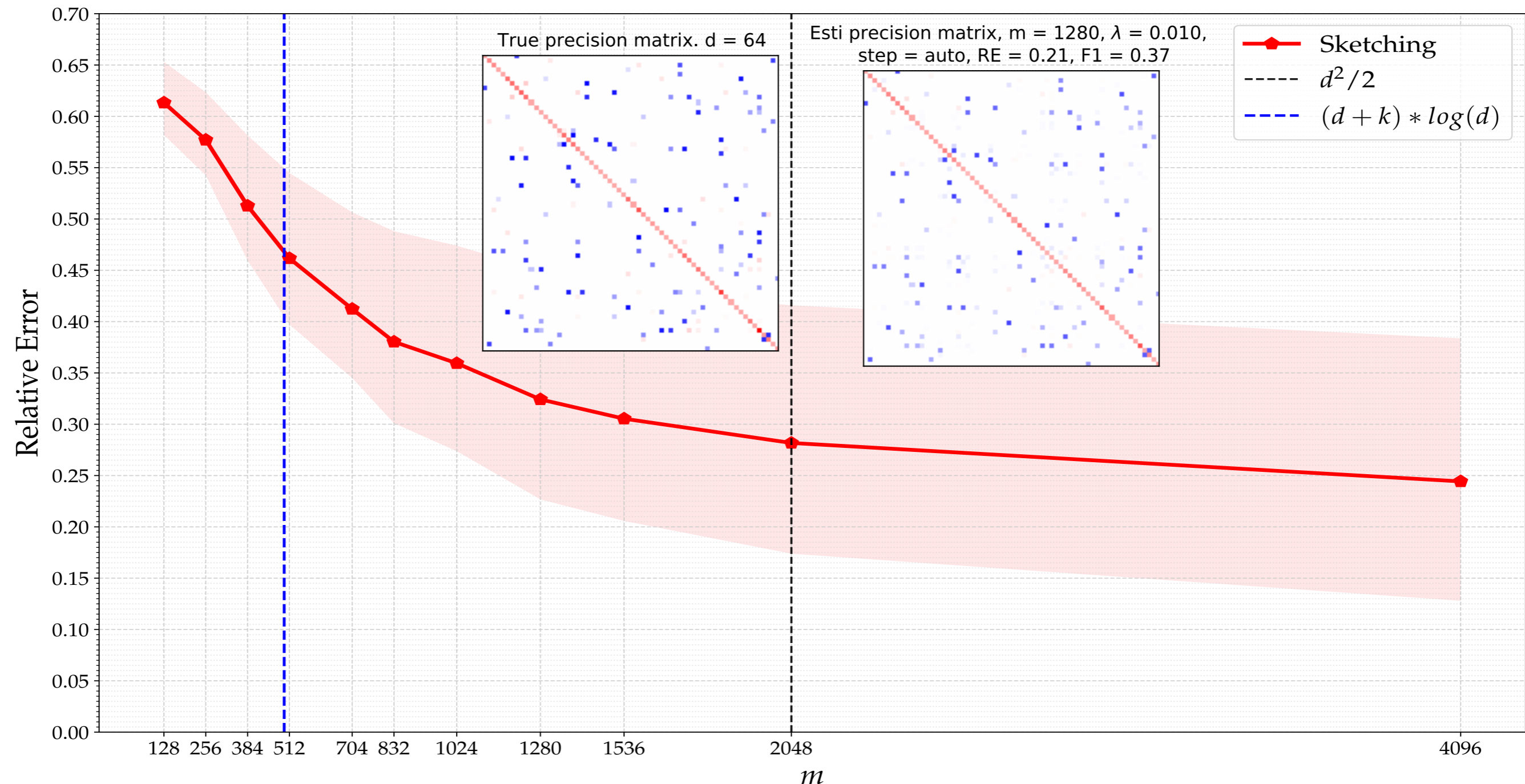
Results

Sketch of the true cov

Sanity-check: $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ $\mathbf{x}_i \sim \mathcal{N}(0, \Theta_\star^{-1})$

$$\mathbf{S} = \mathbf{A}\Sigma_\star$$
$$(n = +\infty)$$

Sklearn $d = 64$

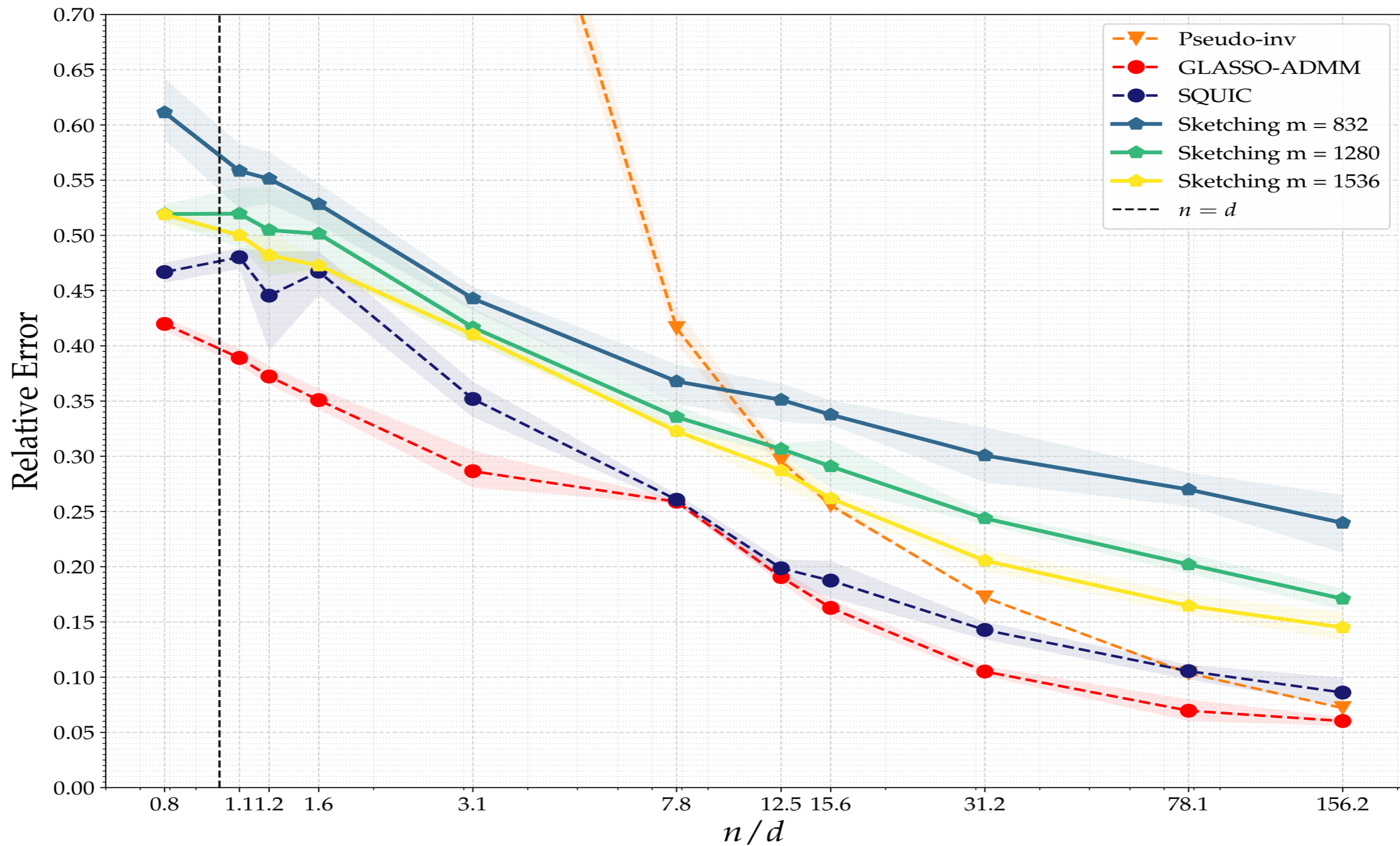


Algorithmic solution

Results

Comparison with GLASSO:

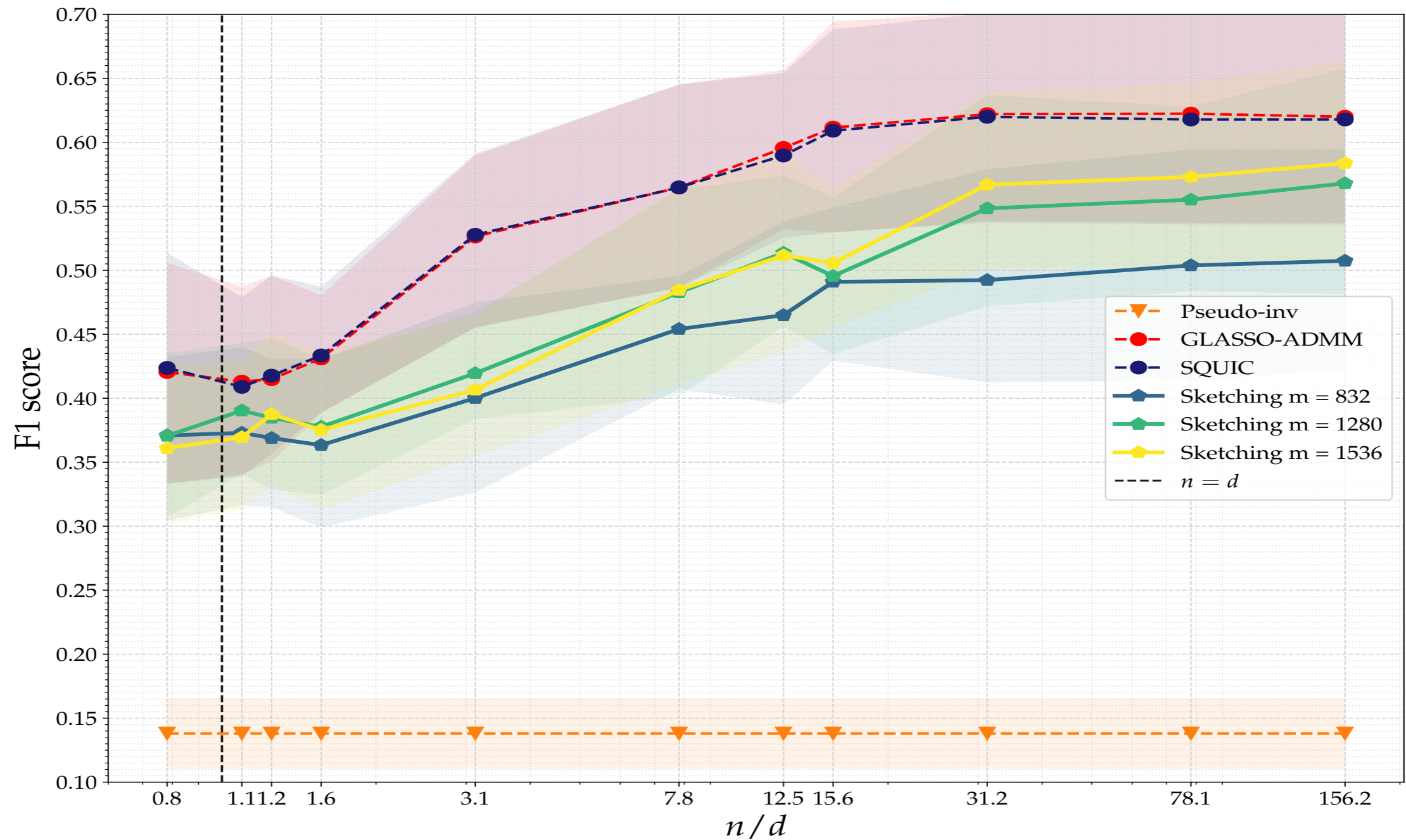
Erdős-Rényi $d = 64$



Results

Comparison with GLASSO:

Erdős-Rényi $d = 64$



| Overview of the talk

- Part I: **Finding graphs from unstructured data**
- Part II: **The sketching approach**
- Part III: **Algorithmic solution**
- Part IV: **Limits, Open questions, partial answers**

| Limitations and perspectives

■ About the complexity:

In memory	In time
$s \dashrightarrow \mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$

Limitations and perspectives

■ About the complexity:

$$s \dashrightarrow m \approx (d + k) \ln(d)$$

In memory	In time
$s \dashrightarrow \mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$

Limitations and perspectives

		In memory	In time
<p>■ About the complexity:</p>		$s \dashrightarrow \mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$
	$s \dashrightarrow m \approx (d+k) \ln(d)$		
	$A_i \dashrightarrow$	Gaussian $\mathcal{O}(m \times d^2)$	
		Rank-one $\mathcal{O}(m \times d)$	

Limitations and perspectives

About the complexity:

		In memory	In time
s	\dashrightarrow	$\mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$
s	\dashrightarrow	$m \approx (d+k) \ln(d)$	
A_i	\dashrightarrow	Gaussian $\mathcal{O}(m \times d^2)$	
	\dashrightarrow	Rank-one $\mathcal{O}(m \times d)$	
			Three op. splitting $\mathcal{O}(d^3)$ $+$ compute S $\mathcal{O}(n \times md)$

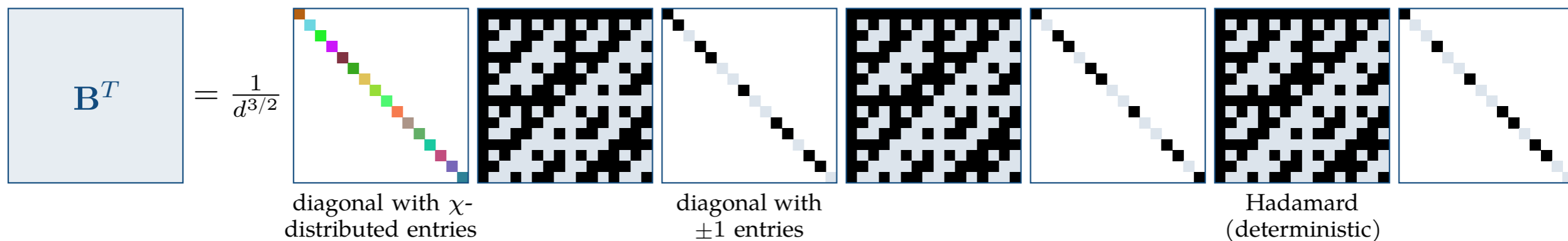
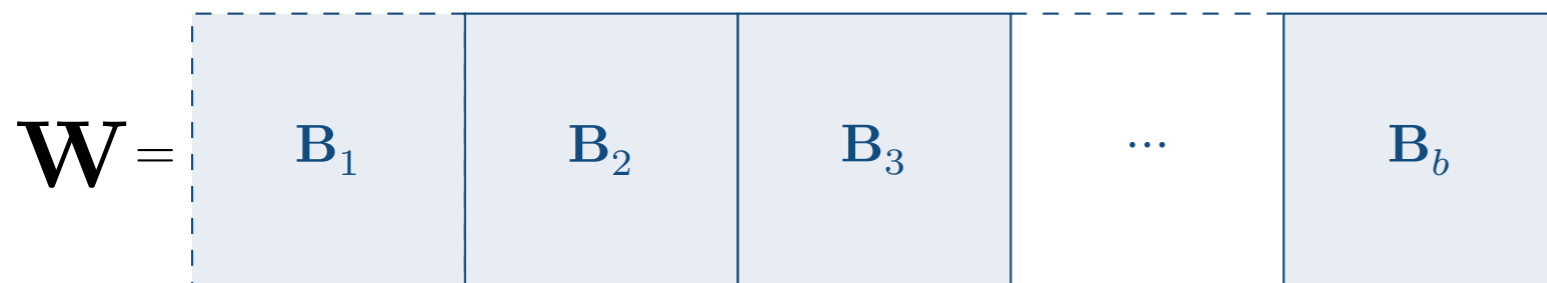
Limitations and perspectives

About the complexity:

		In memory	In time
s	\dashrightarrow	$\mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$
\mathcal{A}_i	\dashrightarrow	$\mathcal{O}(m \times d^2)$	compute S
		$m \approx (d+k) \ln(d)$	$\mathcal{O}(n \times md)$
		Gaussian	$\mathcal{O}(d^3)$
		Rank-one	$\mathcal{O}(m \times d)$
			Three op. splitting

Structured rank-one:

Use random structured matrices:



Limitations and perspectives

About the complexity:

		In memory	In time
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 $A_i \dashrightarrow \mathcal{O}(m \times d^2)$
 $\mathcal{O}(m \times d)$

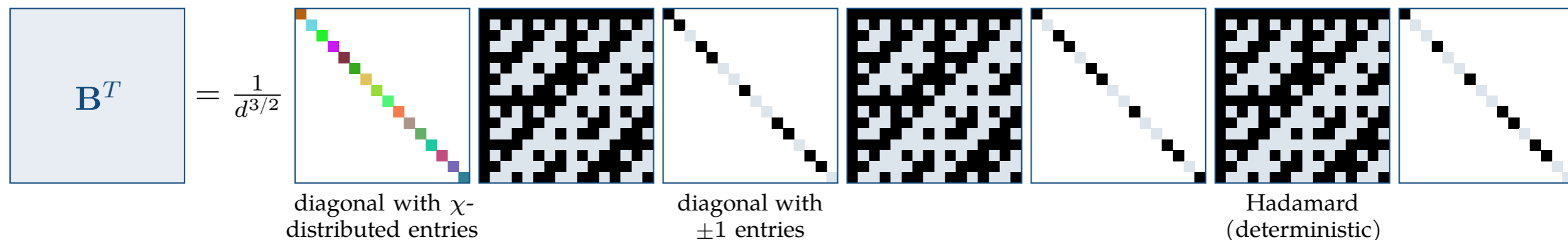
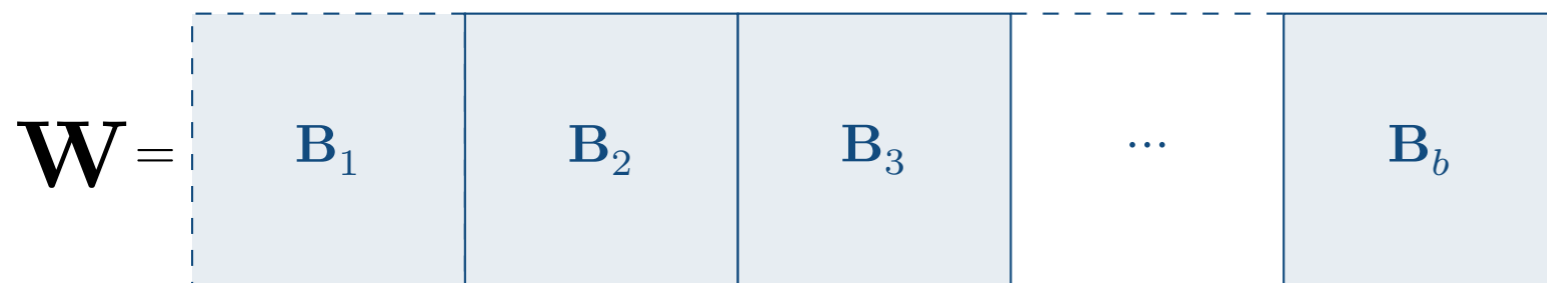
Three op. splitting
 $\mathcal{O}(d^3)$
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Structured rank-one:

Use random structured matrices:

$$\Phi(\mathbf{x}) = (|\langle \mathbf{a}_j, \mathbf{x} \rangle|^2)_{j \in \llbracket m \rrbracket}$$

$$\mathbf{a}_j \sim \text{row}_j(\mathbf{W}) \text{ NOT I.I.D!}$$



Limitations and perspectives

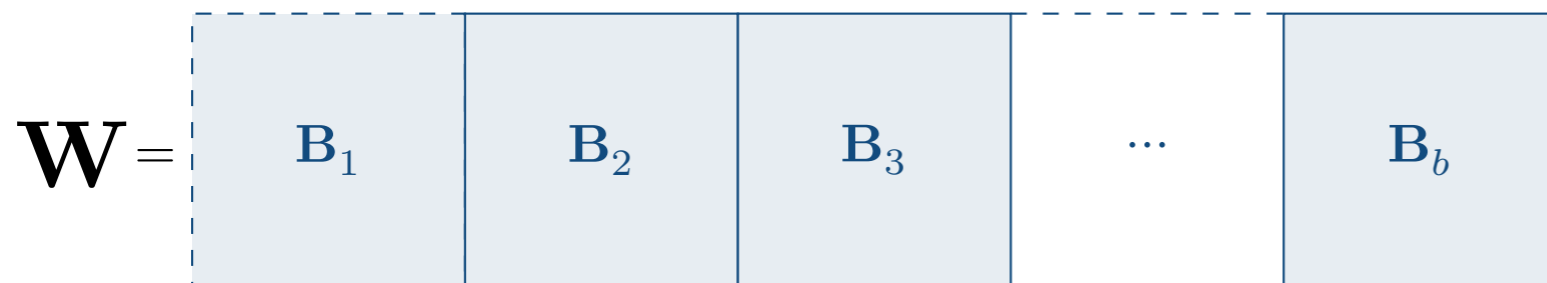
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 $\mathcal{O}(d^3)$
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Structured rank-one:

Use random structured matrices:

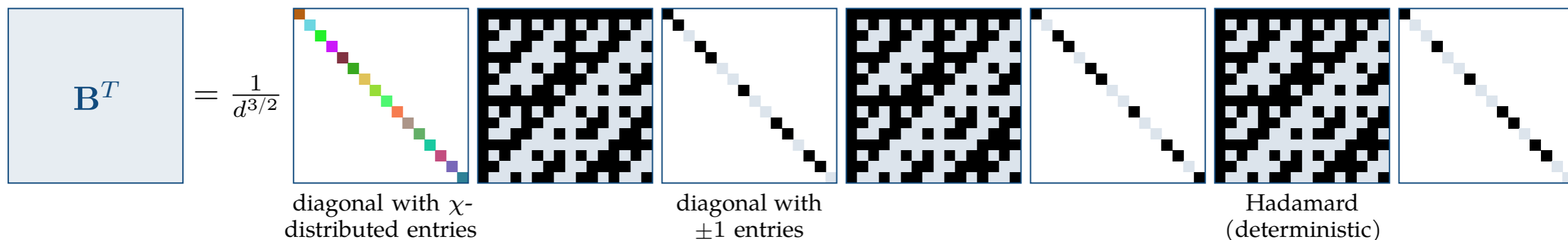


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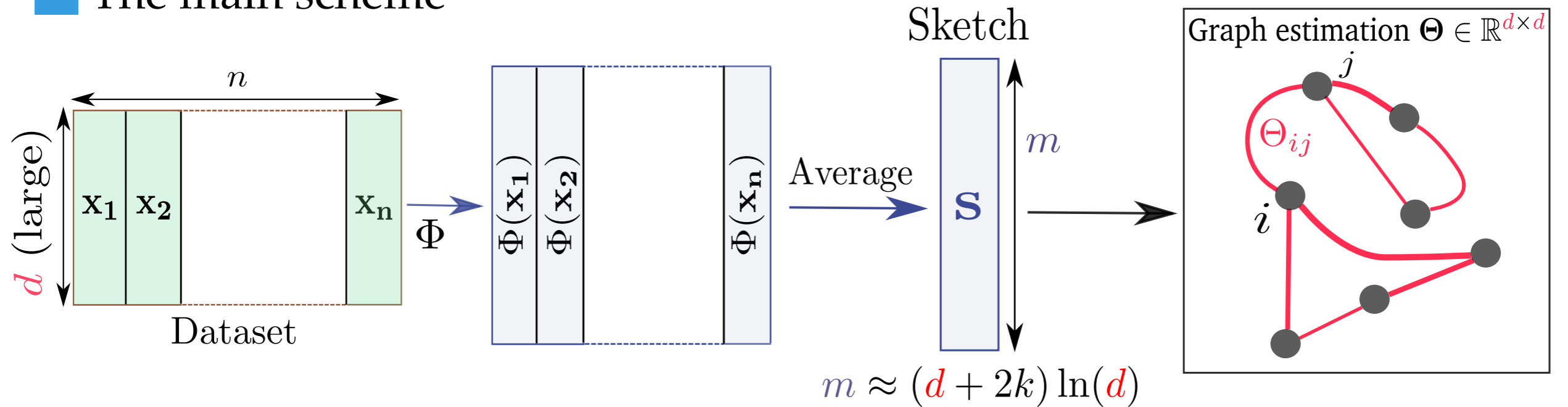
Structured rank-one

Total in memory = $\mathcal{O}(m)$



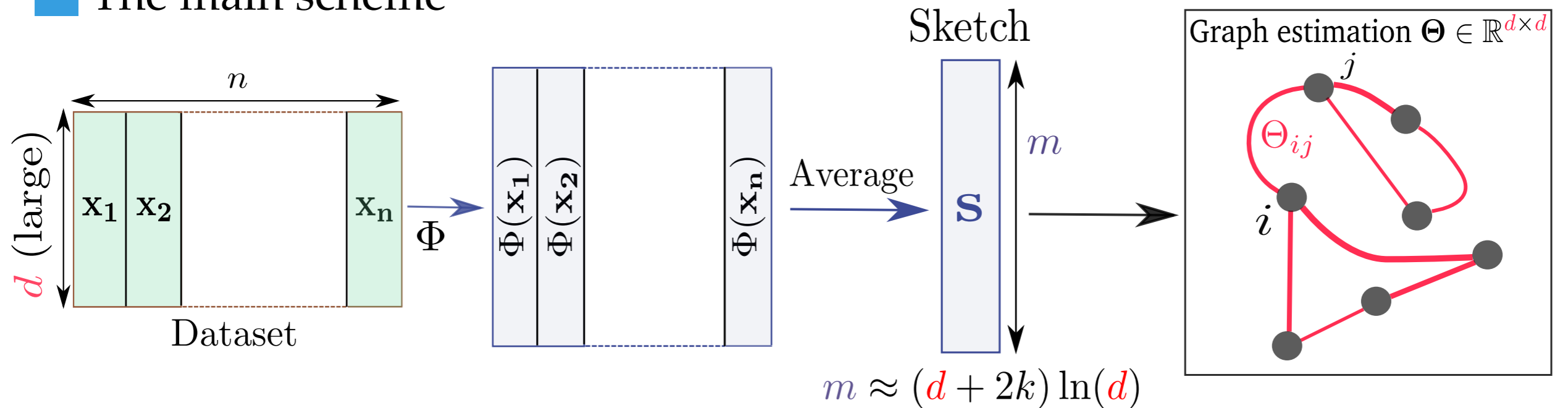
Conclusion

■ The main scheme



Conclusion

The main scheme

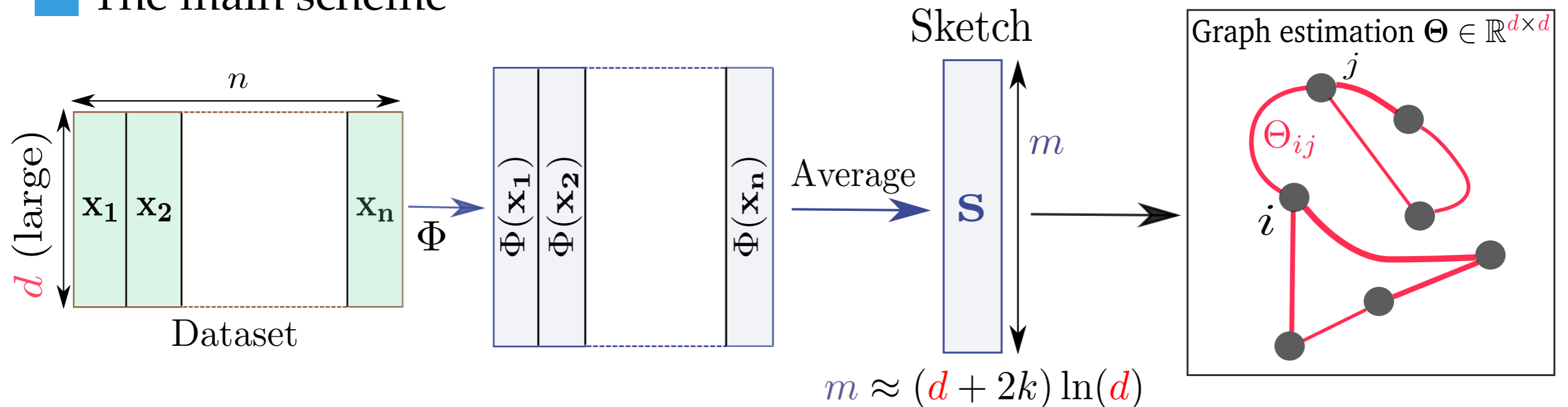


Theoretical guarantees: RIP, optimal decoders

Recovery via Davis & Yin three operator spitting

Conclusion

The main scheme



Theoretical guarantees: RIP, optimal decoders

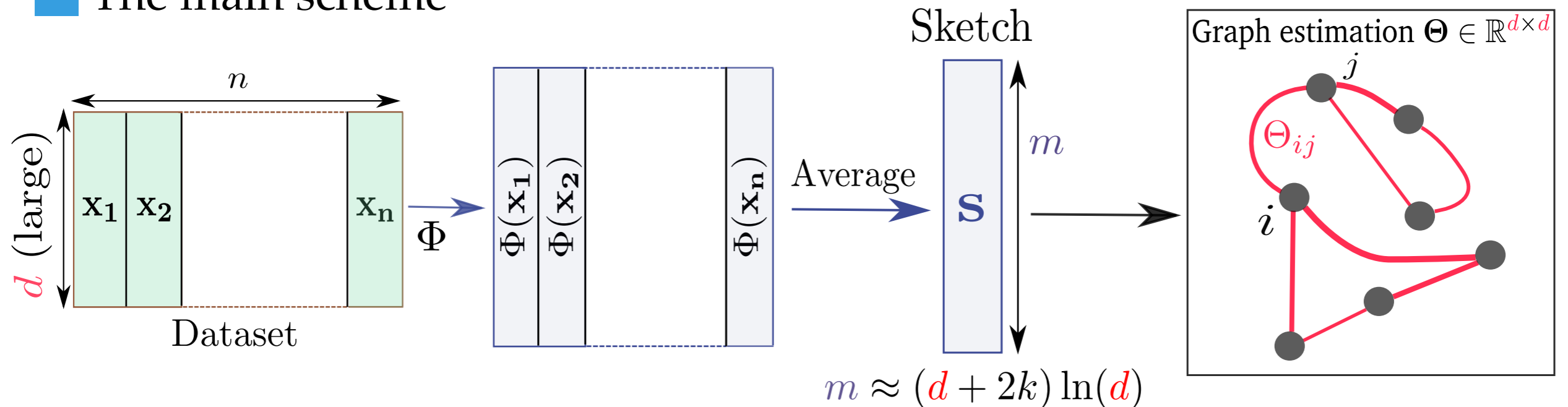
Recovery via Davis & Yin three operator spitting

Limitations: we have to store \mathcal{A} (Gaussian = $\mathcal{O}(d^3)$, rank one = $\mathcal{O}(d^2)$)

Limitations: Algo not that efficient (Greedy approaches ?)

Conclusion

The main scheme



■ Theoretical guarantees: RIP, optimal decoders

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■ Limitations: we have to store \mathcal{A} (Gaussian = $\mathcal{O}(d^3)$, rank one = $\mathcal{O}(d^2)$)

■ Limitations: Algo not that efficient (Greedy approaches ?)

■ Perspectives: structured operators, different algo (greedy approaches ?)

theoretical guarantees ?

Thank you!

