

Inria



ENS DE LYON

Towards Compressive Recovery of Sparse Precision Matrices

Titouan Vayer

joint work with

Rémi Gribonval

Paulo Gonçalves

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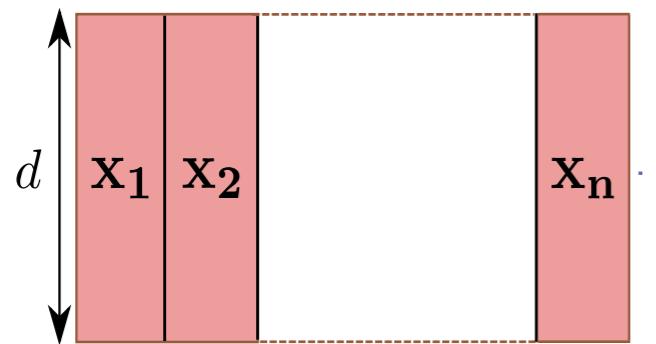
| Overview of the talk

- 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

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

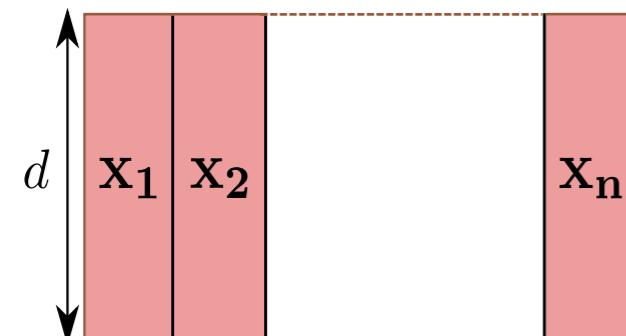


$$\mathbf{x}_i \in \mathbb{R}^d \sim \mu$$

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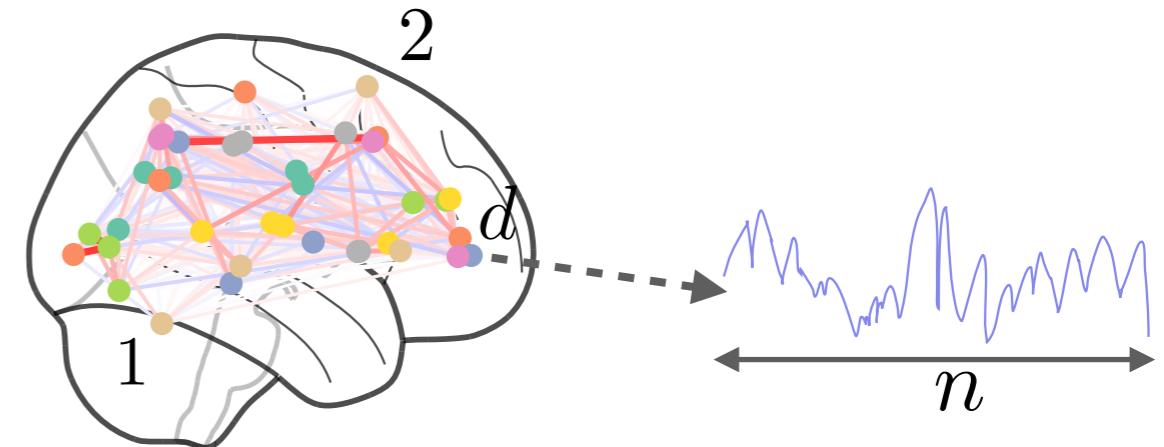
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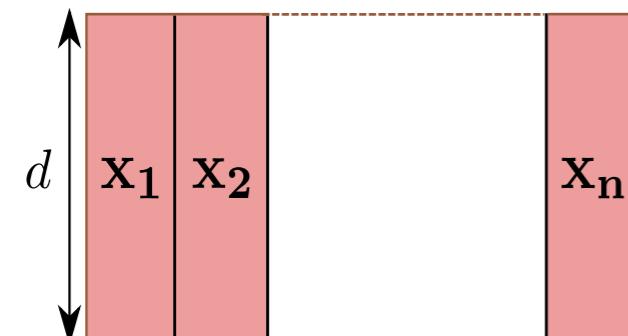
■ Output: graph of **relations between the d variables**



Graph Learning

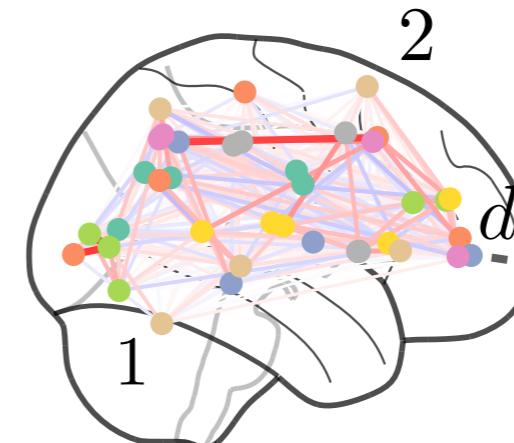
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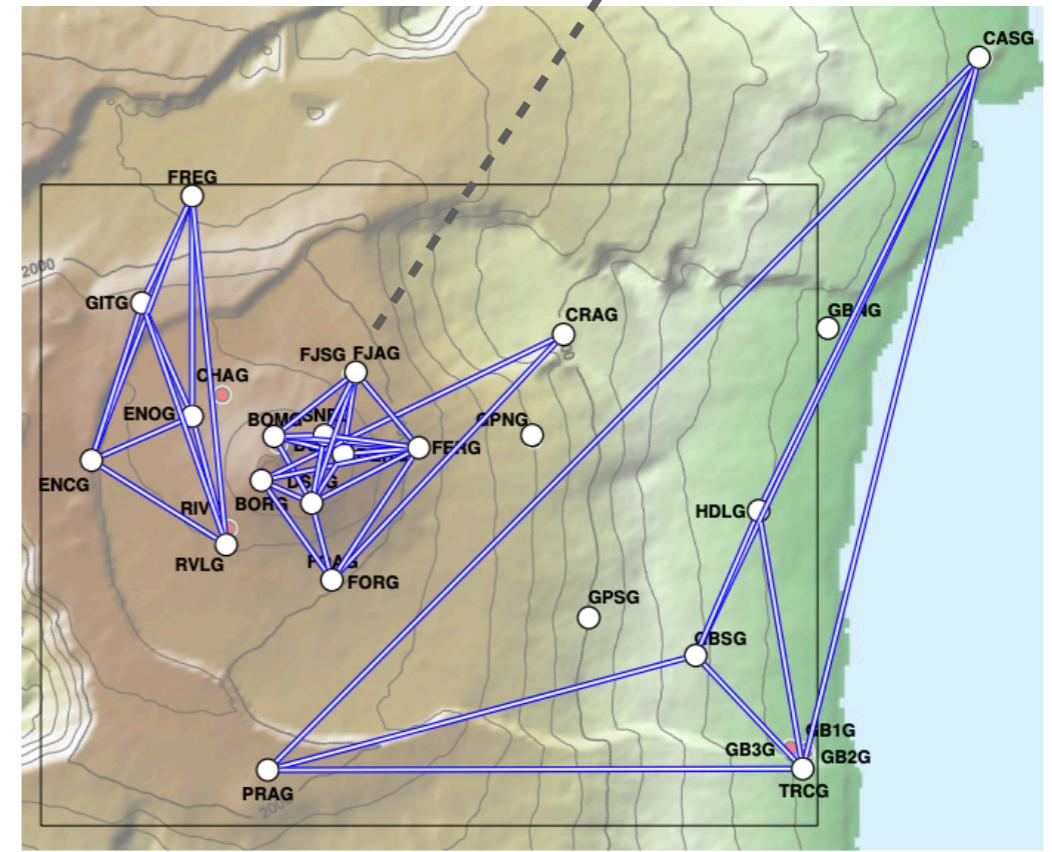
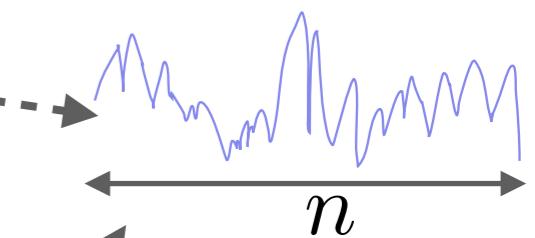


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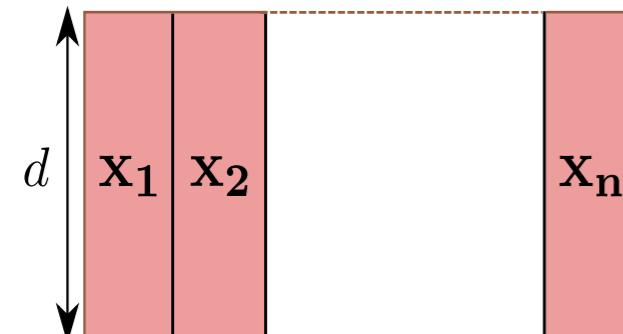
also: genomics,
biological networks, energy...



Graph Learning

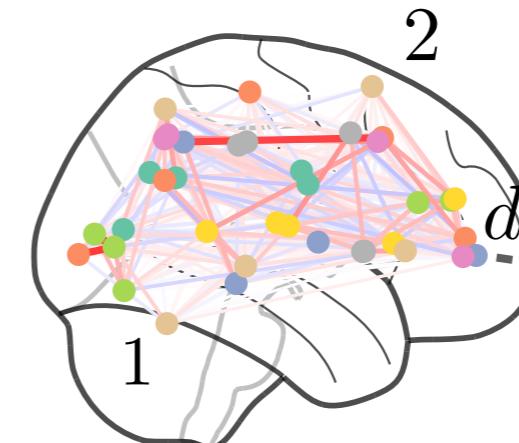
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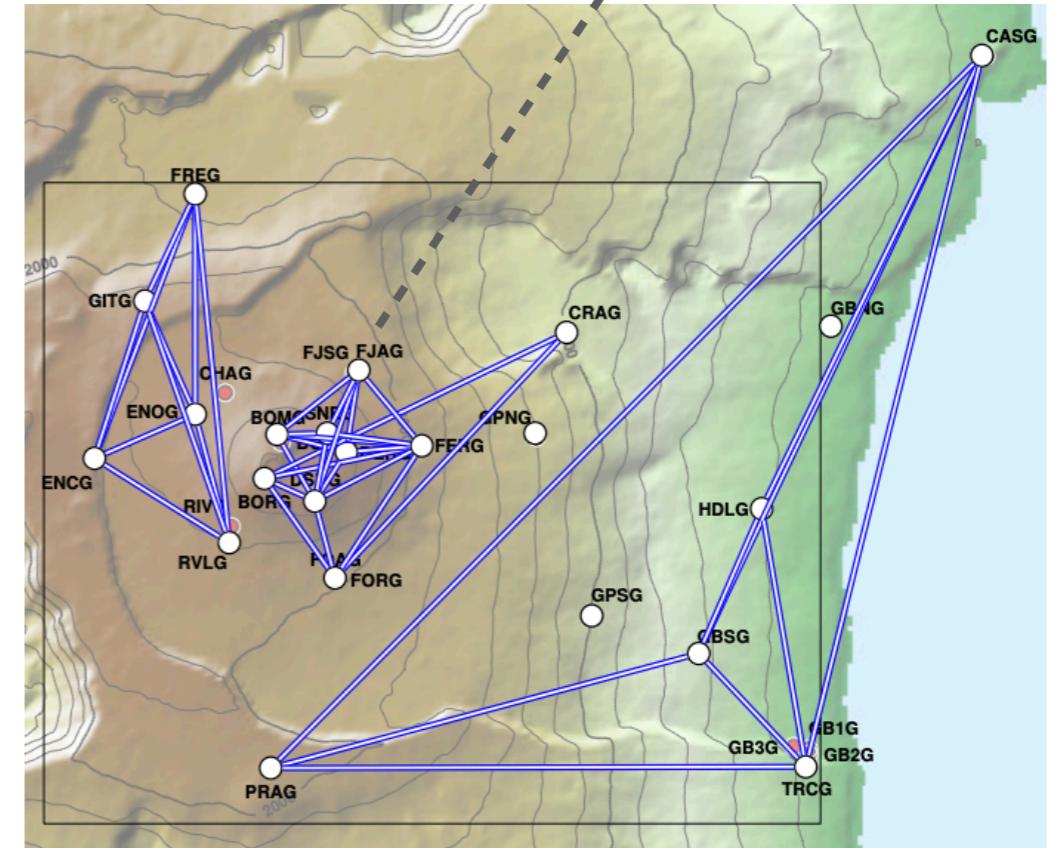


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■ Graph modeled as a matrix:

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

Θ_{ij} : interaction between variable i and j

| statistical correlations

| statistical dependencies

| Graphical LASSO

Side note

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

| Graphical LASSO

■ 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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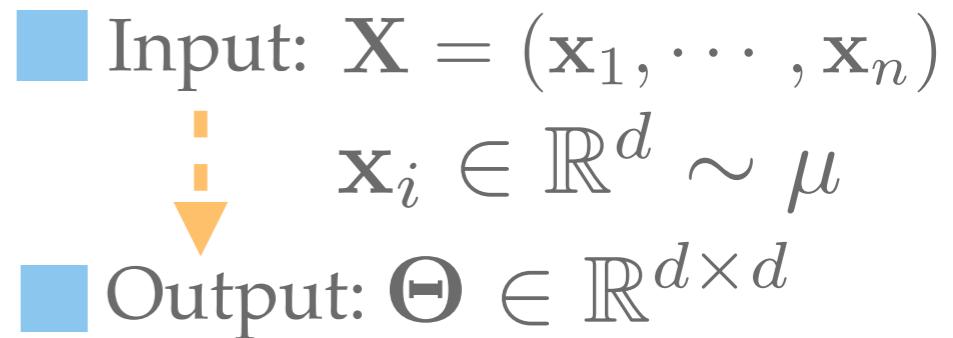
■ Maximum Likelihood estimator

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

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

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

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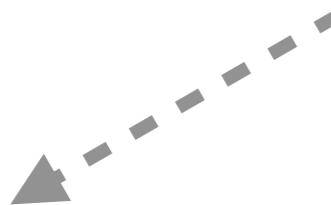
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May not be true
in high dim $n < d$

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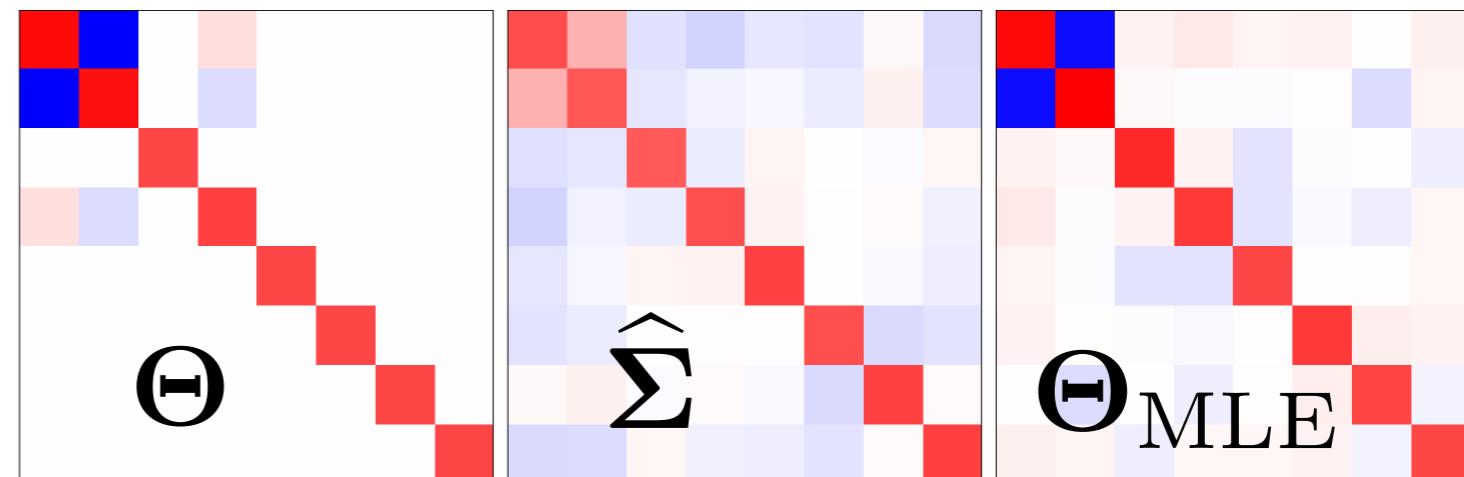
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■ When $\widehat{\Sigma}$ is invertible $\Theta_{MLE} = (\widehat{\Sigma})^{-1}$ \dashrightarrow usually not sparse

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



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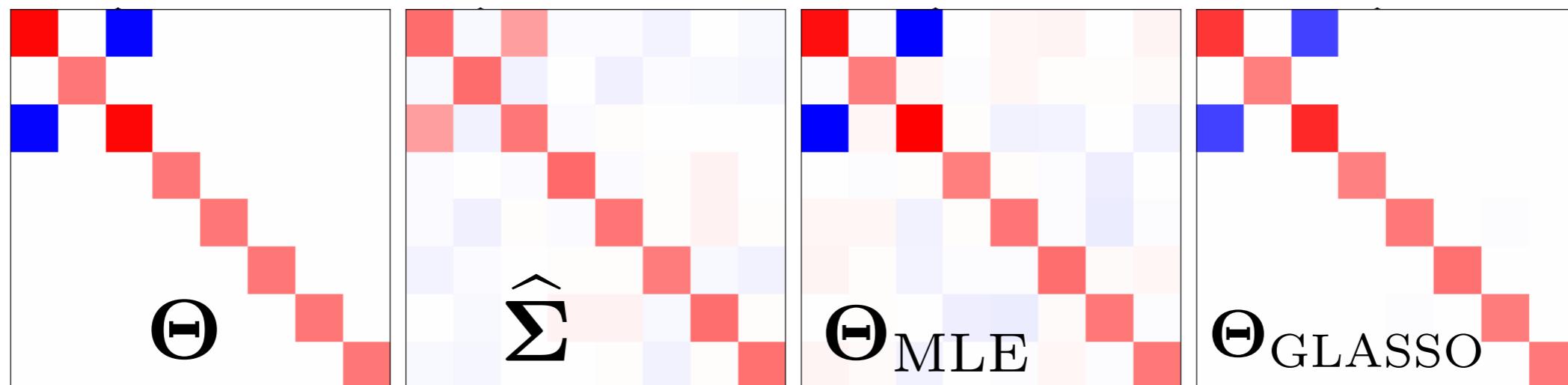
Gaussian assumption $\mu = \mathcal{N}(0, \Sigma = \Theta^{-1})$

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

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

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

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



Side note

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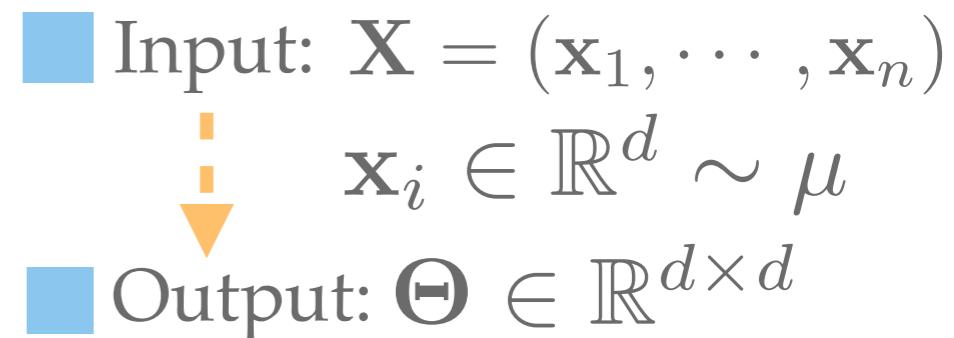
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■ Optimization: convex problem

Coordinate descent

Involves LASSO steps (on the rows)

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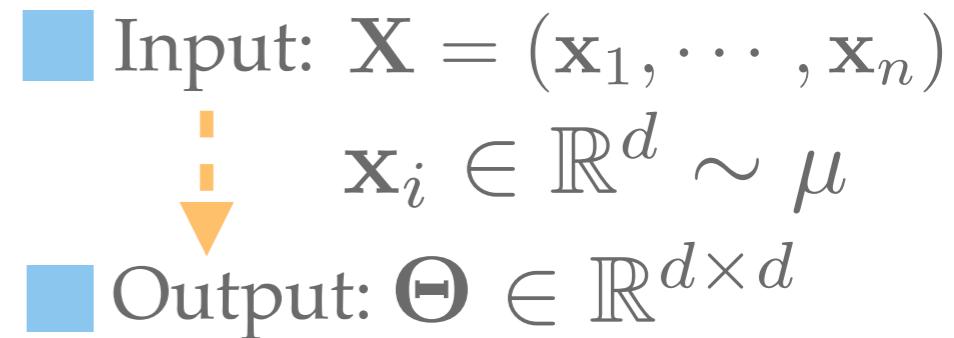
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■ Many large scale variants:

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

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

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$\Theta = \mathcal{L}(\mathcal{G})$ is a Laplacian matrix of a graph

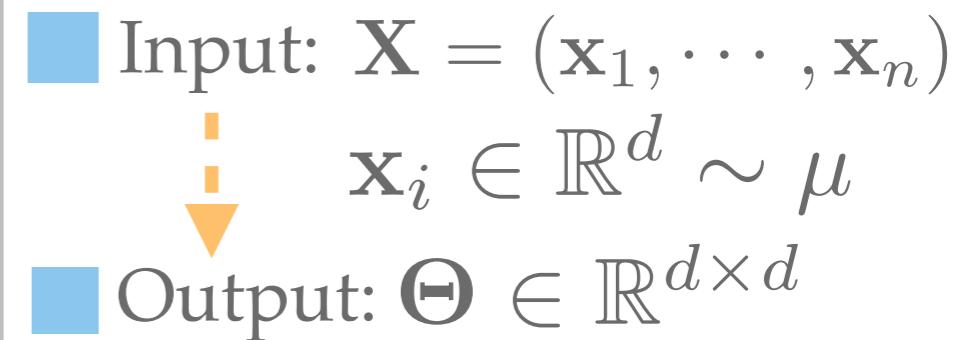
[Kumar, 2020]

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■ Complexity of GLASSO:

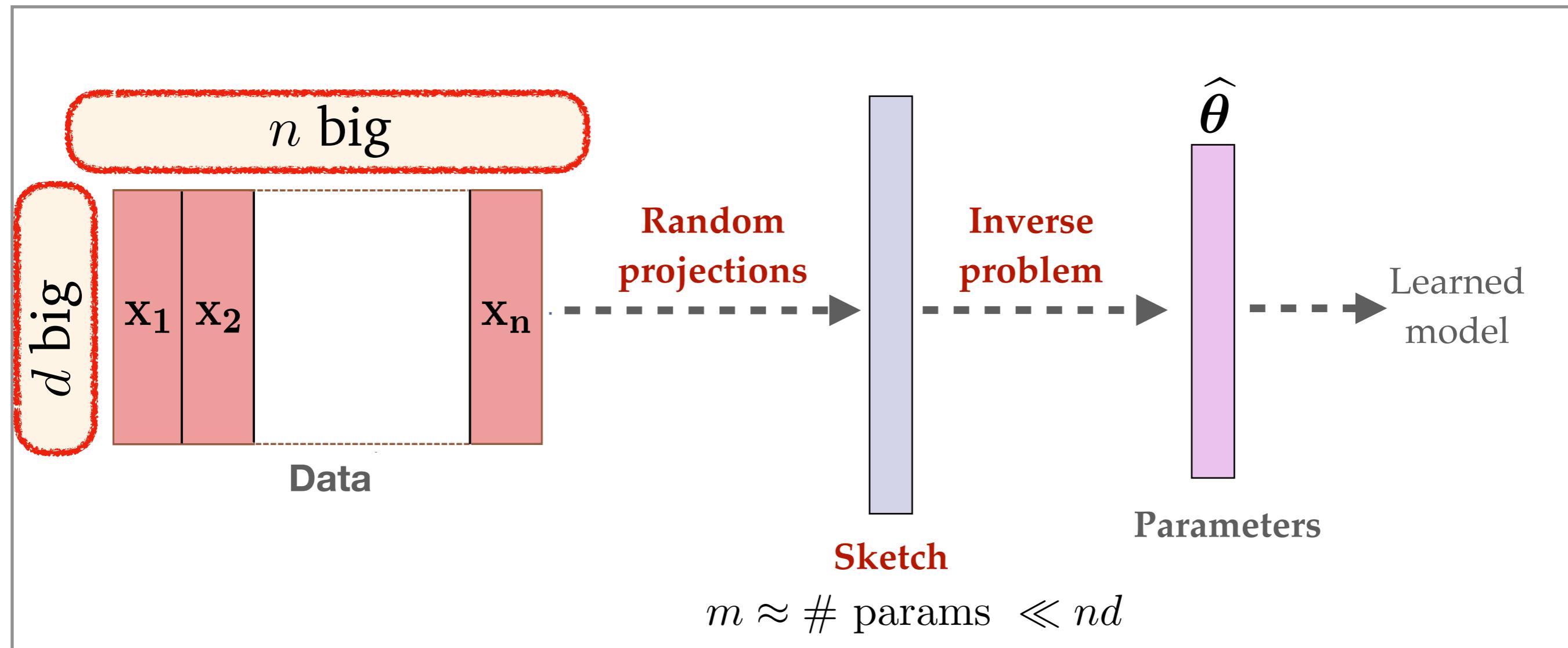


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| The sketching approach

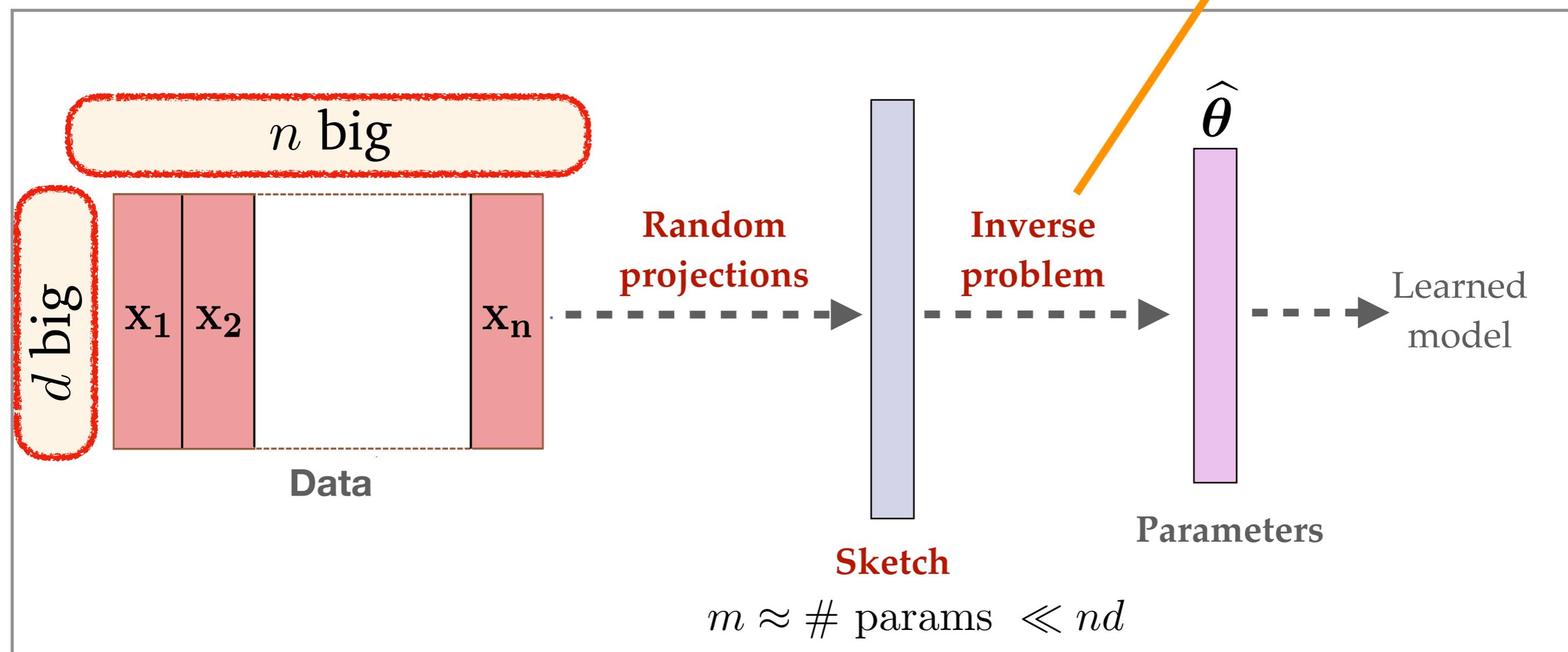
■ High overview:



The sketching approach

generalizes the principles of compressed sensing

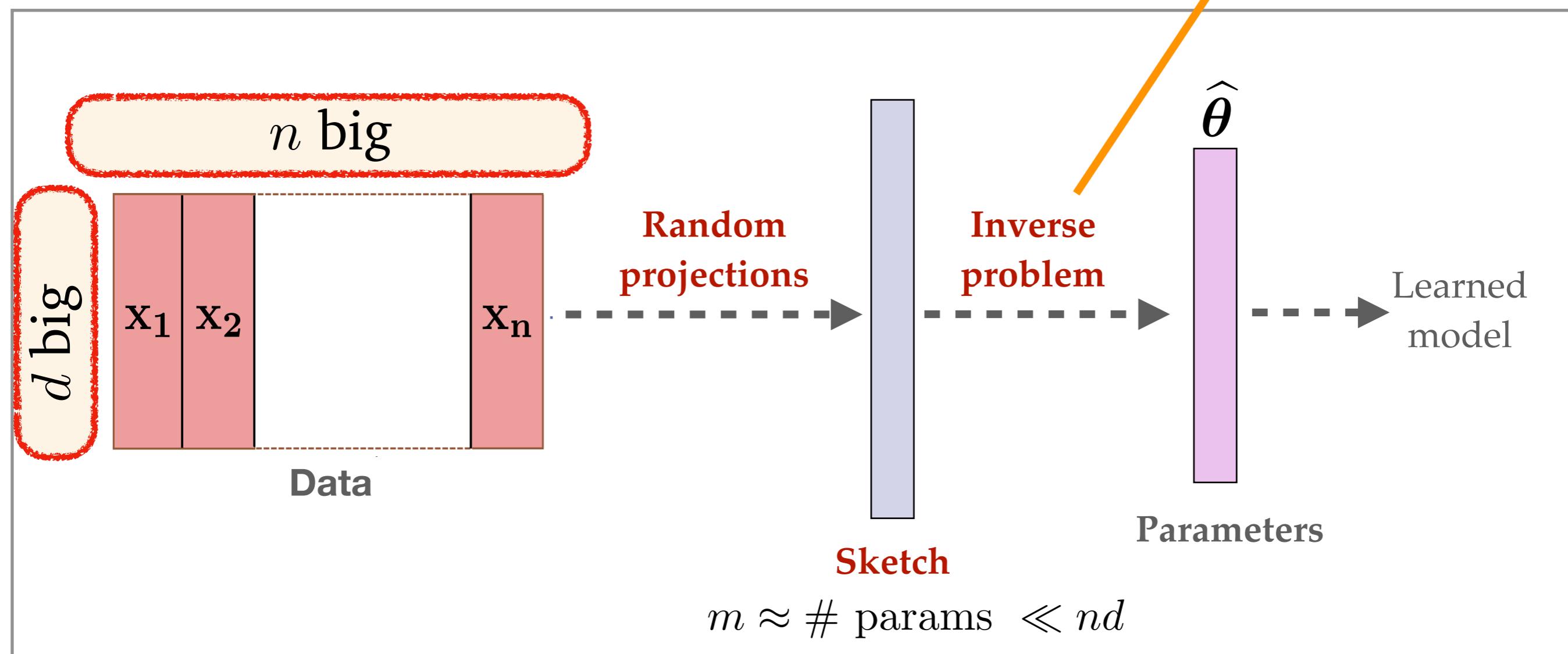
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■ High overview:



■ Advantages for storage and transfer

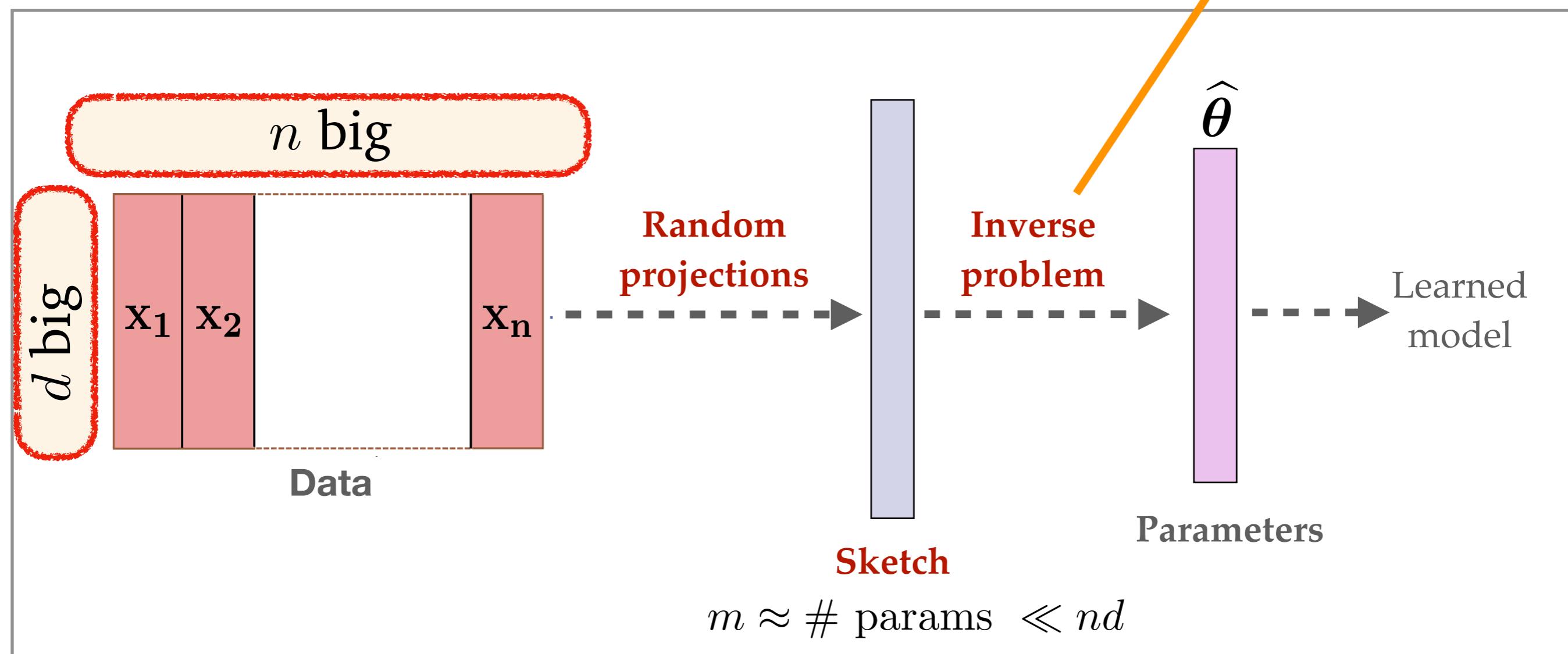
■ Many statistical problems

How to choose Φ ? -> connection to optimal transport

The sketching approach

generalizes the principles of **compressed sensing**

High overview:



■ Advantages for **storage and transfer**

■ Many statistical problems

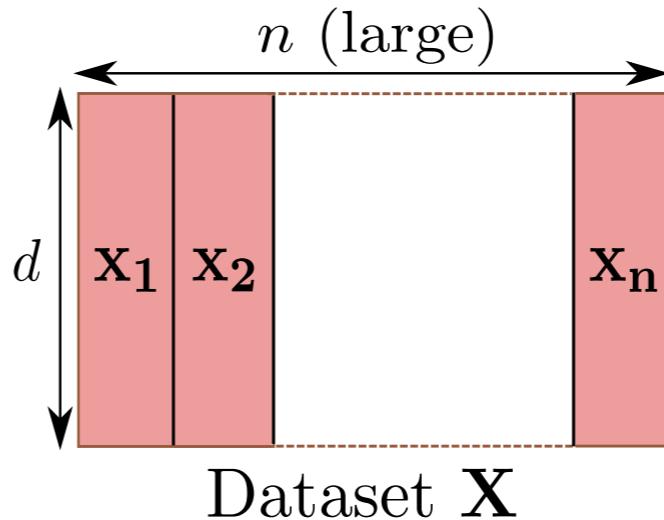
How to choose Φ ? -> connection to **optimal transport**

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, ...

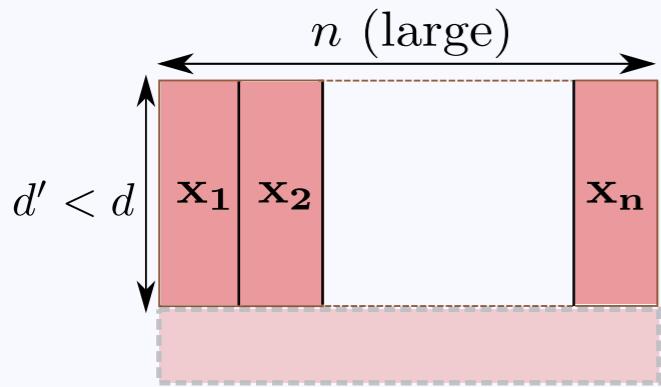
The sketching approach

« Dimension » reduction

- « Low-dim » representation of a dataset

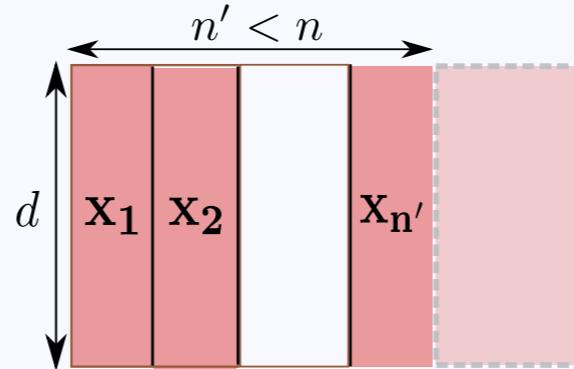


Dimension reduction



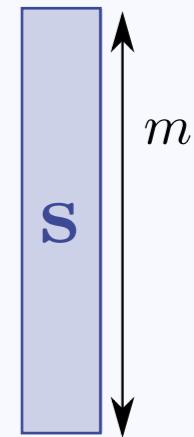
- Random projections (JL lemma)
- Feature selection
- Minimum distortion embedding, PCA

Subsampling



- Coresets
- Importance sampling

Here: linear « sketch »

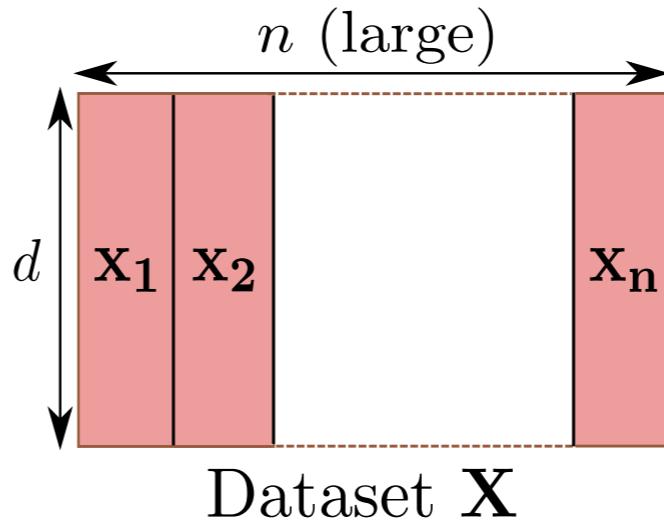


- Only one vector

The sketching approach

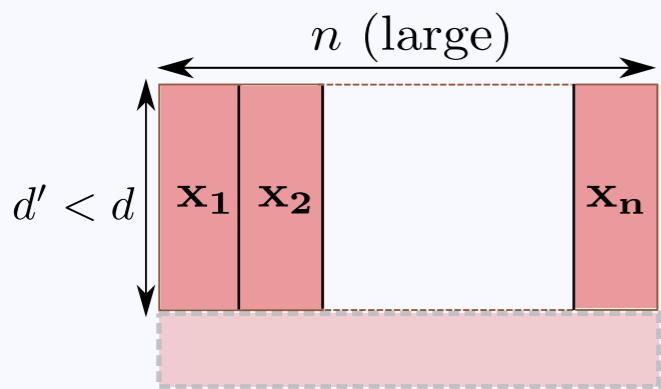
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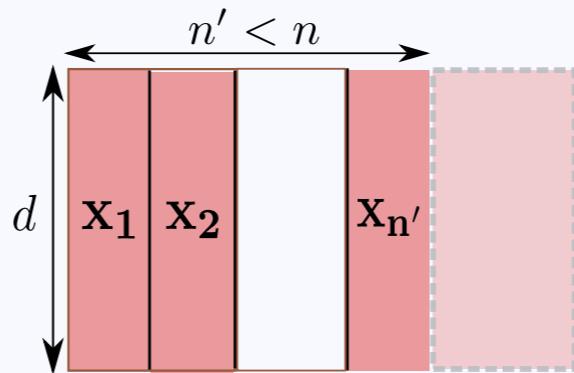
How do we sketch ? How do we learn from sketch ?

Dimension reduction



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Here: linear « sketch »



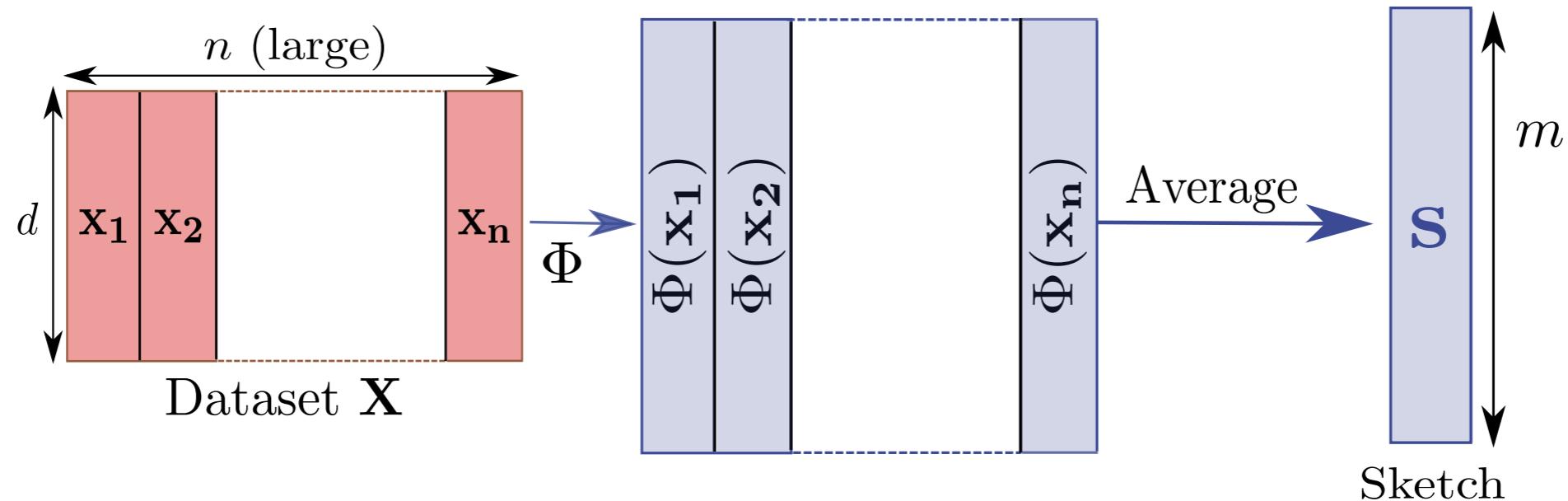
- Only one vector

| The sketching approach

■ Obtaining the sketch

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

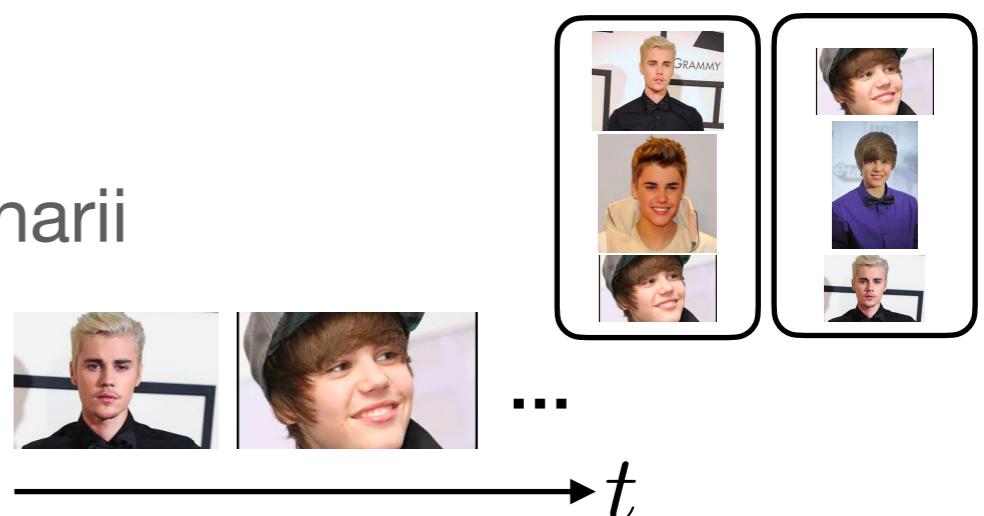
- Averaging **n points** -> $S := \frac{1}{n} \sum_{i=1}^n \Phi(x_i)$



■ Average is a simple idea but

- Suitable for **distributed /streaming** scenarii

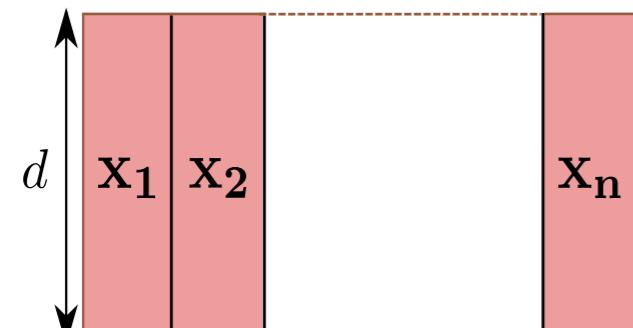
- It can be calculated in **parallel**



| Goal of this talk

■ Input: a dataset

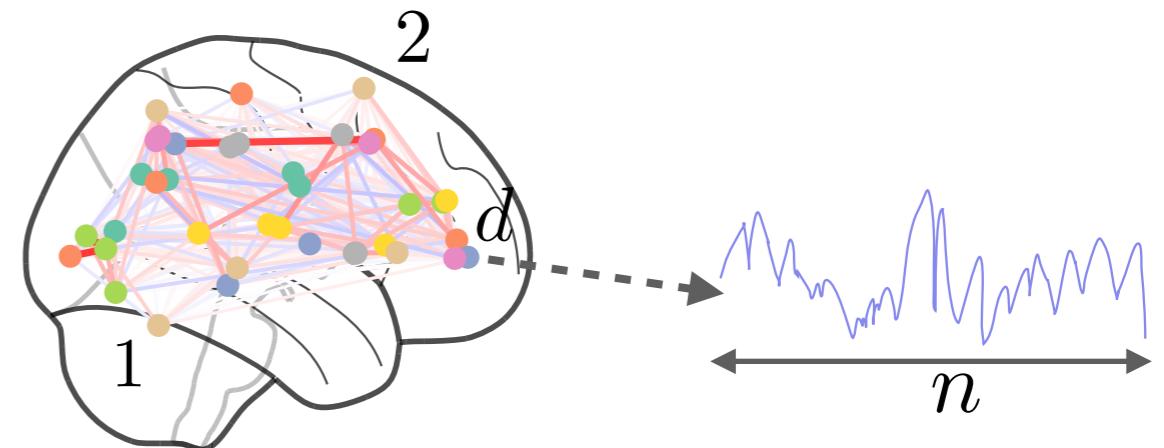
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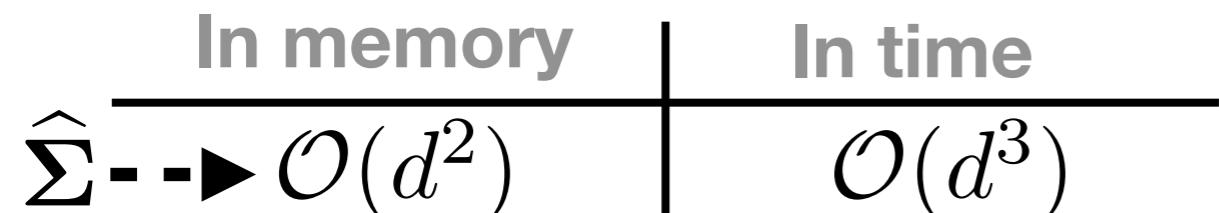
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GLASSO

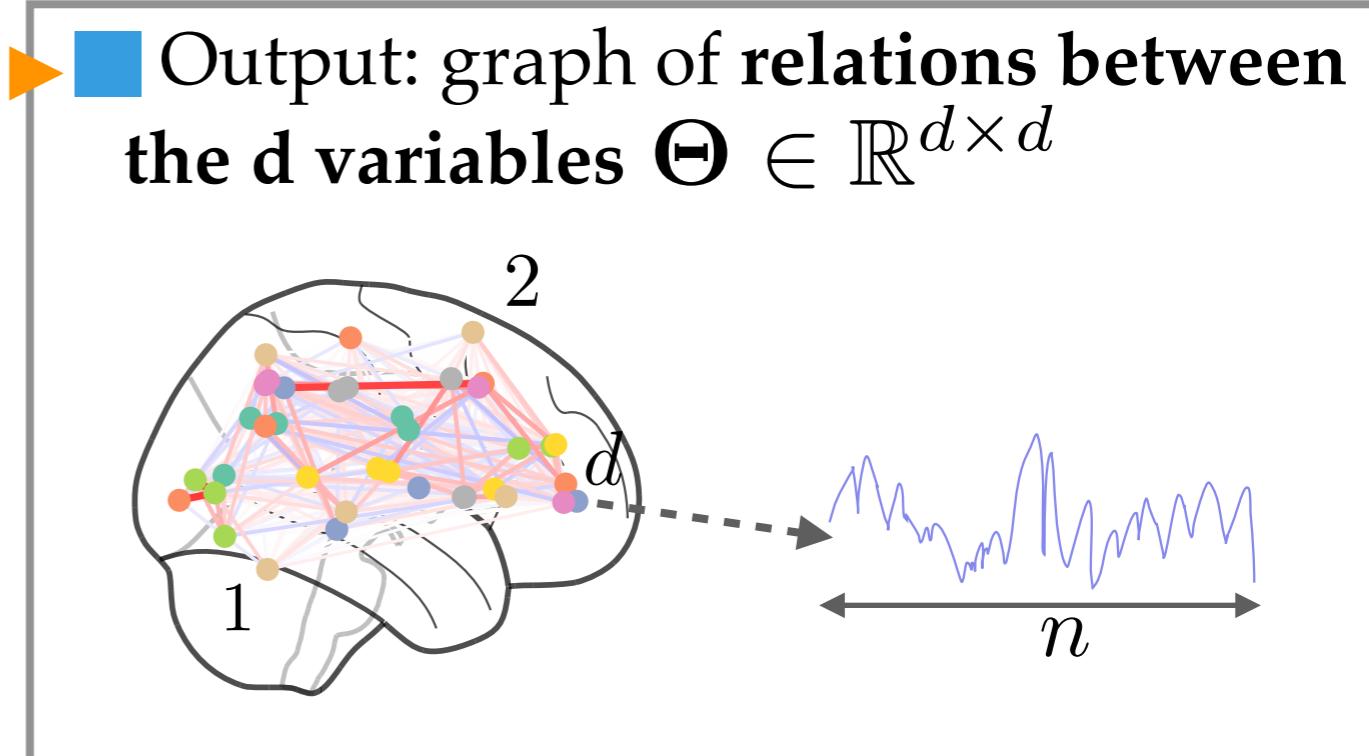
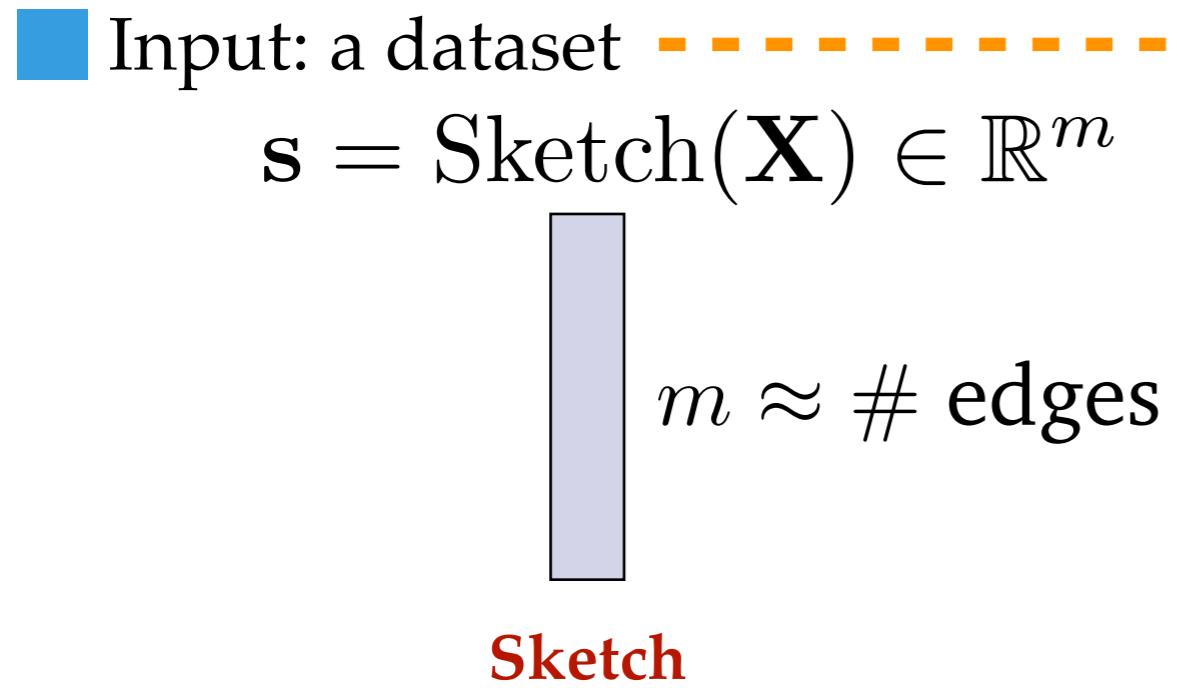
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GLASSO



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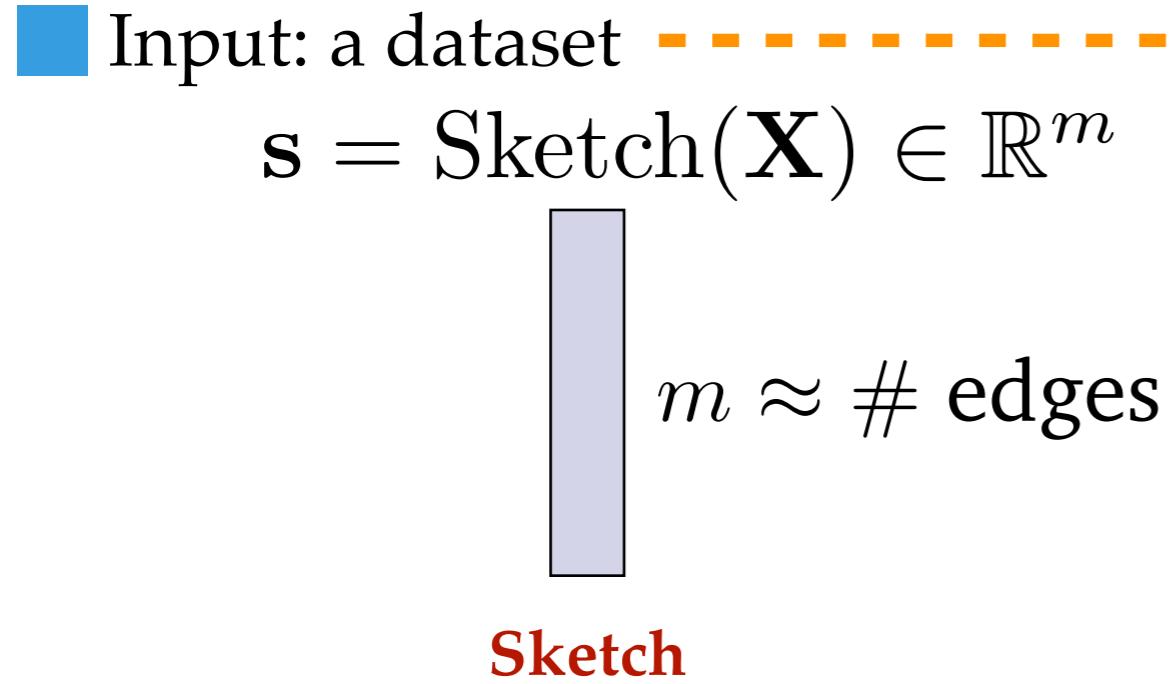
GLASSO

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

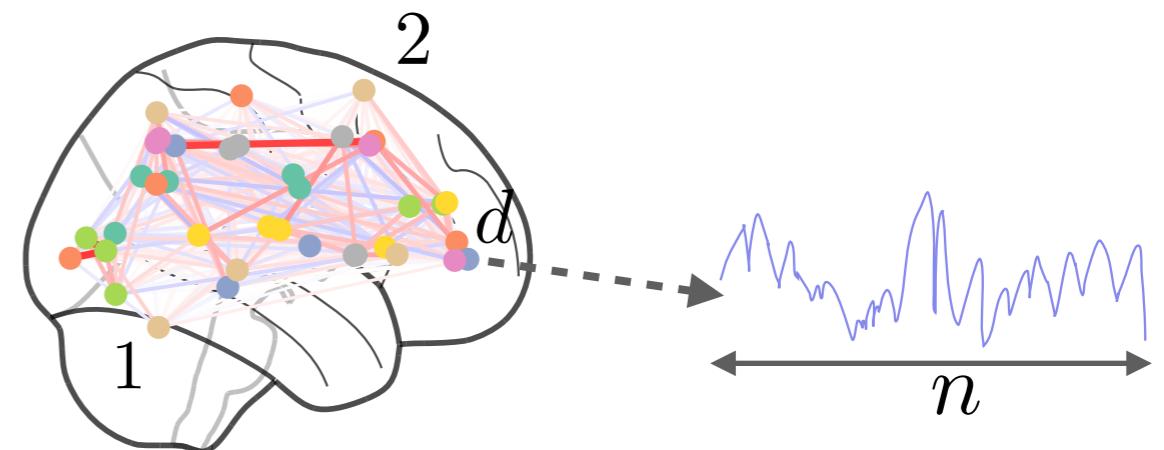
Sketching

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

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

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Structured rank-one

End of presentation

Rank-one measurements

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

Inspired by works on low-rank matrix completion

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Inspired by works on low-rank matrix completion

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

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

Emp. cov.

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

| Towards theoretical compressive recovery

■ Objective/setting

- | $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n) \quad \mathbf{x}_i \in \mathbb{R}^d \sim \mu \quad \text{with} \quad \mathbb{E}_{\mathbf{x} \sim \mu} [\mathbf{x}\mathbf{x}^\top] = \boldsymbol{\Sigma}_\star = \boldsymbol{\Theta}_\star^{-1}$
- | $\boldsymbol{\Theta}_\star \in \mathfrak{S}$ in some **low-dim. space** (e.g. sparse p.d matrices = sparse graph)
- The objective is to find $\boldsymbol{\Theta}_\star$ from the sketch $\mathbf{s} \in \mathbb{R}^m$

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■ The objective is to find $\boldsymbol{\Theta}_*$ from the sketch $\mathbf{s} \in \mathbb{R}^m$

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

$$\boxed{\text{Find } \boldsymbol{\Theta}_* \text{ from } \mathbf{s} = \mathcal{A}\widehat{\boldsymbol{\Sigma}} = \mathcal{A}\boldsymbol{\Sigma}_* + \mathbf{e}}$$

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- Notable difference

We want **the inverse of the matrix**

that is measured

not find $\boldsymbol{\Sigma}_*$ given $\mathcal{A}\boldsymbol{\Sigma}_* + \mathbf{e}$

| Towards theoretical compressive recovery



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



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

Towards theoretical compressive recovery

■ Objective/setting

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

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not find $\boldsymbol{\Sigma}_*$ given $\mathcal{A}\boldsymbol{\Sigma}_* + \mathbf{e}$

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

Key assumption:
 $\boldsymbol{\Theta}_*$ lies in some **low-dim. space**

| Towards theoretical compressive recovery

■ Example of low-dim space

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

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

sym. positive definite matrices

localized spectrum

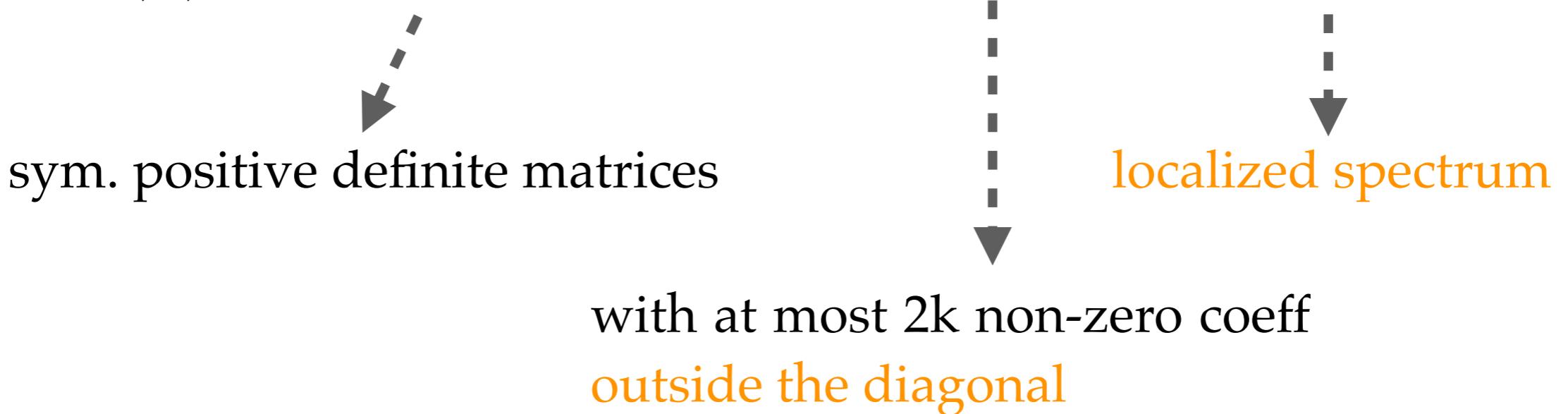
with at most $2k$ non-zero coeff
outside the diagonal

| Towards theoretical compressive recovery

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- Sparse precision (= sparse graph) matrices with known spectrum
- Called the model set

| The Restricted Isometric Property

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invRIP

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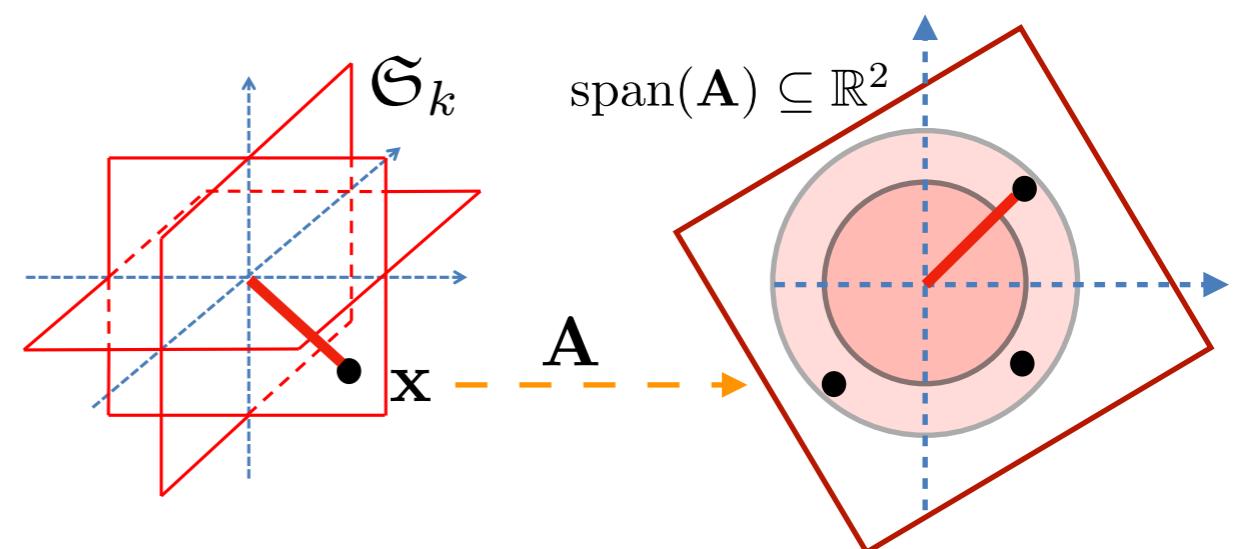
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■ The restricted isometric property (RIP) [Candes & Tao, 2005]

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

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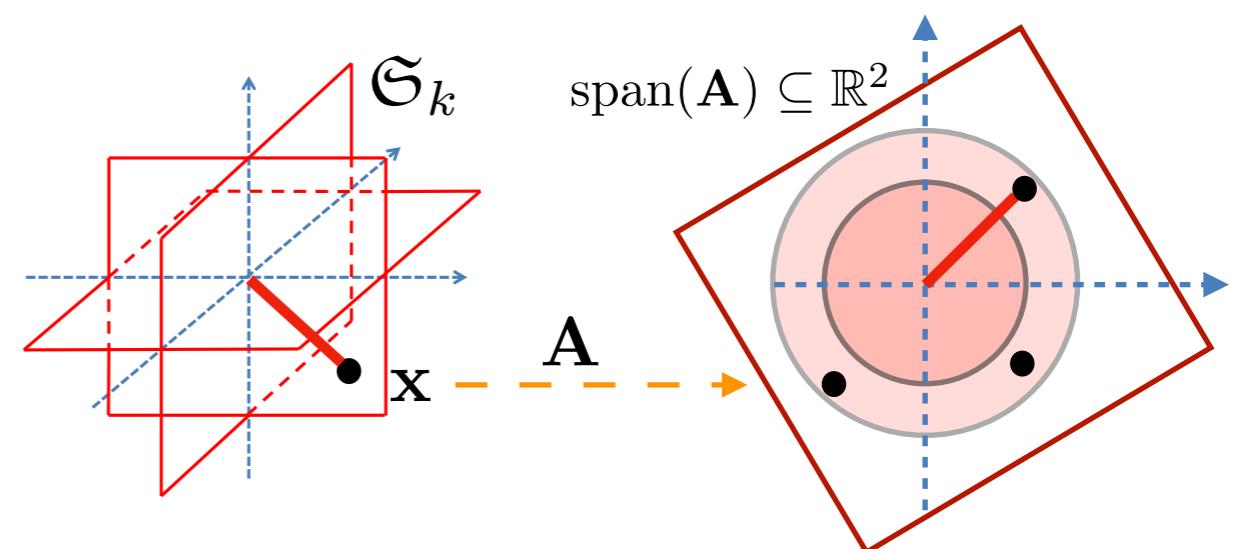
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- E.g. **Gaussian matrices**

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

... also Johnson-Lindenstrauss Lemma

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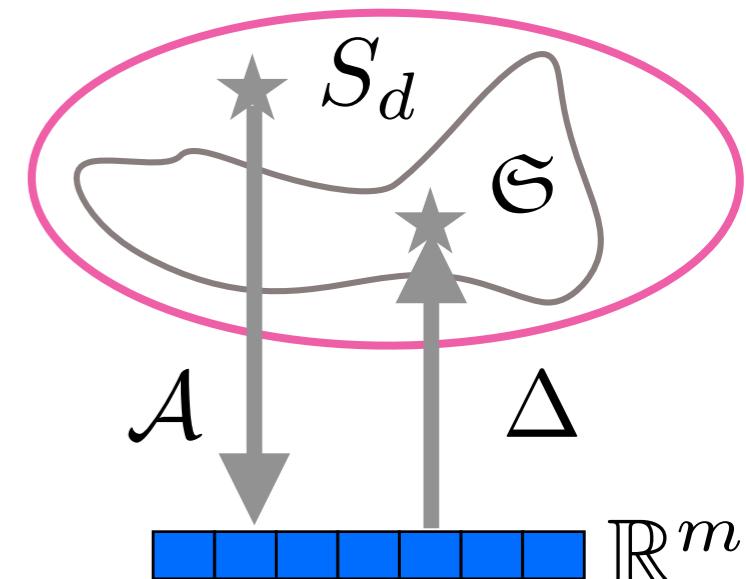
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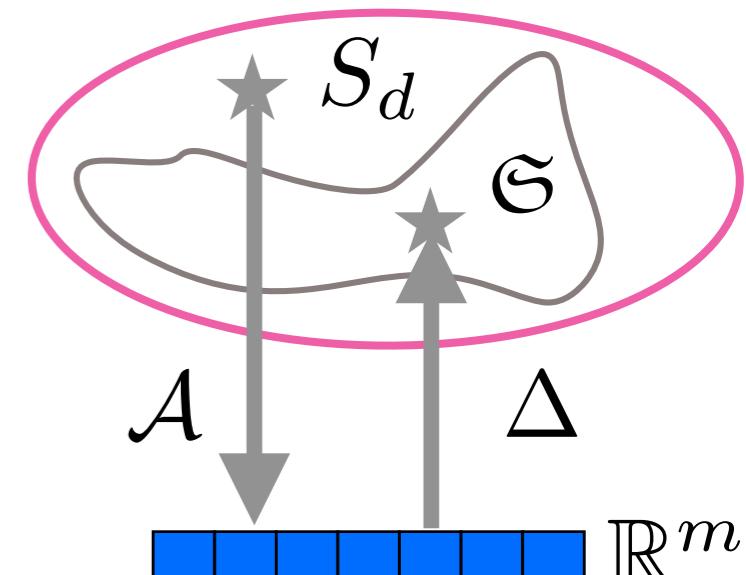
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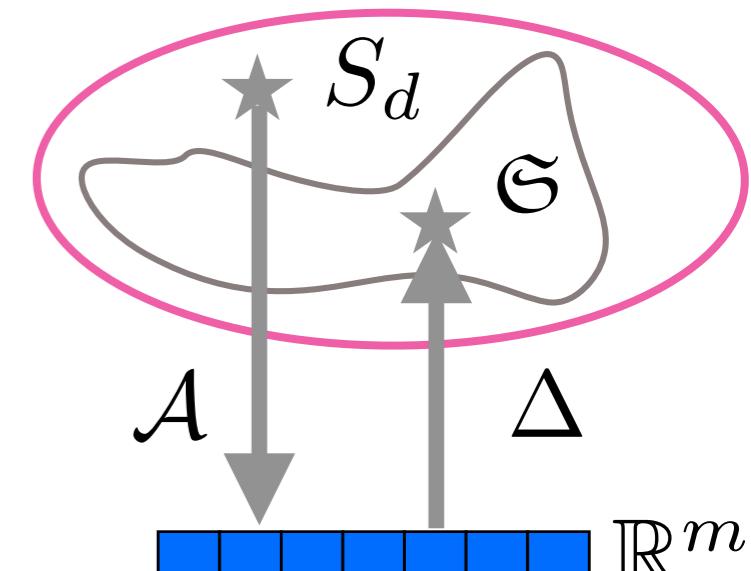
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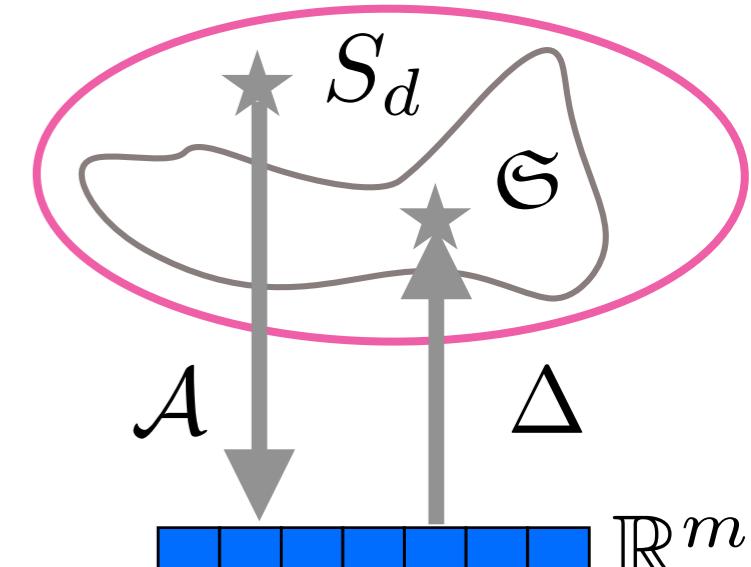
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Happiness and joy

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$\mathcal{A}\mathbf{S} = \frac{1}{\sqrt{m}} (\langle \mathbf{A}_j, \mathbf{S} \rangle_F)_{j \in [\![m]\!]}$ **is random** \dashrightarrow **invRIP** with high prob.



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■ Two ingredients

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

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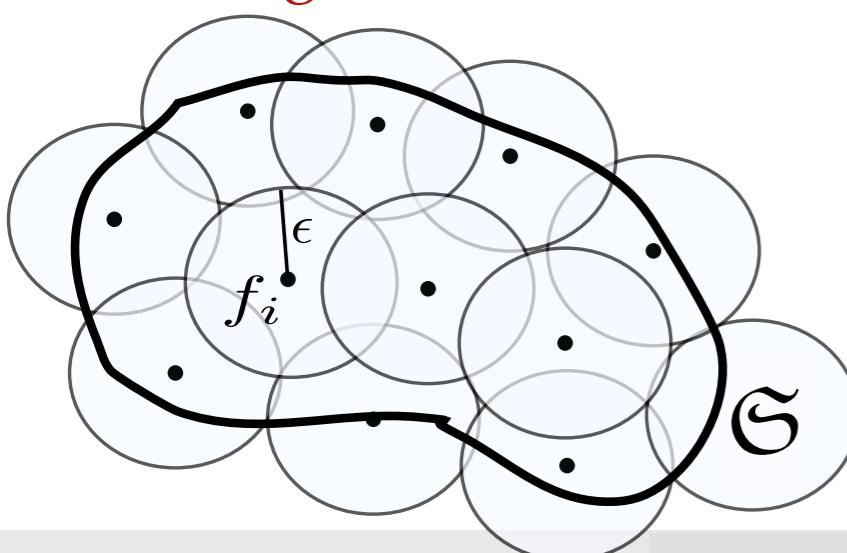
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- The set \mathfrak{S} is sufficiently « low-dim », has « low complexity »

Covering numbers $\dashleftarrow \mathcal{N}(\mathfrak{S}, \varepsilon)$ is sufficiently small



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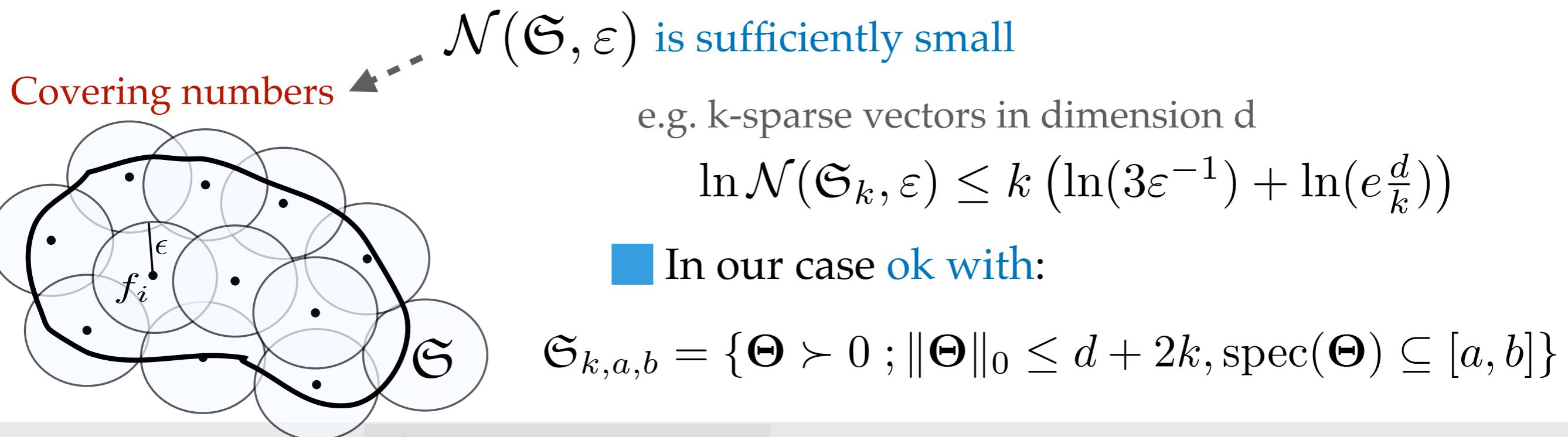


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Main results

Gaussian measurements

- Sketch with $\mathbf{A}_j \underset{i.i.d}{\sim} \mathcal{N}(0, \mathbf{I}_{d \times d})$
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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: $\Delta[\mathbf{s}] \in \arg \min_{\Theta \in \mathfrak{S}} \|\mathcal{A}(\Theta^{-1}) - \mathbf{s}\|_2$
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$$\widetilde{\Theta} \in \arg \min_{\substack{\Theta \in S_d(\mathbb{R}) \\ a\mathbf{I}_d \preceq \Theta \preceq b\mathbf{I}_d}} \frac{1}{2} \|\mathcal{A}(\text{inv}(\Theta)) - \mathbf{s}\|_2^2 + \lambda \|\Theta\|_{1,\text{off}}$$

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■ Non-convex with non-smooth penalty + smooth fidelity term $\rightarrow \nabla f$

■ We use Davis & Yin three-operator splitting scheme

$$\text{prox}_{\lambda\varphi}(\Theta) \triangleq \arg \min_{\mathbf{A} \in \mathbb{R}^{d \times d}} \varphi(\mathbf{A}) + \frac{1}{2\lambda} \|\mathbf{A} - \Theta\|_F^2$$

[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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■ We know the prox

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

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

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

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

[Davis & Yin, 2017]

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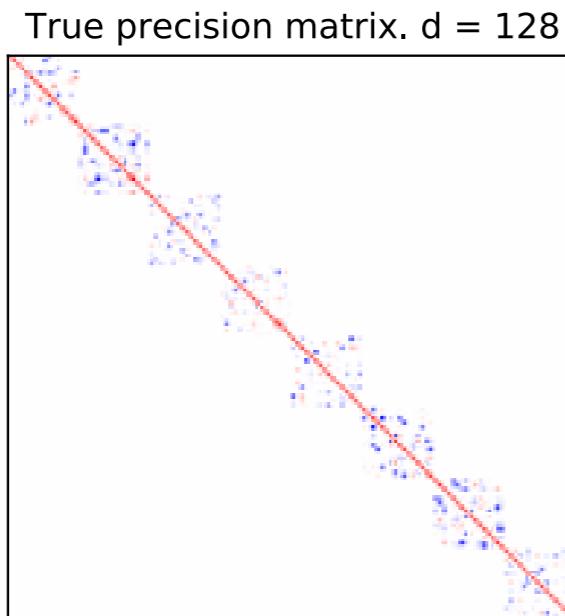
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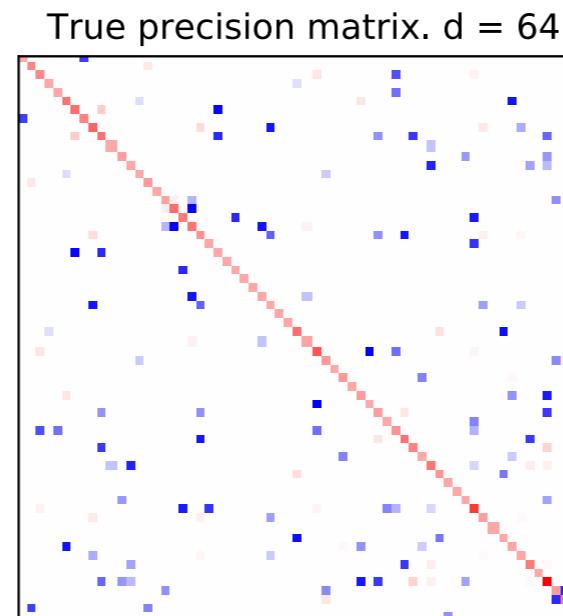
Setting:

- We generate sparse Θ_\star according to some laws

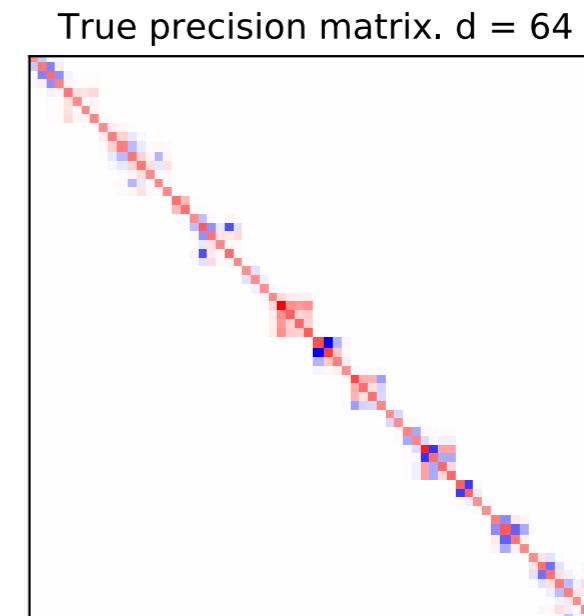
Erdös-Réyni



Sklearn



Powerlaw



- 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

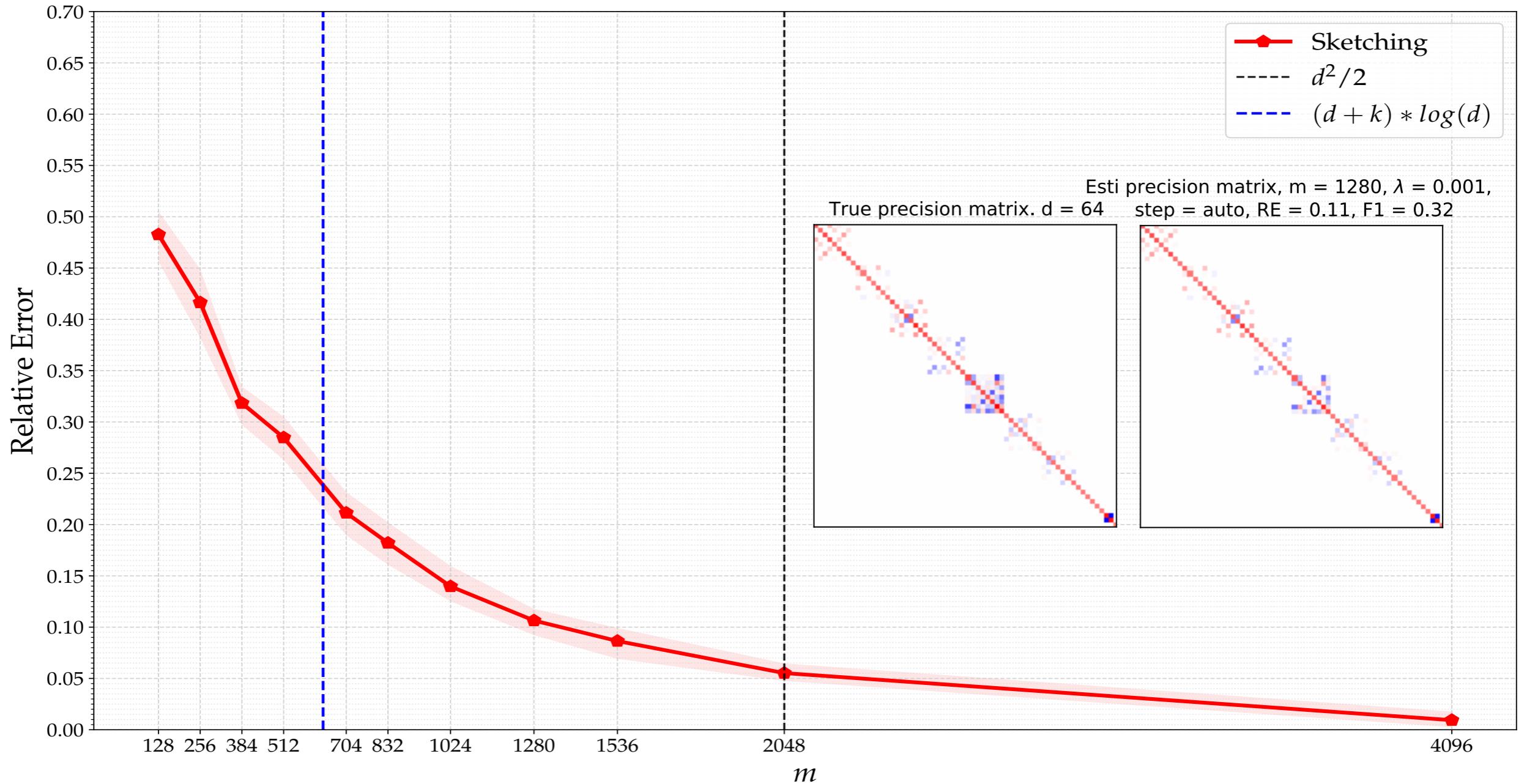
Sketch of the true cov

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

$$\mathbf{s} = \mathcal{A}\Sigma_\star$$

$$(n = +\infty)$$

Erdős-Réyni $d = 64$



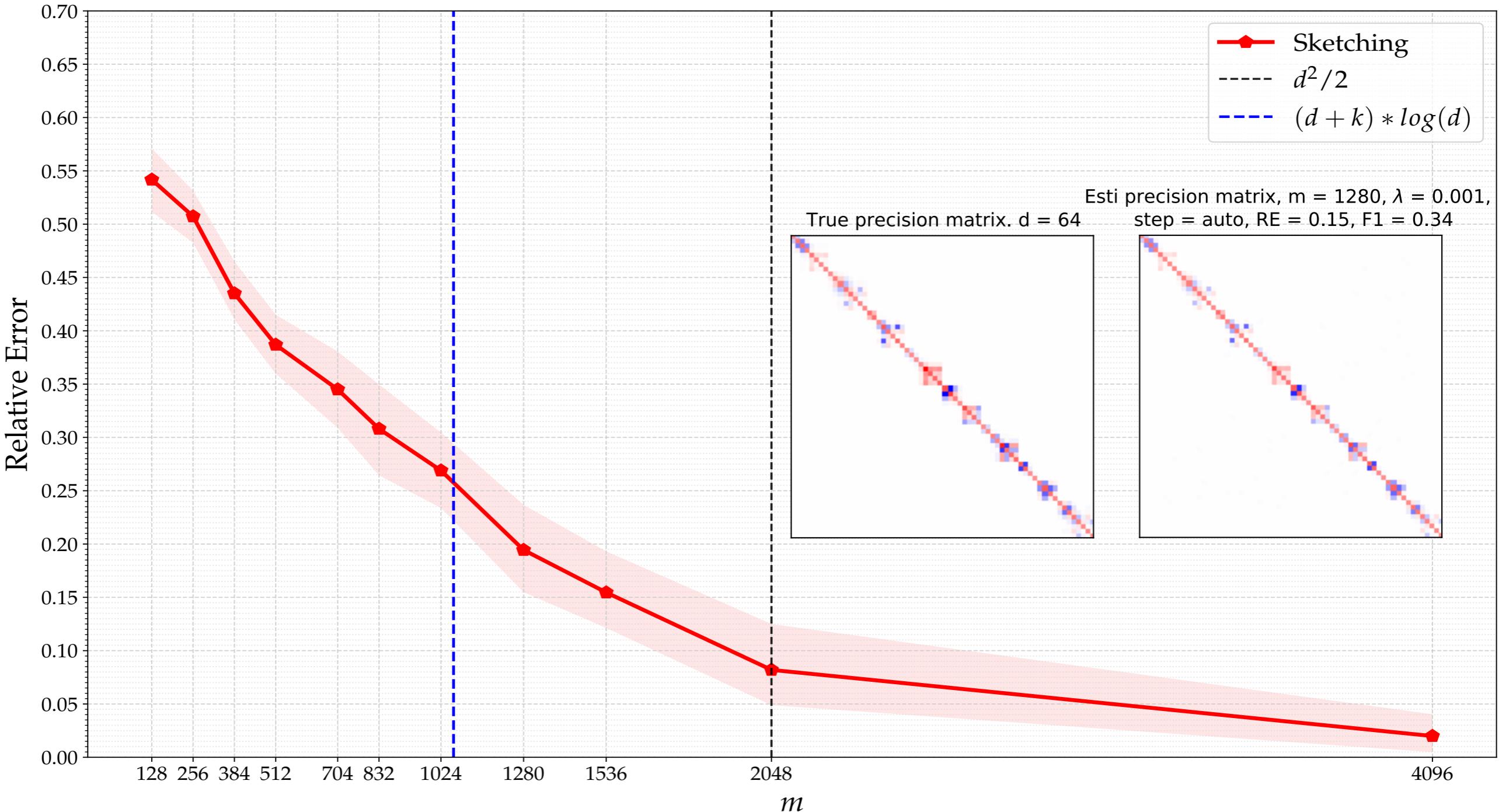
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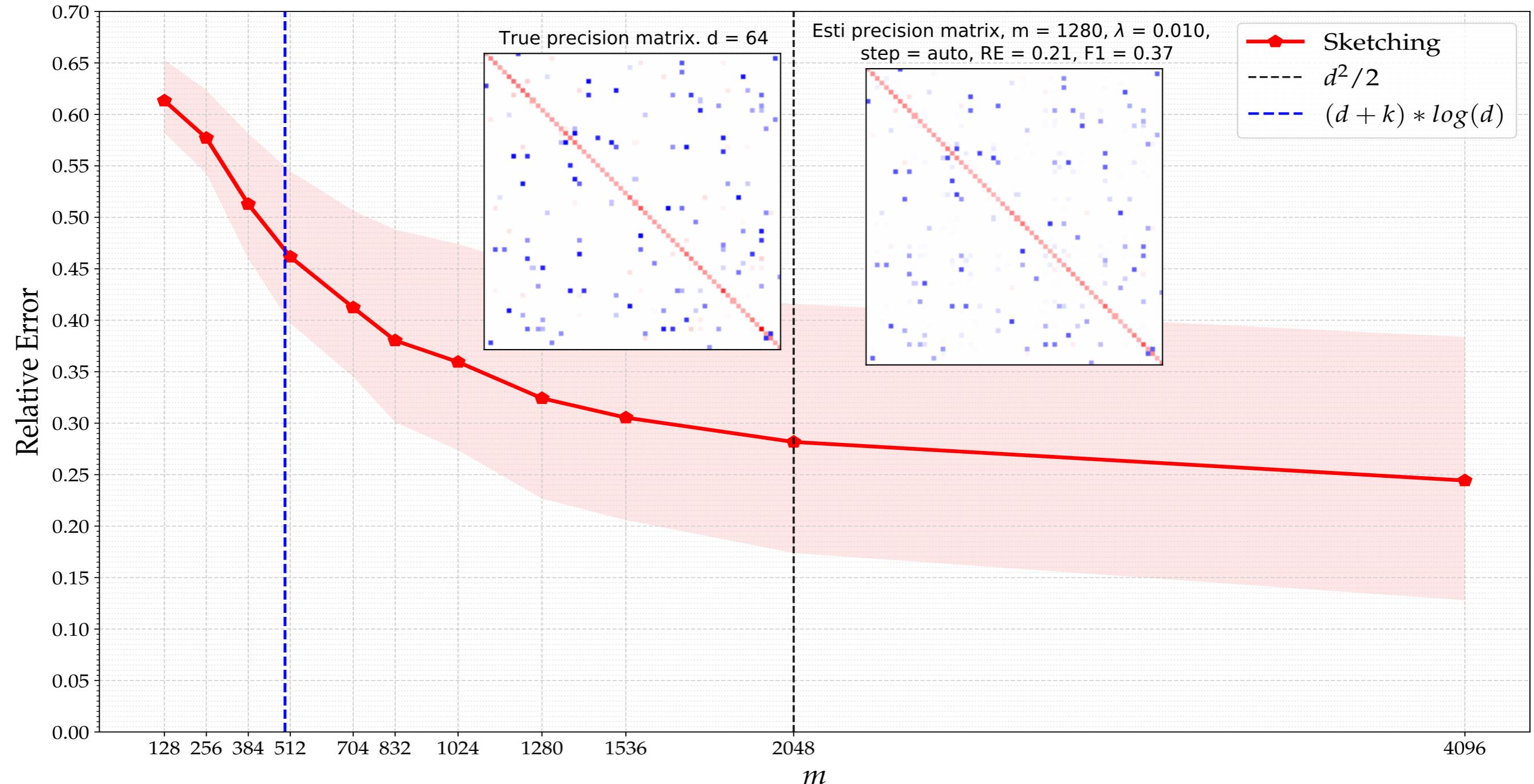
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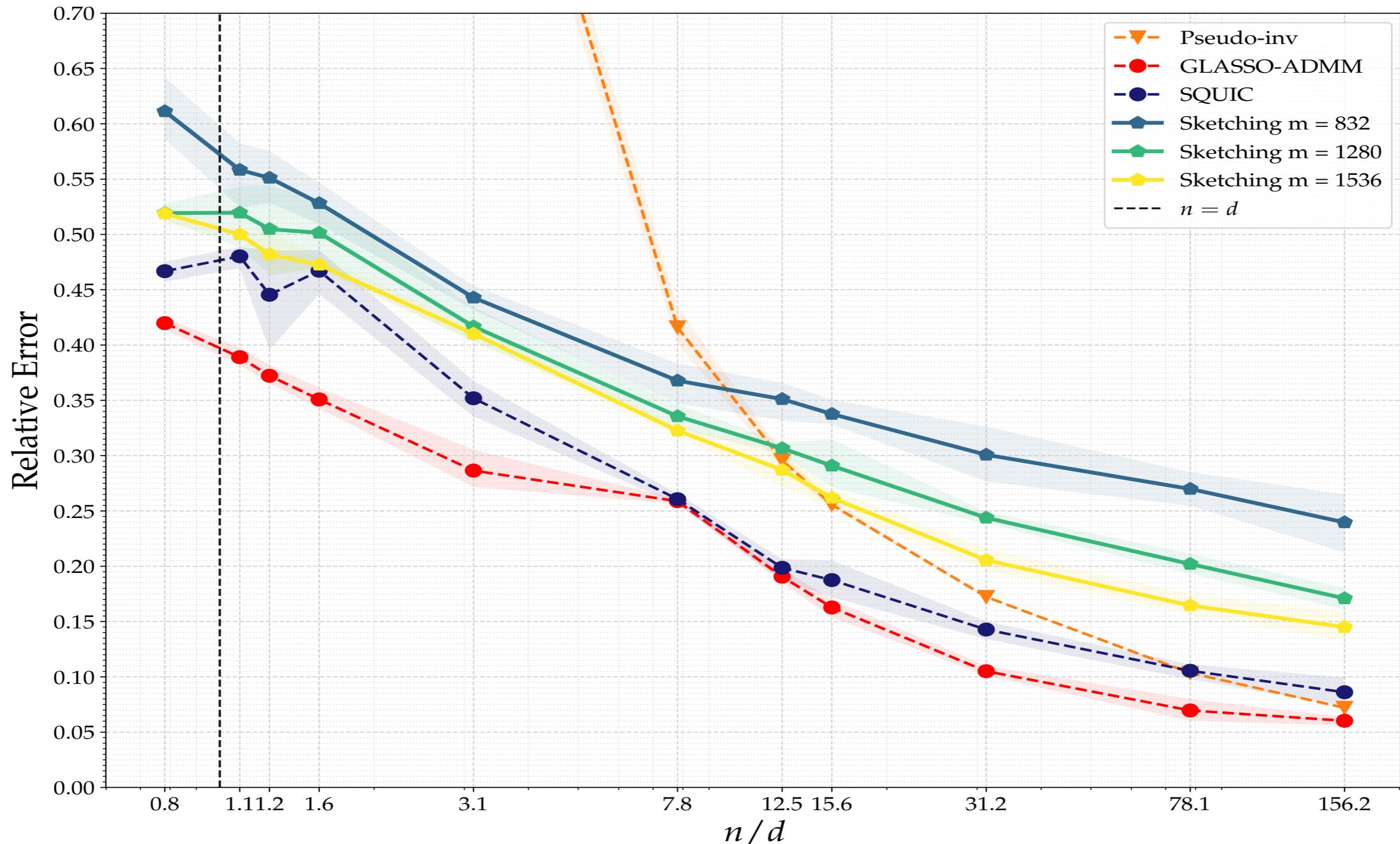
Sklearn $d = 64$



Results

Comparison with GLASSO:

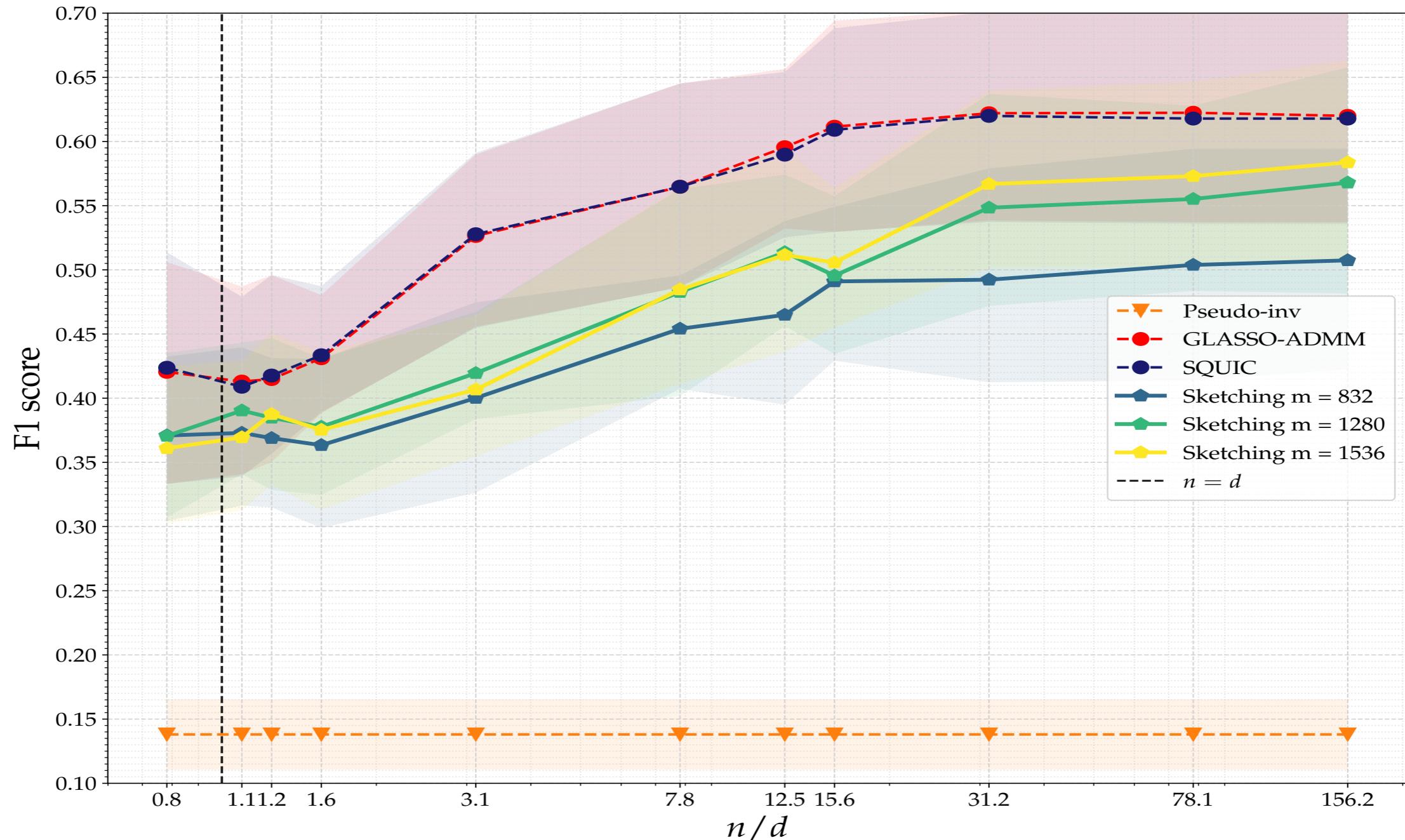
Erdős-Réyni $d = 64$



Results

Comparison with GLASSO:

Erdös-Réyni $d = 64$



| 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:

$$\frac{\text{In memory}}{\text{s} \rightarrow \mathcal{O}(m) \ll d^2} \quad \frac{\text{In time}}{\mathcal{O}(?)}$$

Limitations and perspectives

About the complexity:

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

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

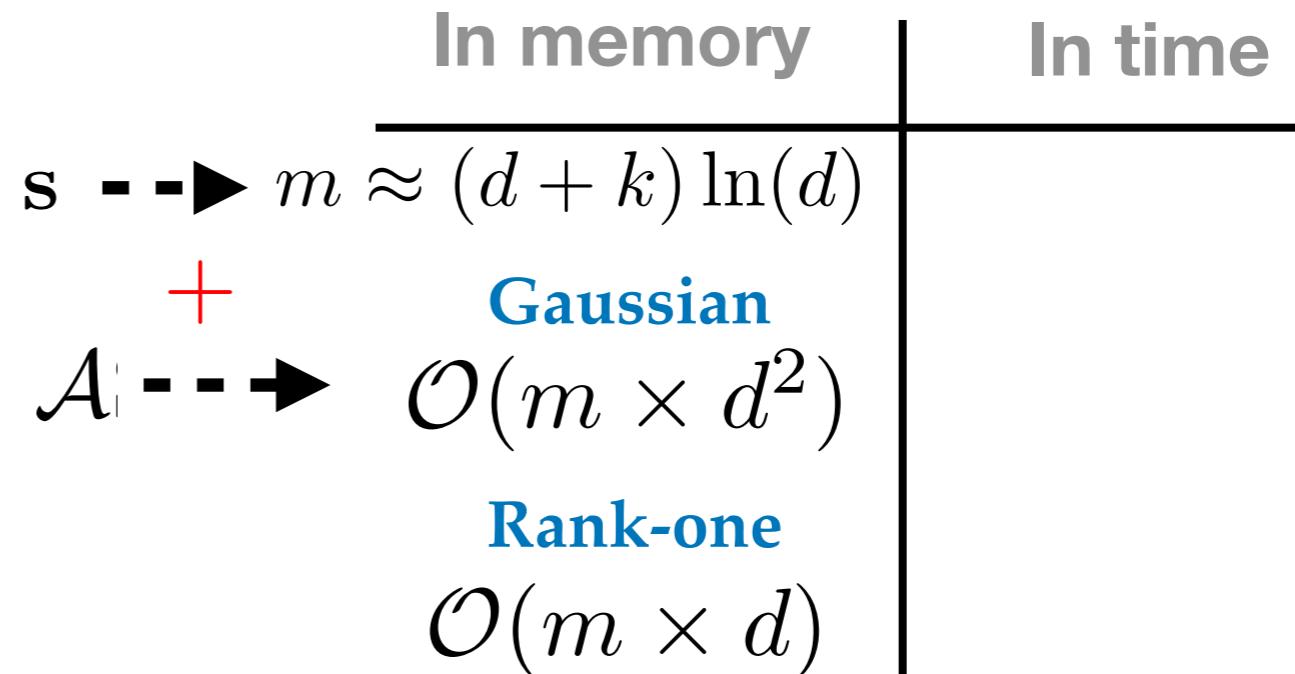
In memory

In time

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:

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

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

Limitations and perspectives

About the complexity:

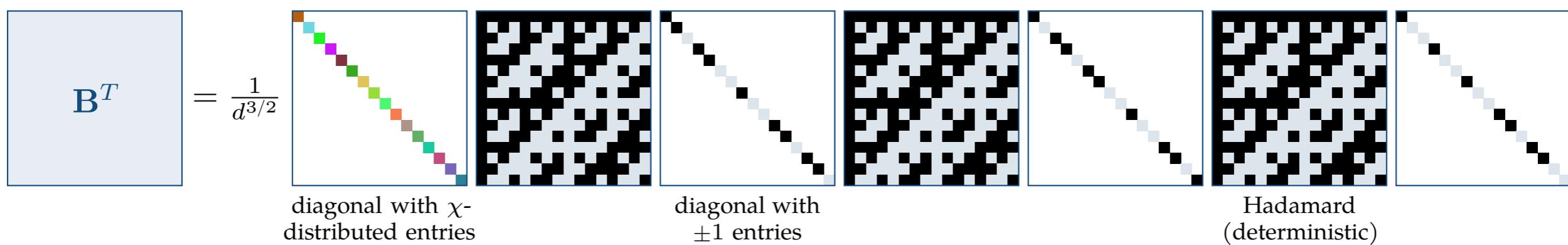
In memory	In time
$\mathcal{O}(m) \ll d^2$	$\mathcal{O}(?)$

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

Structured rank-one:

- Use random structured matrices:

$$\mathbf{W} = \begin{array}{|c|c|c|c|c|} \hline & \mathbf{B}_1 & \mathbf{B}_2 & \mathbf{B}_3 & \cdots & \mathbf{B}_b \\ \hline \end{array}$$



Limitations and perspectives

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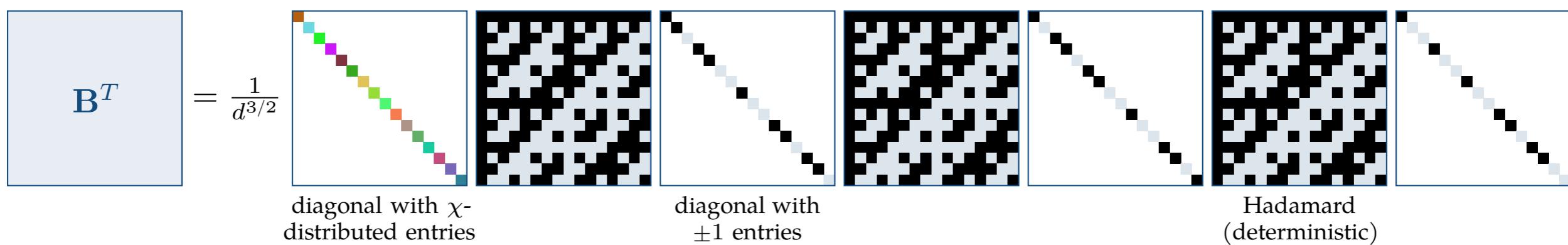
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$$\mathbf{a}_j \sim \text{row}_j(\mathbf{W}) \text{ NOT I.I.D !}$$



Limitations and perspectives

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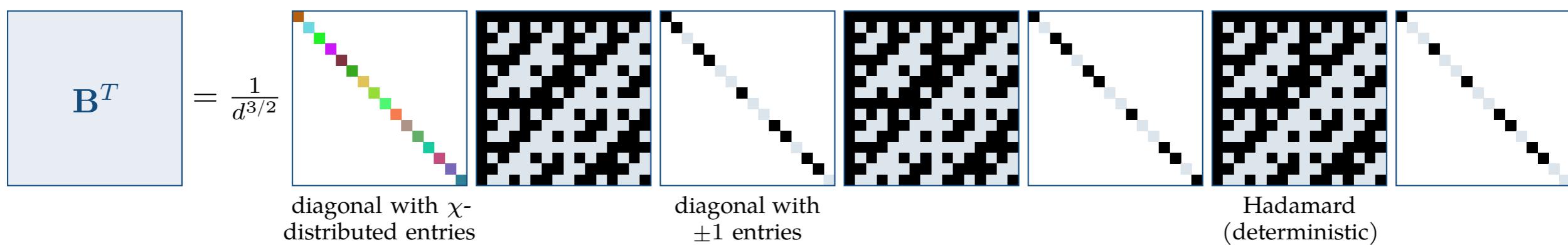
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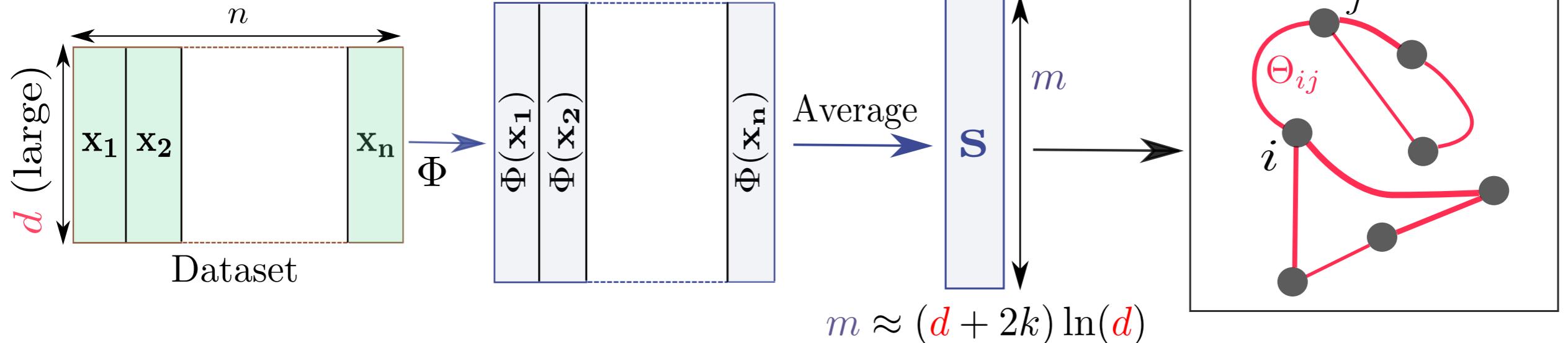
Structured rank-one

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



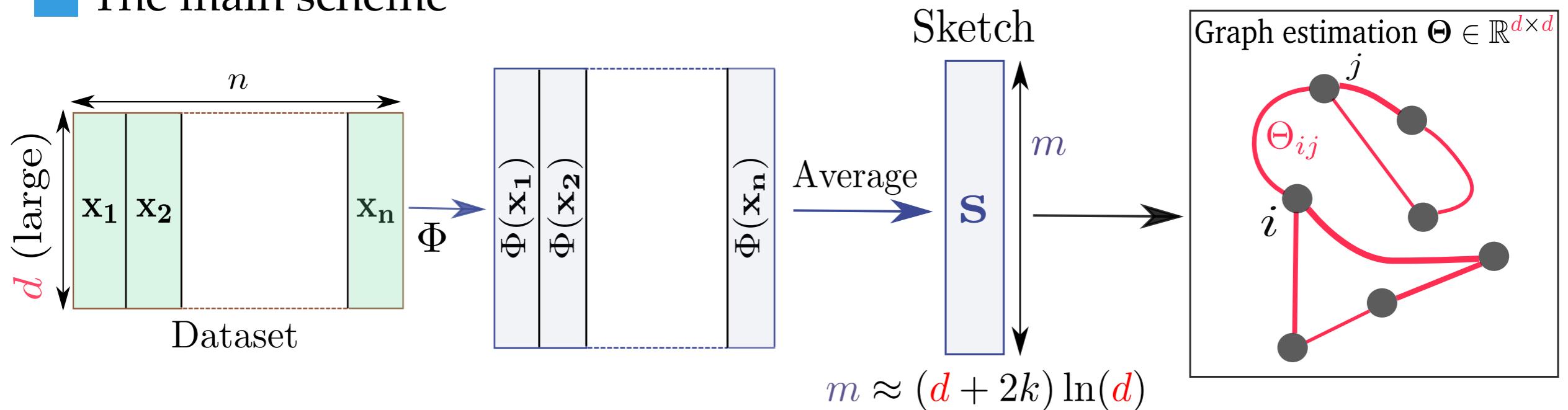
Conclusion

The main scheme



Conclusion

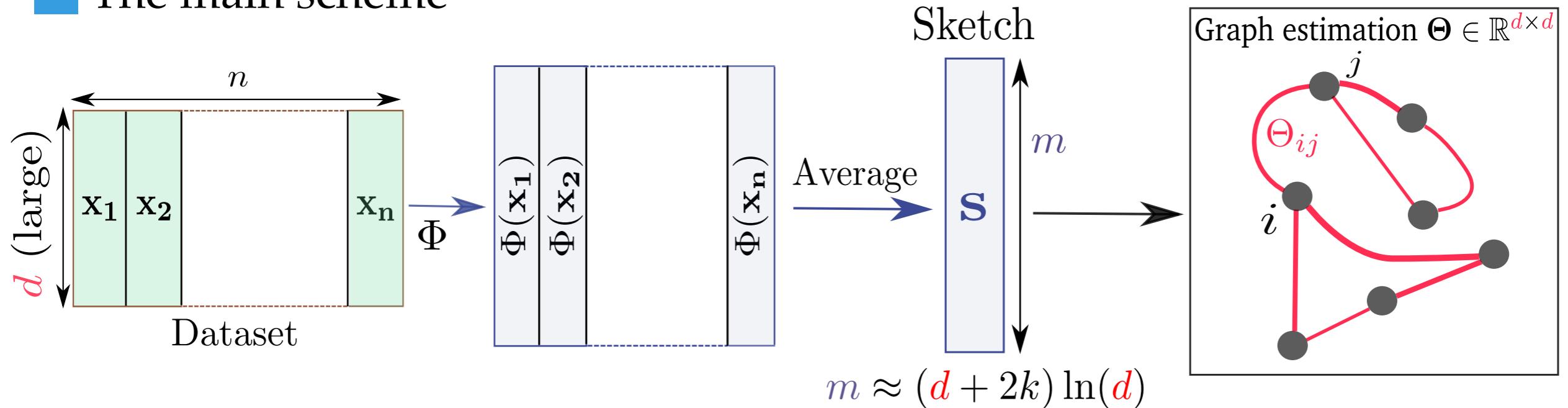
The main scheme



- Theoretical guarantees: RIP, optimal decoders
- Recovery via Davis & Yin three operator splitting

Conclusion

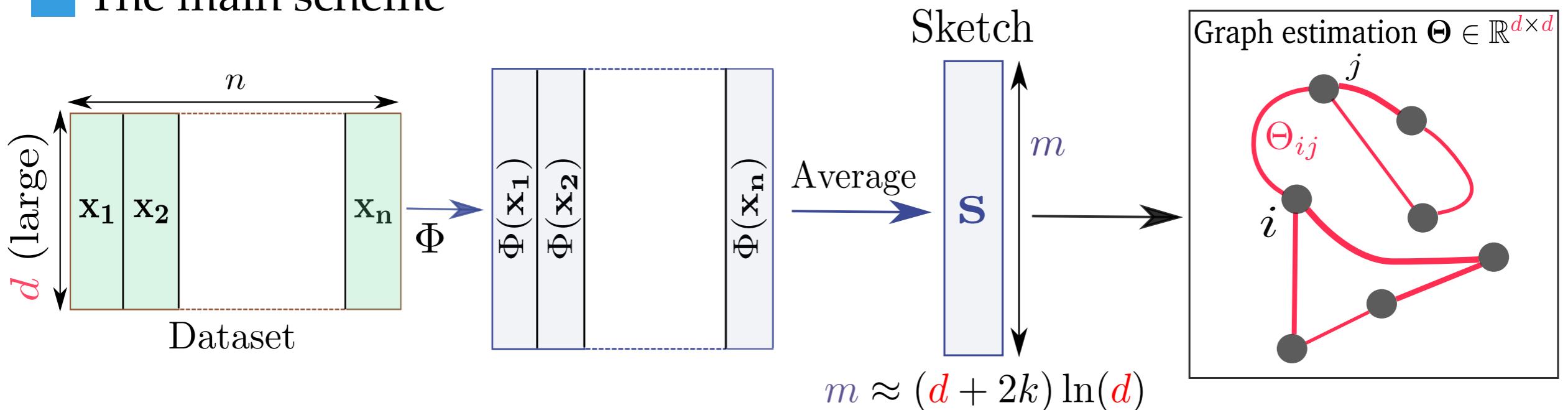
The main scheme



- Theoretical guarantees: RIP, optimal decoders
- Recovery via Davis & Yin three operator splitting
- 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!

