Gaussian Graphical Models.

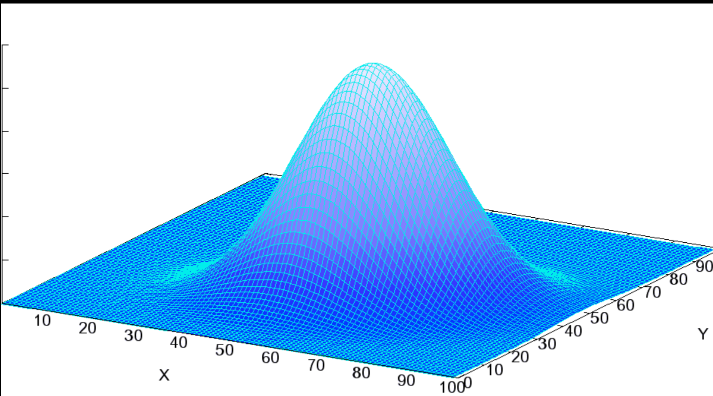
SUMMARY:

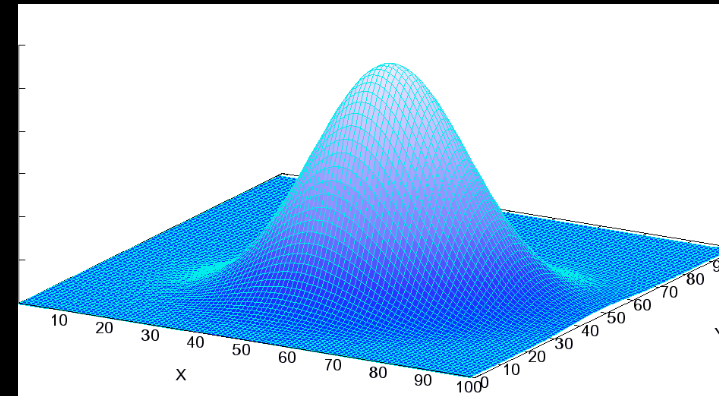
Can learn Attractive and Walk-Summable GGMs with $O(d^2 \log p / \kappa^6)$ samples and quadratic run-time.

d - degree (max)
p - total number of parameters

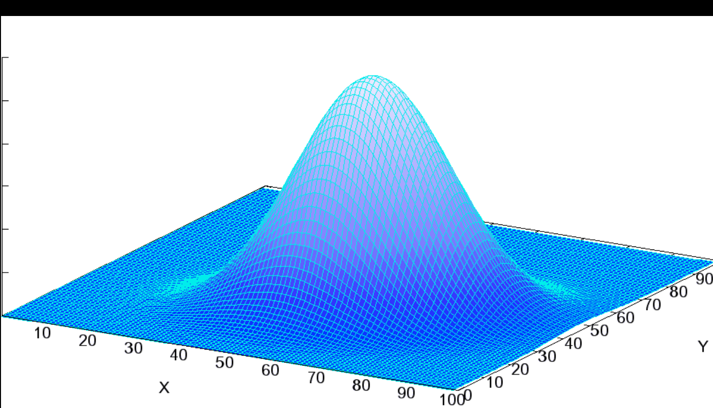
Open: Can any sparse GGM be learnt with $O\left(\frac{d \log p}{\kappa^2}\right)$ samples and a fixed polynomial run-time?

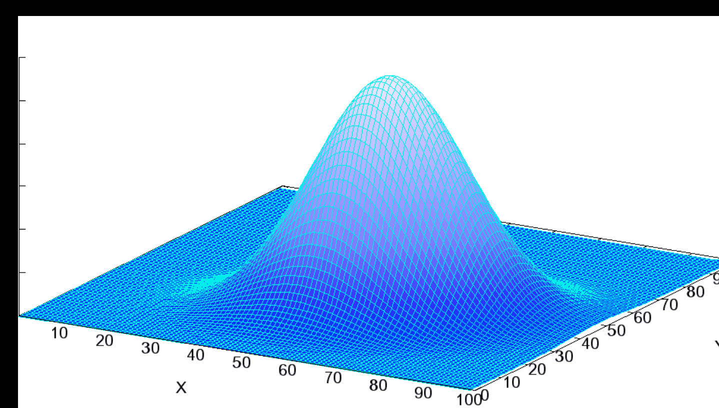
$$\kappa(\Theta) = \min_{i,j:\Theta_{ij}\neq 0} \frac{|\Theta_{ij}|}{\sqrt{\Theta_{ii}\Theta_{jj}}}$$



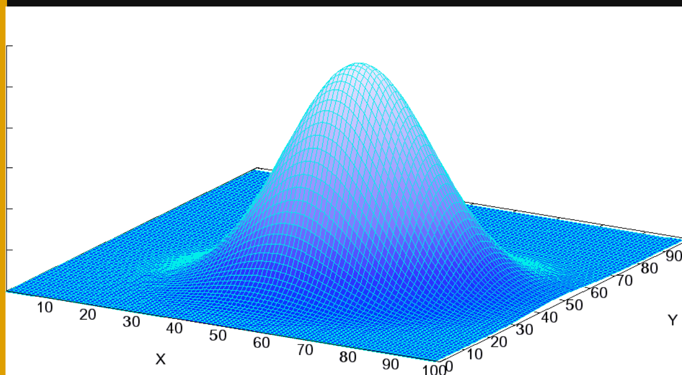


Learning Gaussian Graphical Models w/o condition number bounds





GGMs



Motivation

Algorithm

While $|S| < t$:

Add $\arg\min_{j} Var(X_i \mid X_{S \cup j})$.

Special Models

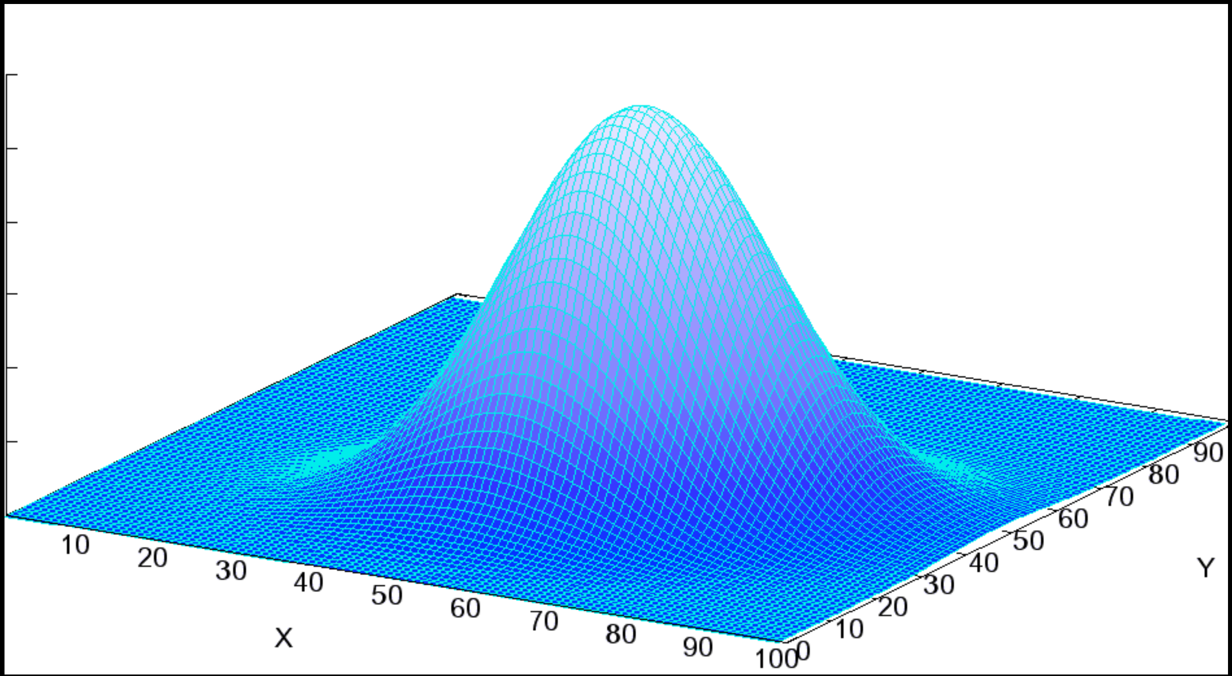
Analysis

Attractive. SDD

Gaussian Graphical Models (GGMs)

$X \sim N(0, \Sigma)$. $\Sigma \in R^{p \times p}$ covariance matrix.

p = number of features.



$$Pr[X = x] = \frac{1}{\sqrt{(2\pi)^p det(\Sigma)}} exp(-x^T \Sigma^{-1} x/2)$$

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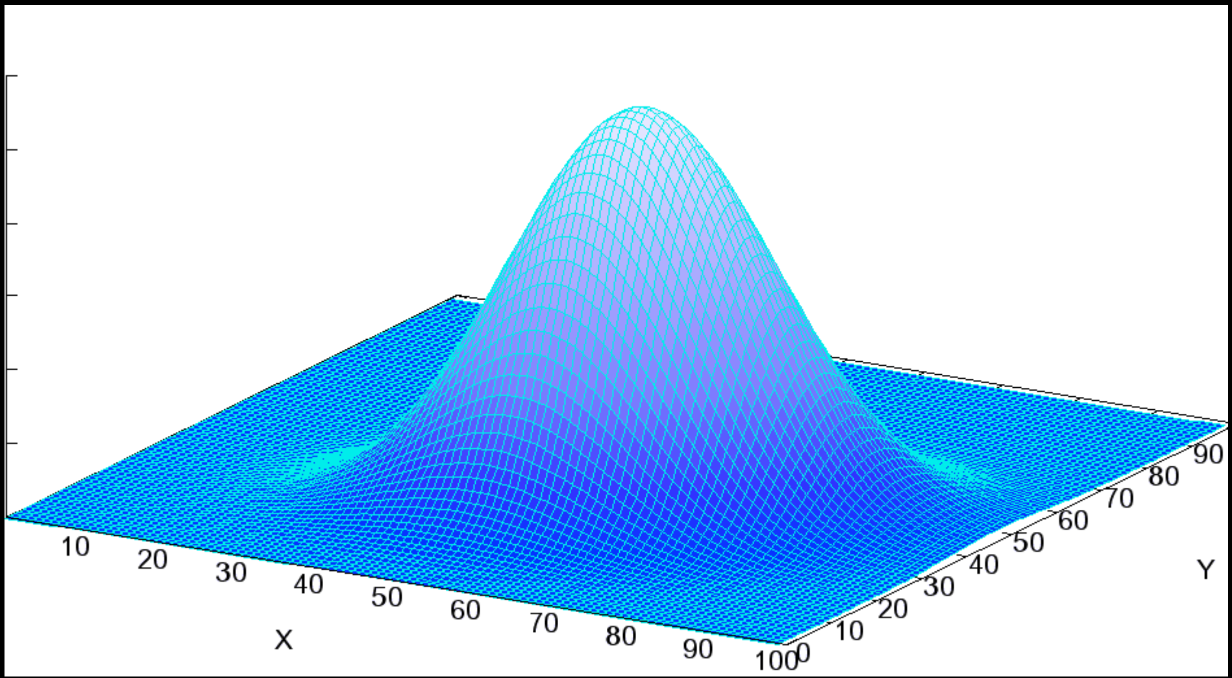

Today's Focus: Precision Matrix $\Theta = \Sigma^{-1}$.

$Cov(x)_{ij} = E[x_i, x_j]$

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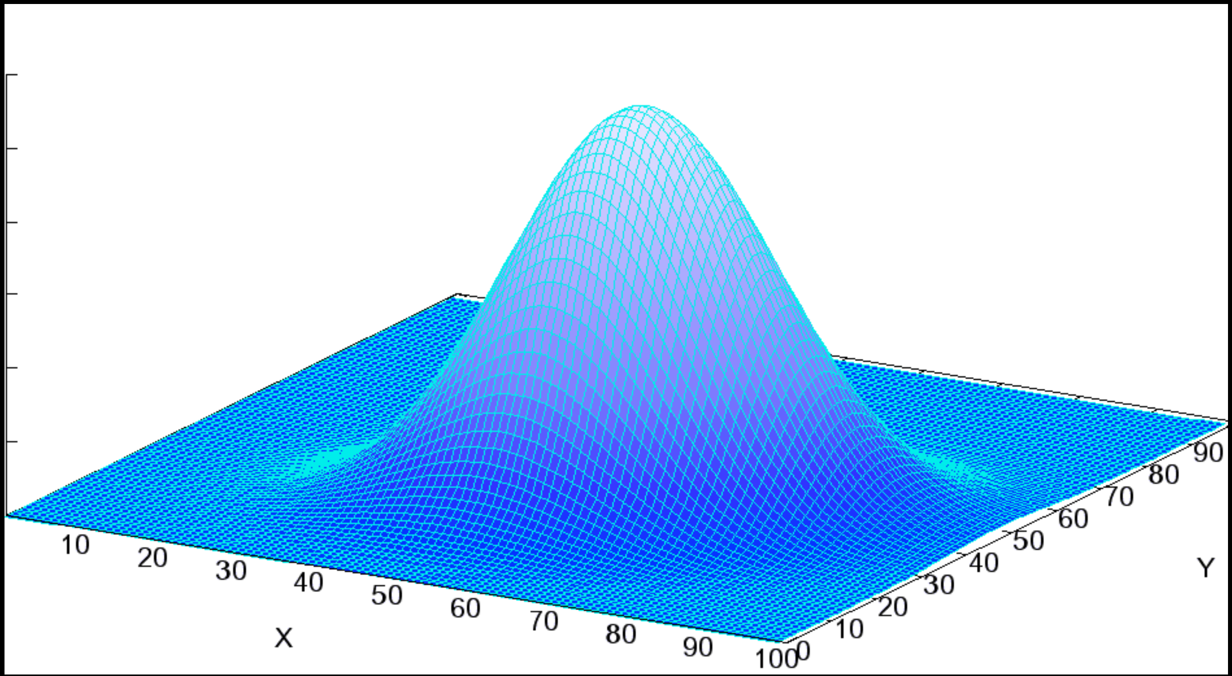

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Dempster 72: Encodes conditional independence structure

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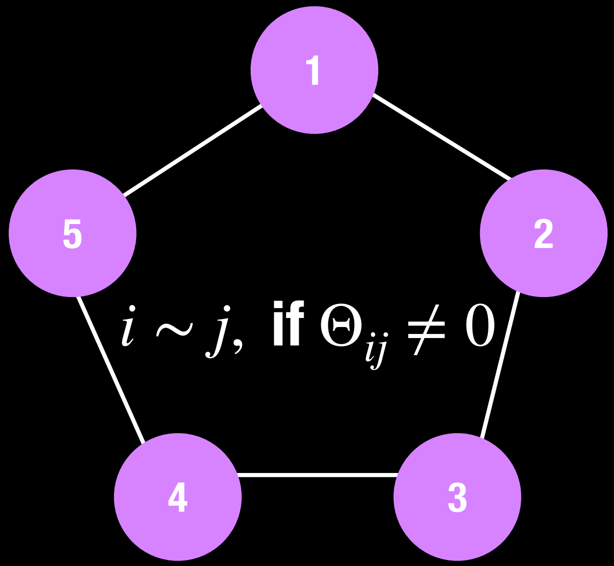

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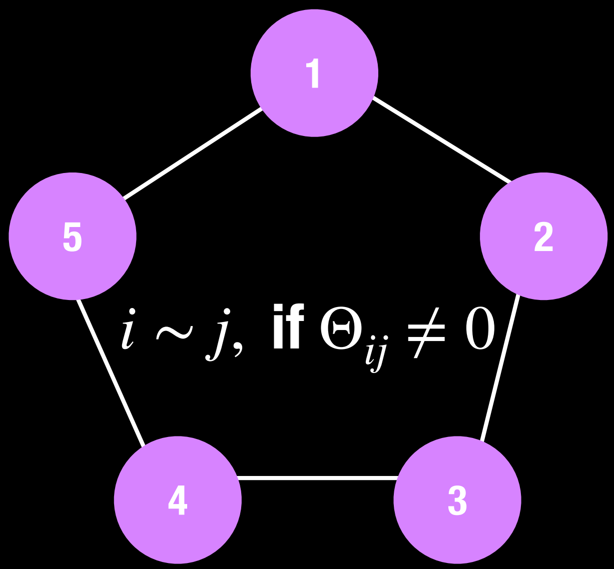

Markov property: $\Theta_{ij} = 0 \Rightarrow X_i, X_j$ **are independent conditioned on neighbors of** i**.**

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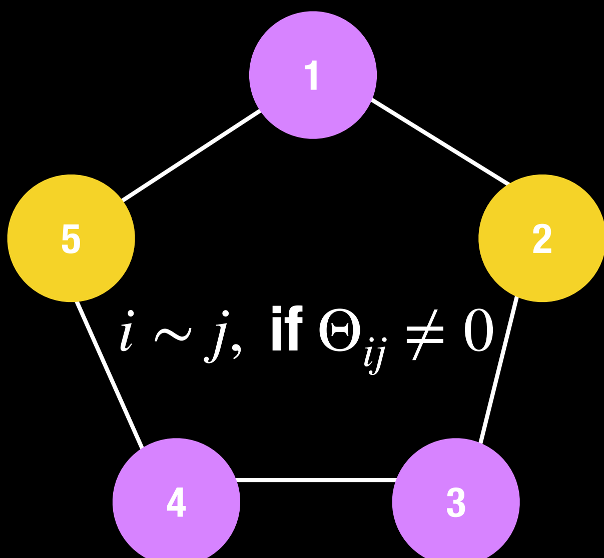

Example: $(X_1 \mid X_2, X_5)$ **independent of** $(X_3 \mid X_2, X_5)$

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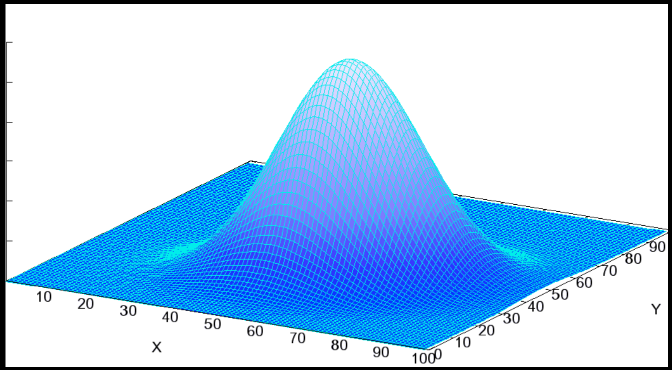
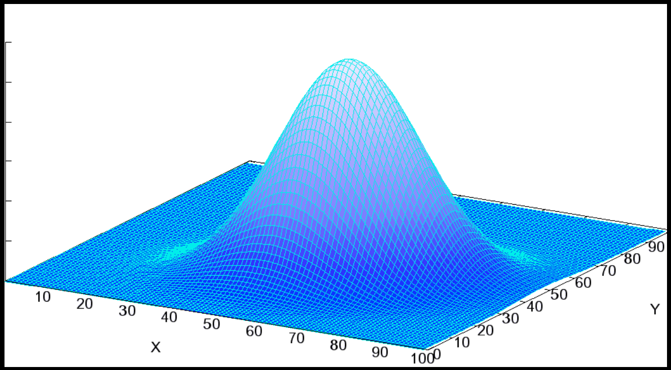
The assumption that makes the formalism non-trivial and useful …

Why?



Fundamental model for modeling statistical relations between variables



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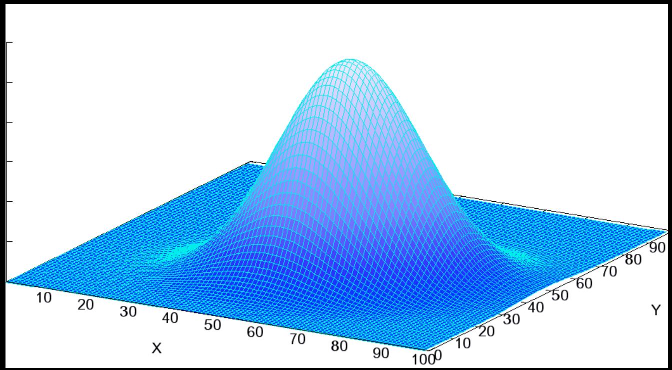

Many applications in machine learning, sciences:

Gene-regulatory networks

Brain connection networks from fMRI

...

Bigger Picture

Can we learn sparse dependency graphs from few samples?

(aka learning Markov random fields, undirected graphical models)

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Can we learn sparse dependency graphs from few samples?

(aka learning Markov random fields, undirected graphical models)

$$X \sim \{1, -1\}^p\,.$$

Dependency graph of X: $i \nsim j \Rightarrow X_i, X_j$ **are independent conditioned on neighbors of** i.

Example: "Random Walk" Model

$$X_i = X_{i-1} + Z_i, \text{ where } Z_1, \ldots, Z_p \text{ i.i.d } N(0,1)$$

1	1	1	1	1	1	1	1	1	1
1	2	2	2	2	2	2	2	2	2
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1	2	3	4	4	4	4	4	4	4
1	2	3	4	5	5	5	5	5	5
1	2	3	4	5	6	6	6	6	6
1	2	3	4	5	6	7	7	7	7
1	2	3	4	5	6	7	8	8	8
1	2	3	4	5	6	7	8	9	9
1	2	3	4	5	6	7	8	9	10

Σ : Covariance Matrix

$E[x_1, x_2] = 1$

$E[x_2, x_3] = 2$

$x_1 = z_1 \quad x_2 = z_1 + z_2 \quad x_3 = z_1 + z_2 + z_3$

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2	-1	0	0	0	0	0	0	0	0
-1	2	-1	0	0	0	0	0	0	0
0	-1	2	-1	0	0	0	0	0	0
0	0	-1	2	-1	0	0	0	0	0
0	0	0	-1	2	-1	0	0	0	0
0	0	0	0	-1	2	-1	0	0	0
0	0	0	0	0	-1	2	-1	0	0
0	0	0	0	0	0	-1	2	-1	0
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Dependency graph

2	-1	0	0	0	0	0	0	0	0
-1	2	-1	0	0	0	0	0	0	0
0	-1	2	-1	0	0	0	0	0	0
0	0	-1	2	-1	0	0	0	0	0
0	0	0	-1	2	-1	0	0	0	0
0	0	0	0	-1	2	-1	0	0	0
0	0	0	0	0	-1	2	-1	0	0
0	0	0	0	0	0	-1	2	-1	0
0	0	0	0	0	0	0	-1	2	-1
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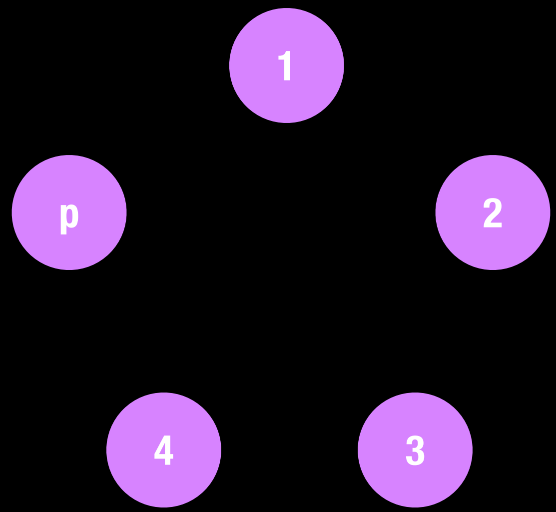
Θ : Precision Matrix

Learning Sparse GGMs

- Structure learning - learn dependency graph.
- Parameter learning - learn the matrix.

Structure Learning for GGMs

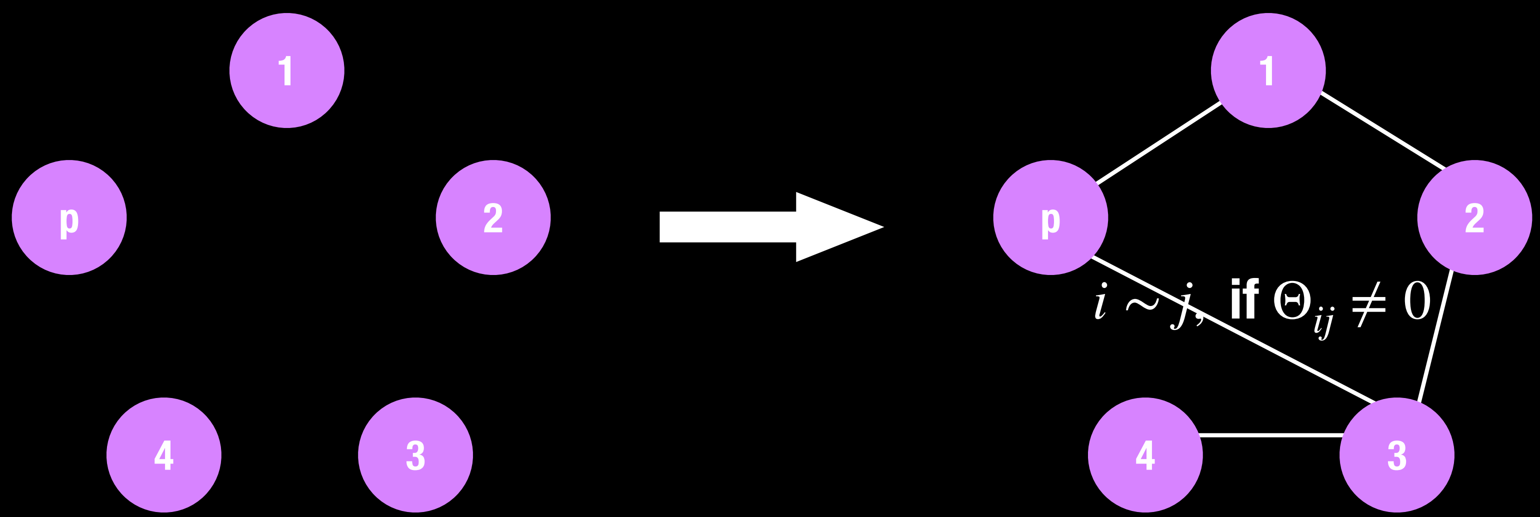
- Structure learning - learn dependency graph.



Input: Given samples $X^1, X^2, \ldots, X^n$ from a GGM
Output: Dependency graph of the GGM.

Structure Learning for GGMs

- **Structure learning - learn dependency graph.**



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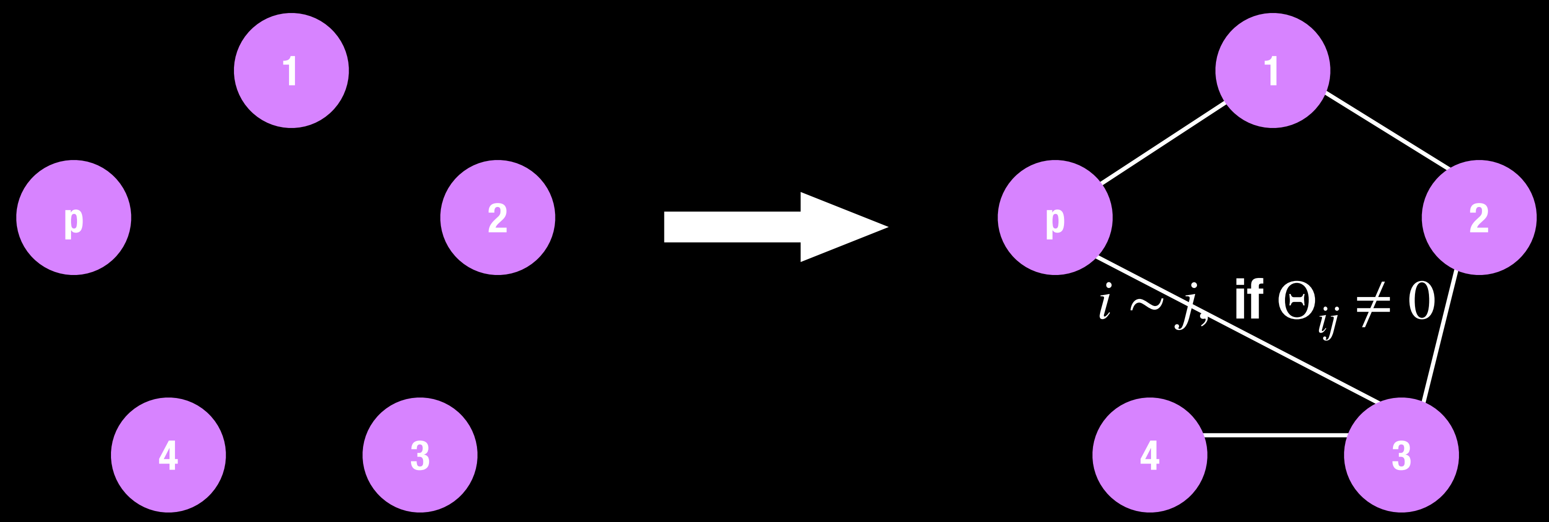

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Challenge: Often $n \ll p$.

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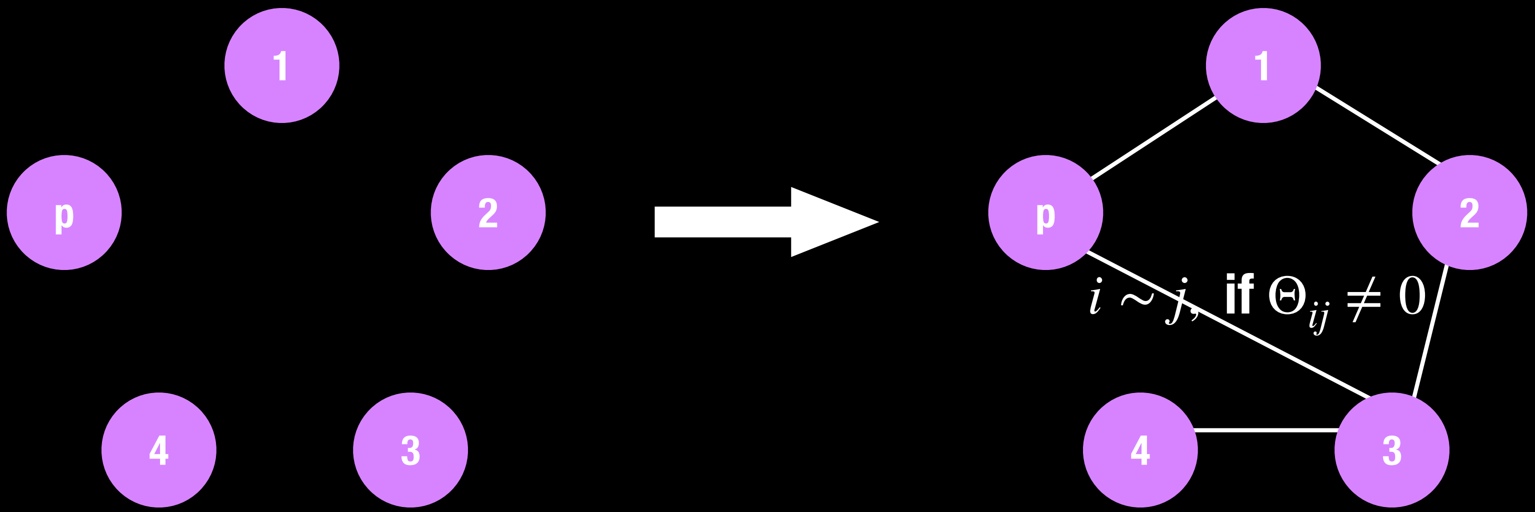

Assumption: Unknown dependency graph is sparse - each vertex has at most d edges.

Challenge: Often $n \ll p$.

Structure Learning for GGMs

Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

(Think: $n = O_d(\log p)$. **)**

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Core of problem. Can learn parameters easily afterward.

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(Think: $n = O_d(\log p)$. **)**

Ideal: Practical algorithms with provable guarantees.

Example: Unknown order Random Walk

$$X_{\pi(i)} = X_{\pi(i-1)} + Z_i, \text{ where } Z_1, \ldots, Z_p \text{ i.i.d } N(0,1)$$

7	1	5	6	7	4	3	7	2	7
1	1	1	1	1	1	1	1	1	1
5	1	5	5	5	4	3	5	2	5
6	1	5	6	6	4	3	6	2	6
7	1	5	6	8	4	3	8	2	8
4	1	4	4	4	4	3	4	2	4
3	1	3	3	3	3	3	3	2	3
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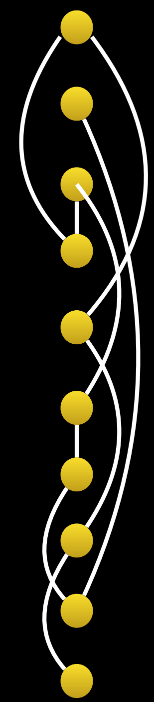

Dependency graph?

2	0	0	-1	-1	0	0	0	0	0
0	2	0	0	0	0	0	0	-1	0
0	0	2	-1	0	-1	0	0	0	0
-1	0	-1	2	0	0	0	0	0	0
-1	0	0	0	2	0	0	-1	0	0
0	0	-1	0	0	2	-1	0	0	0
0	0	0	0	0	-1	2	0	-1	0
0	0	0	0	-1	0	0	2	0	-1
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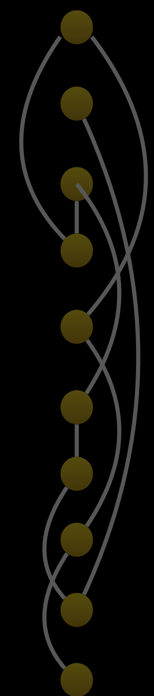

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-1	0	-1	2	0	0	0	0	0	0
-1	0	0	0	2	0	0	-1	0	0
0	0	-1	0	0	2	-1	0	0	0
0	0	0	0	0	-1	2	0	-1	0
0	0	0	0	-1	0	0	2	0	-1
0	-1	0	0	0	0	-1	0	2	0
0	0	0	0	0	0	0	-1	0	1

Θ : Precision Matrix

How many samples of X to find the hidden permutation?

Previous Work

Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

Well studied with several popular software packages:
GLASSO, CLIME, ACLIME

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- **GLASSO: Friedman, Hastie, Tibshirani 08**

  Can learn with $O(d^2 \log p)$ samples if precision matrix is incoherent.

Previous Work

Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

Strong assumption: Violated by random walk …

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Previous Work

$\boxed{\text{Given samples } X^1, X^2, \ldots, X^n \text{ from a GGM of degree } d \ll p\text{, can we efficiently find the dependency graph with } n \ll p?}$

Summary: GLASSO, CLIME, ACLIME need `well-conditioned' precision matrix.

Previous Work

Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

Summary: GLASSO, CLIME, ACLIME need `well-conditioned' precision matrix.

- Violated by simple models
- Not scale invariant
- Not just analysis … **fail empirically**

Previous Work

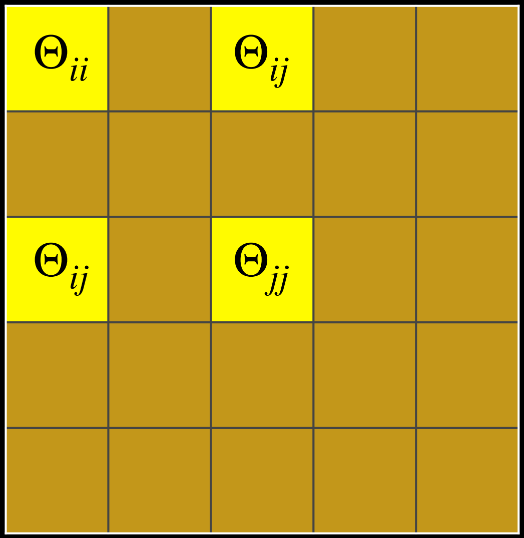
Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

What is possible information theoretically?

Previous Work: MVL18

Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

$$\kappa(\Theta) = \min_{i,j:\Theta_{ij}\neq 0} \frac{|\Theta_{ij}|}{\sqrt{\Theta_{ii}\Theta_{jj}}}$$



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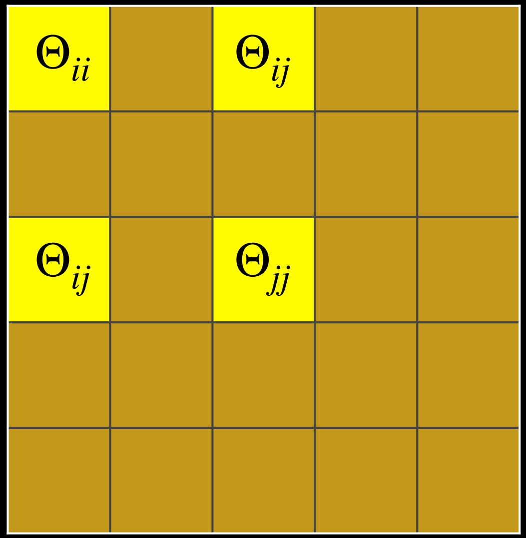
Measures signal in 2x2 submatrices … not whole matrix.



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MVL18: $\kappa(\Theta) = \min_{i,j:\Theta_{ij}\neq 0} \frac{|\Theta_{ij}|}{\sqrt{\Theta_{ii}\Theta_{jj}}}$

Dependency graph identifiable with $n = O(d \log p / \kappa^2)$ samples!

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Example: Random walk model - $\kappa = 1/2$.

Information-Theoretic Limits: MVL18

Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

MVL18: $\kappa(\Theta) = \min_{i,j:\Theta_{ij}\neq 0} \frac{|\Theta_{ij}|}{\sqrt{\Theta_{ii}\Theta_{jj}}}$

Dependency graph identifiable with $n = O(d \log p/\kappa^2)$ samples!

Wang, Wainwright, Ramachandran 10: Need $n = \Omega(\log p/\kappa^2)$.

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Problematic for even moderate sized instances
… Can we do better?

GGMS: Main Learning Challenge

Given n samples from a GGM of degree $d \ll p$,
can we find the dependency graph with $n \approx d \log p / \kappa^2$, and
run-time fixed polynomial in p? (Or even $p^{o(d)}$.)

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Attractive, SDD,… more generally, Walk-Summable

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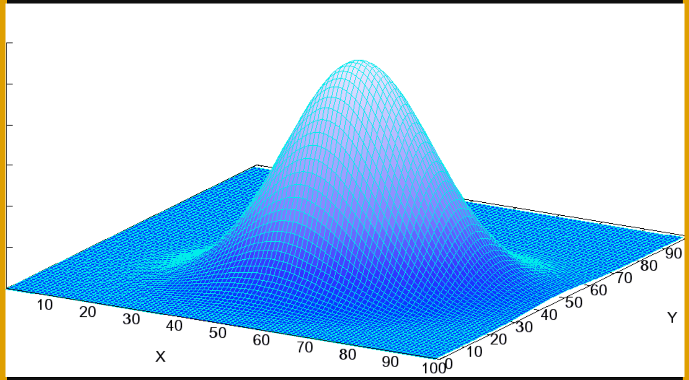
Main: A simple greedy algorithm solves above ill-conditioned cases
(and recovers guarantees of GLASSO, CLIME, …)

GGMs



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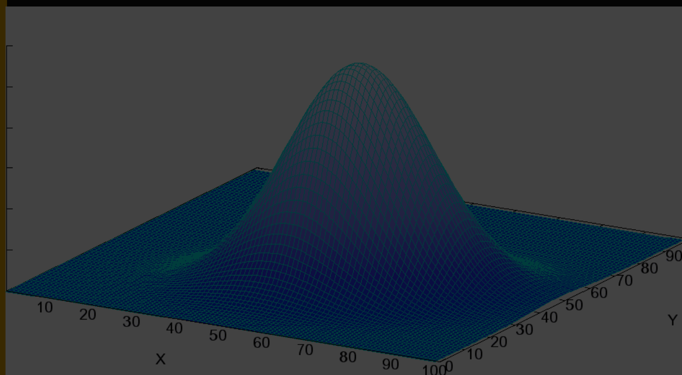
$$\boxed{\begin{array}{c}\text{While } |S| < t : \\ \text{Add } \arg\min_j Var(X_i \mid X_{S \cup j}) \,.\end{array}}$$

Special Models

Analysis

Attractive. SDD.

GGMs



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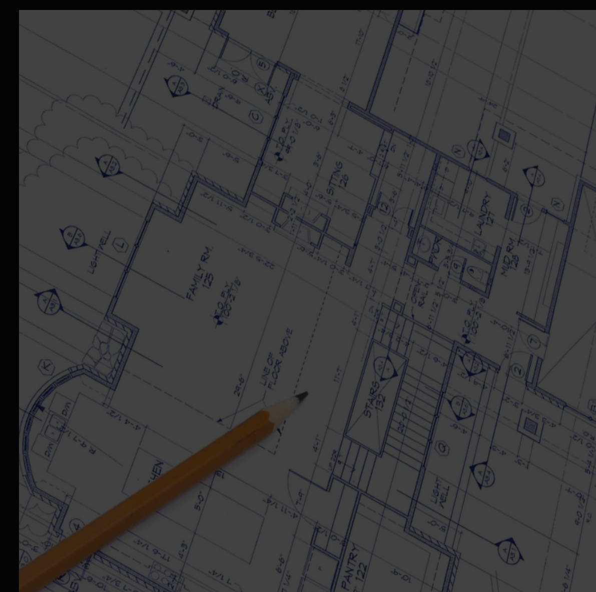

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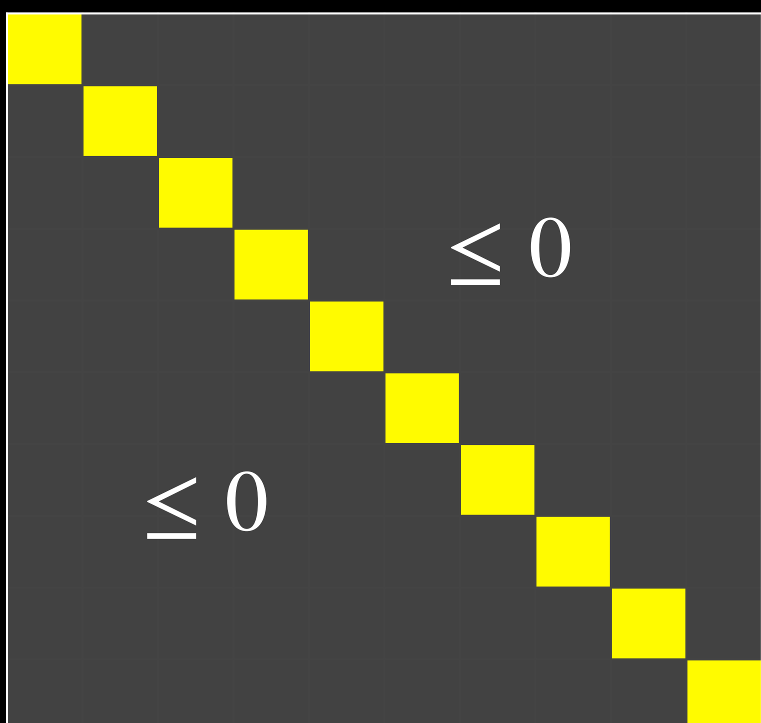
Attractive GGMs

GGM is attractive if all covariances are non-negative.

(Equivalently, Θ has non-positive off-diagonals.)



Θ : Precision Matrix

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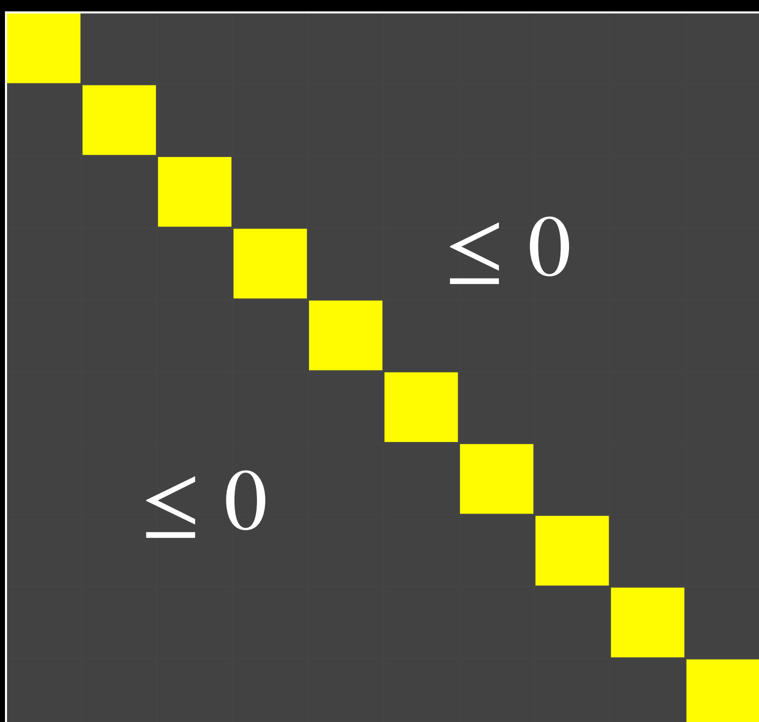

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Ex: Gaussian Free Fields

- **Many applications via Gaussian processes**

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0	-1	2	-1	0	0	0	0	0	0
0	0	-1	2	-1	0	0	0	0	0
0	0	0	-1	2	-1	0	0	0	0
0	0	0	0	-1	2	-1	0	0	0
0	0	0	0	0	-1	2	-1	0	0
0	0	0	0	0	0	-1	2	-1	0
0	0	0	0	0	0	0	-1	2	-1
0	0	0	0	0	0	0	0	-1	2

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- Many applications via Gaussian processes
- Ex: Random walk model
- Ill-conditioned if ‘long paths’

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GGM is attractive if all covariances are non-negative.

Previous: No efficient algorithms with $O_d(\log p)$ sample complexity known.

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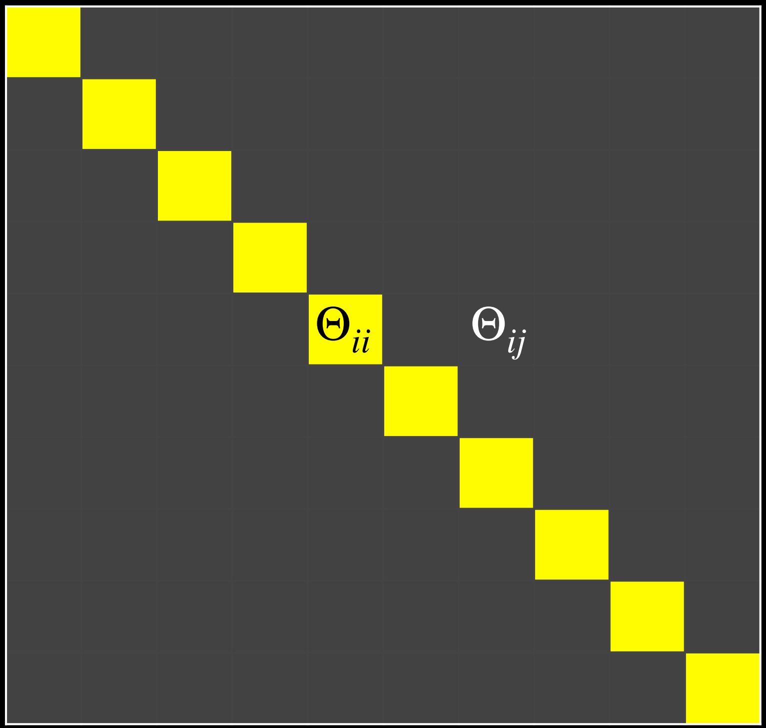
Walk-Summable GGMs

GGM walk-summable if making off-diagonals of precision matrix negative preserves positive semi-definiteness.



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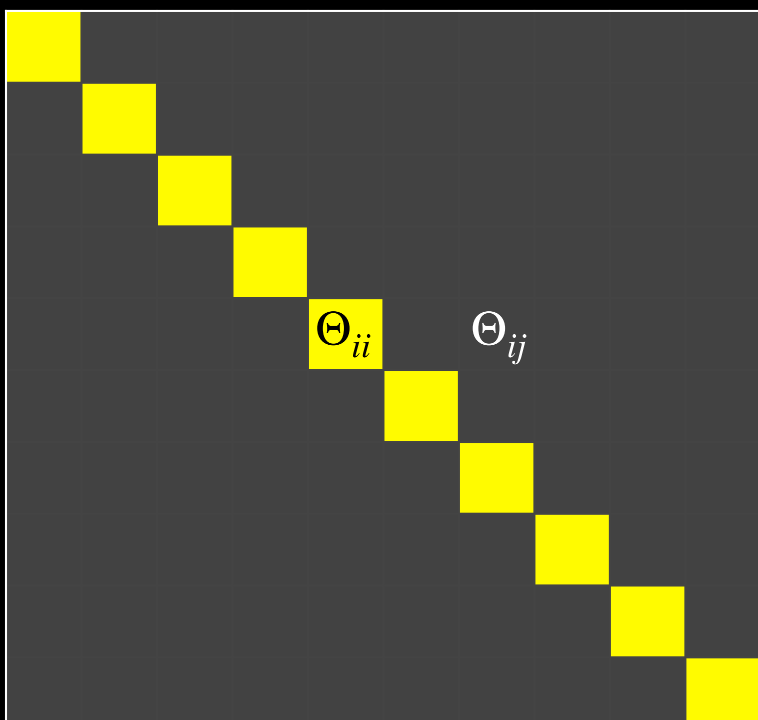

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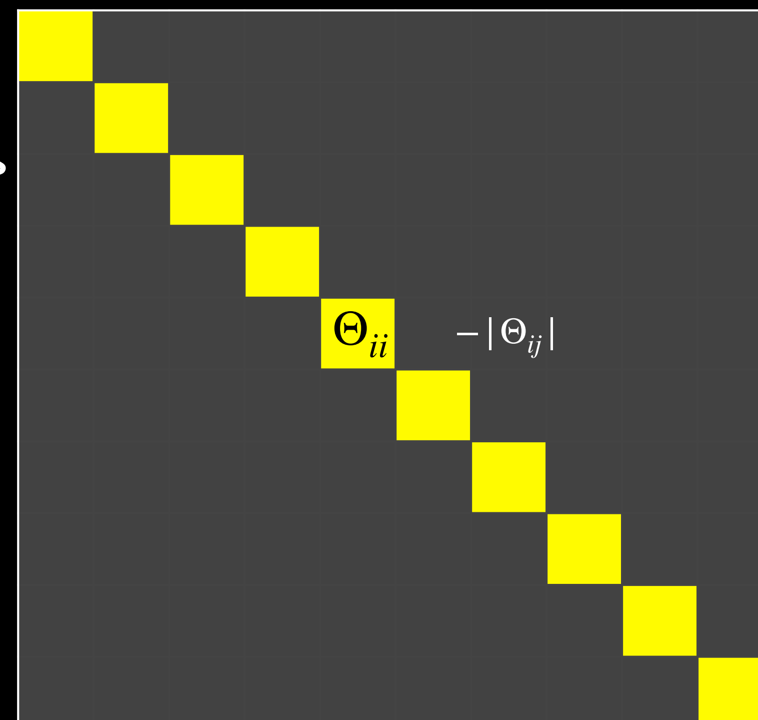
all eigenvalues > 0



Offdiagonals negative $\succeq 0$

Walk-Summable GGMs

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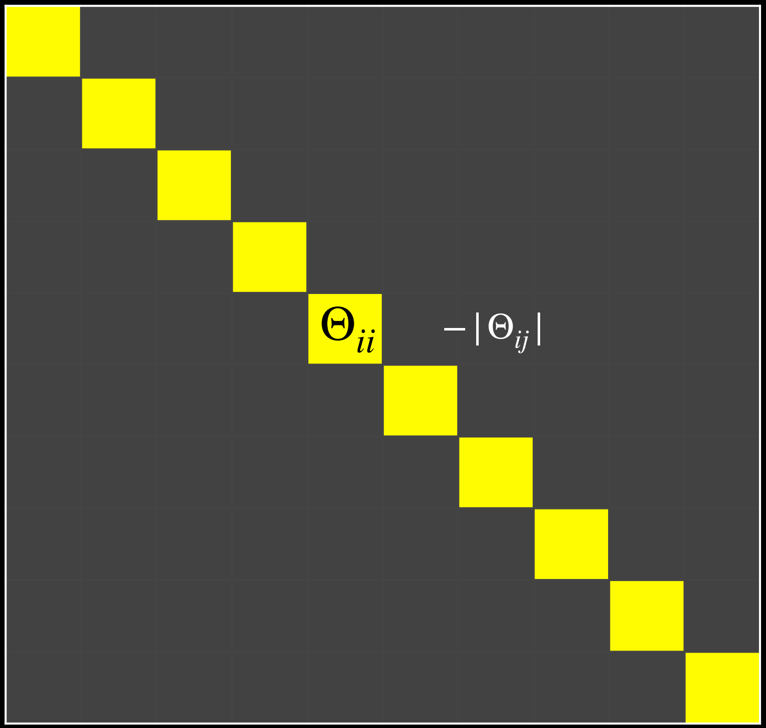
- Introduced by Maliutov, Johnson, Willsky 2006
- Generalize many classes
  - Attractive
  - Pairwise normalizable
  - Non-frustrated
  - Symmetric diagonally-dominant



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Walk-Summable GGMs

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KKMM: **Hybrid** (Greedy+Lasso) learns walk-summable models with $O(d \log p / \kappa^4)$ samples.

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Learning GGMs Greedily

Input: Samples from a sparse GGM ~ X.
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Similar greedy approaches for discrete GMs: [Bresler10], [HKM17], [BKM19]

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Input: Samples from a sparse GGM ~ X.
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GREEDYPRUNE

1. **Recover neighborhood of each vertex in parallel.**
2. **Grow a candidate neighborhood.**
3. **Prune out some vertices.**

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Phase 1: Growing a neighborhood

Input: Samples from a sparse GGM ~ X.
Goal: Neighborhood of vertex 1.

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Input: Samples from a sparse GGM ~ X.
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GREEDY-GROWING

1. **Set** $S \leftarrow \emptyset$
2. **While S is small enough:**
   1. **Find j to minimize estimate of** $Var(X_1 \,|\, X_{S \cup j})$.

      ↳ For each $var(x_1 | x_{S \cup j})$ we need $1/\varepsilon^2$ samples to get $(1-\varepsilon)$ accuracy.
   2. $S \leftarrow S \cup \{j\}$.

Intuition: Add vertex that gives maximum decrease in conditional variance.

Phase 2: Pruning a neighborhood

Input: Samples from a sparse GGM ~ X.
Goal: Neighborhood of vertex 1.

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Input: Samples from a sparse GGM ~ X.
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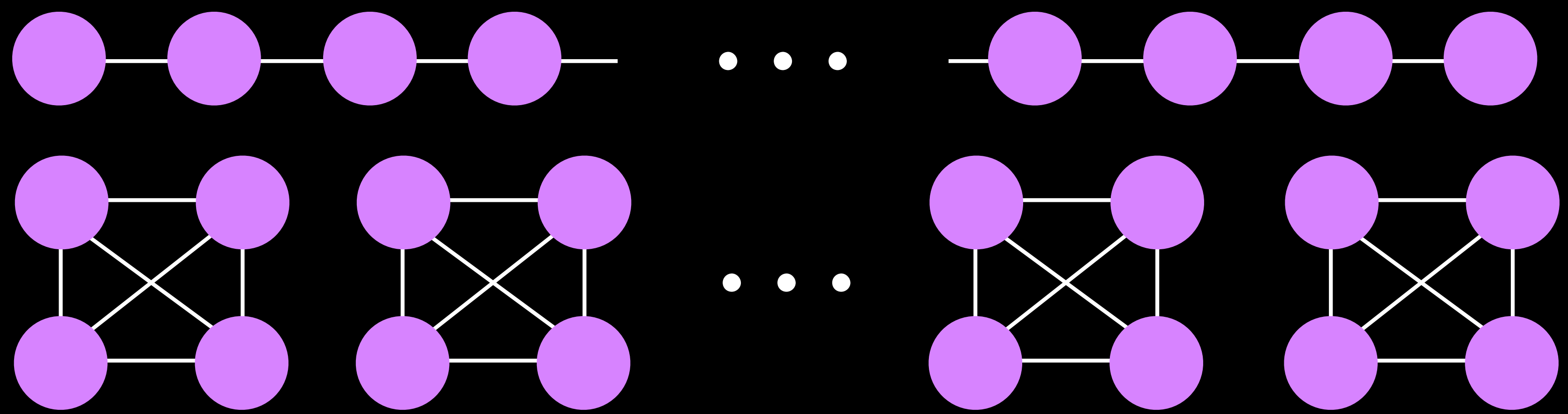
GREEDY-PRUNING

1. For each j in S:
    1. If $Var(X_1 \,|\, X_{S\setminus\{j\}}) < (1+\tau)Var(X_1 \,|\, X_S)$, drop j from S.

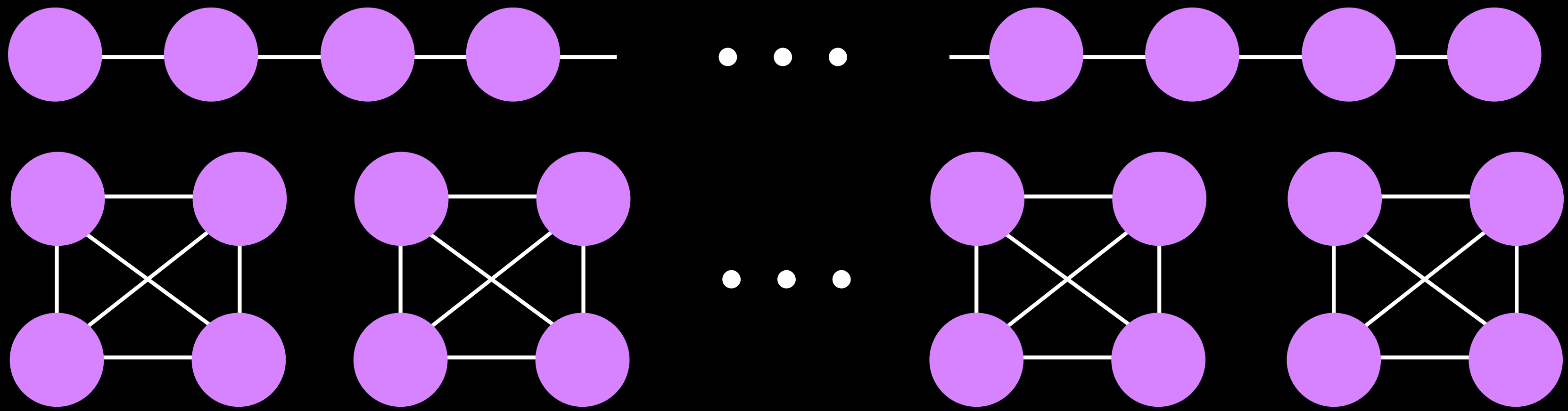
Intuition: If dropping a vertex, does not hurt too much, drop it.

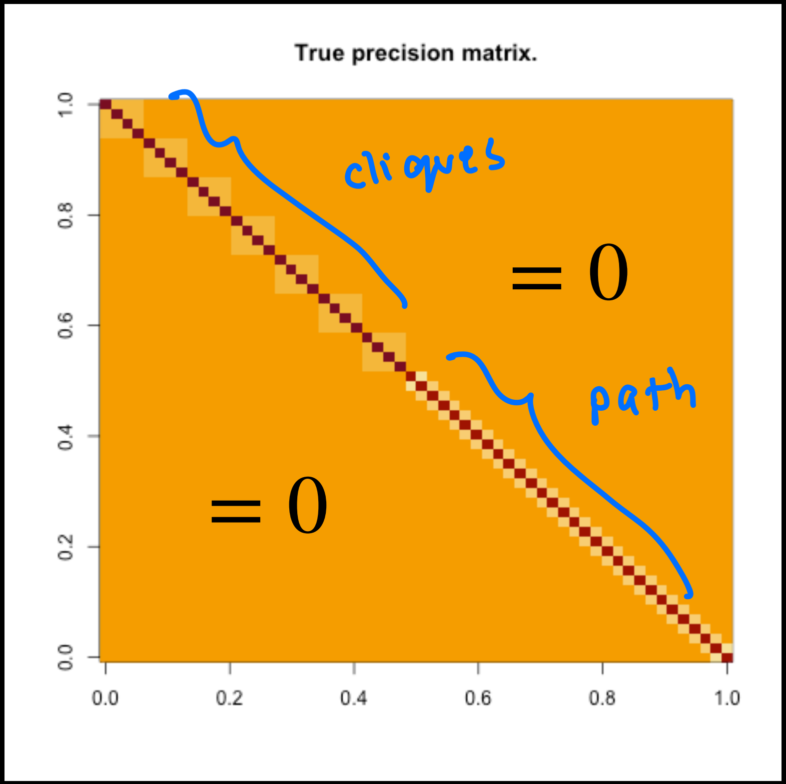
Experiments: A Simple Challenge



Precision: Path + Cliques
Max-degree = 3
Ill-conditioned

Experiments: A Simple Challenge





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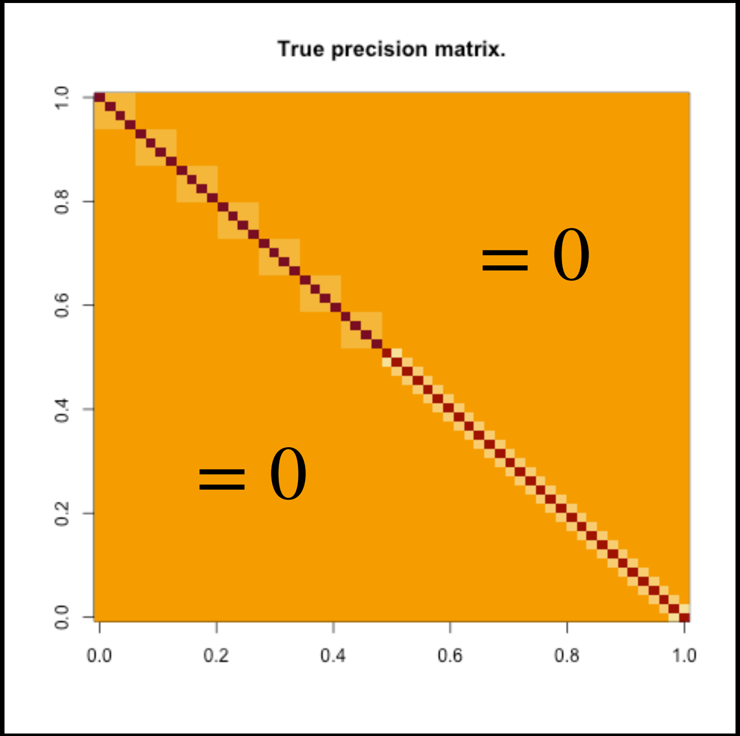
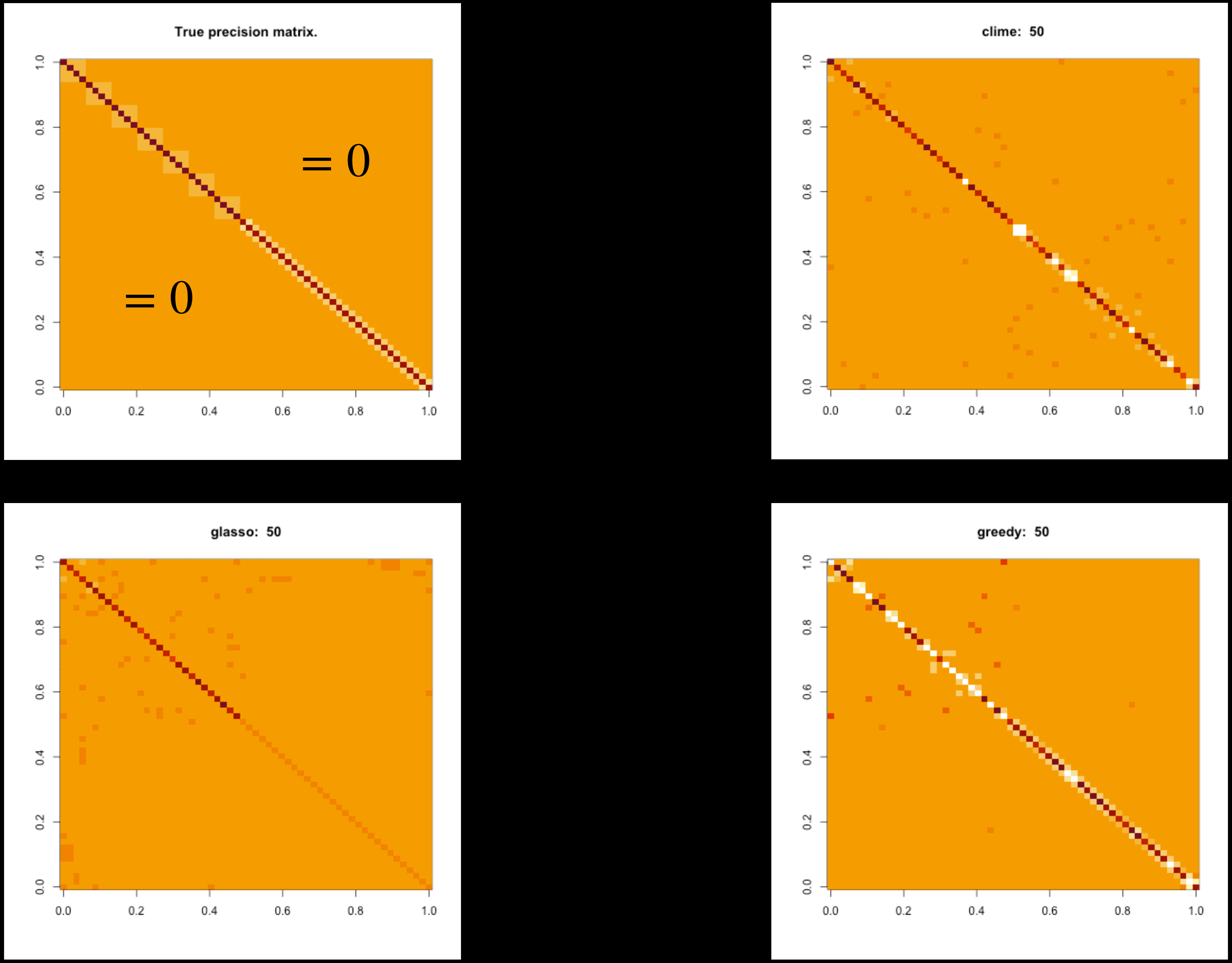

True precision matrix.
= 0
= 0
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.2
0.4
0.6
0.8
1.0


True precision matrix.
= 0
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clime: 50
glasso: 50
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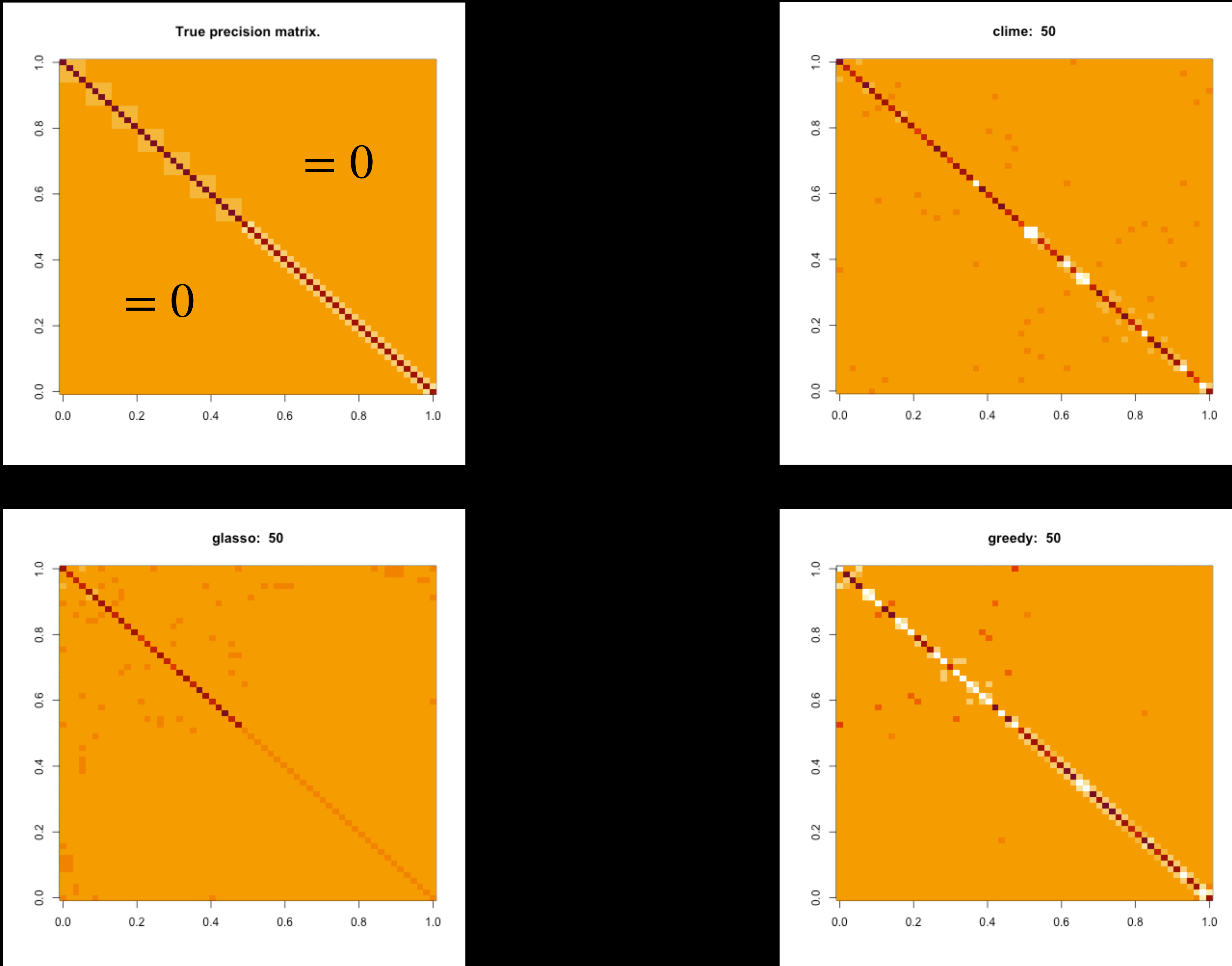
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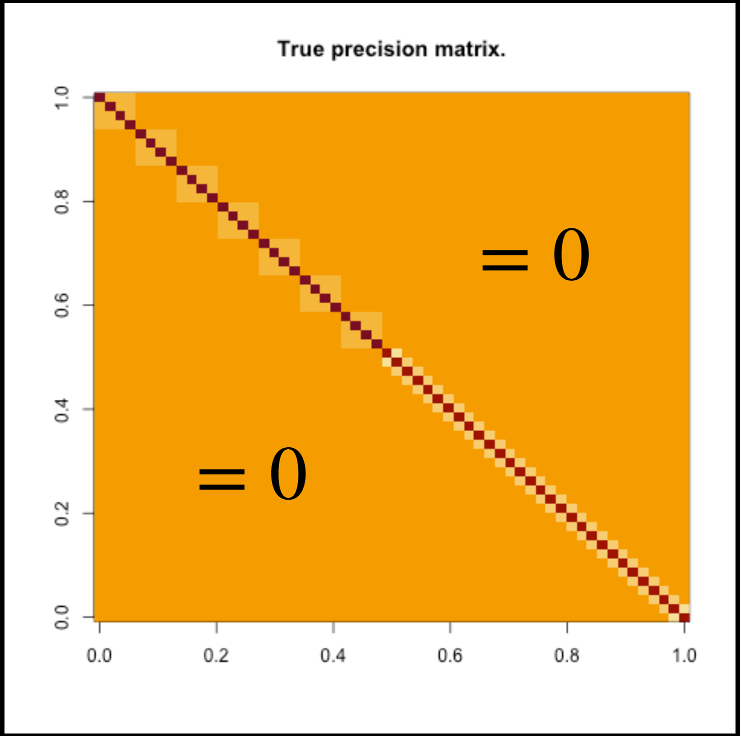
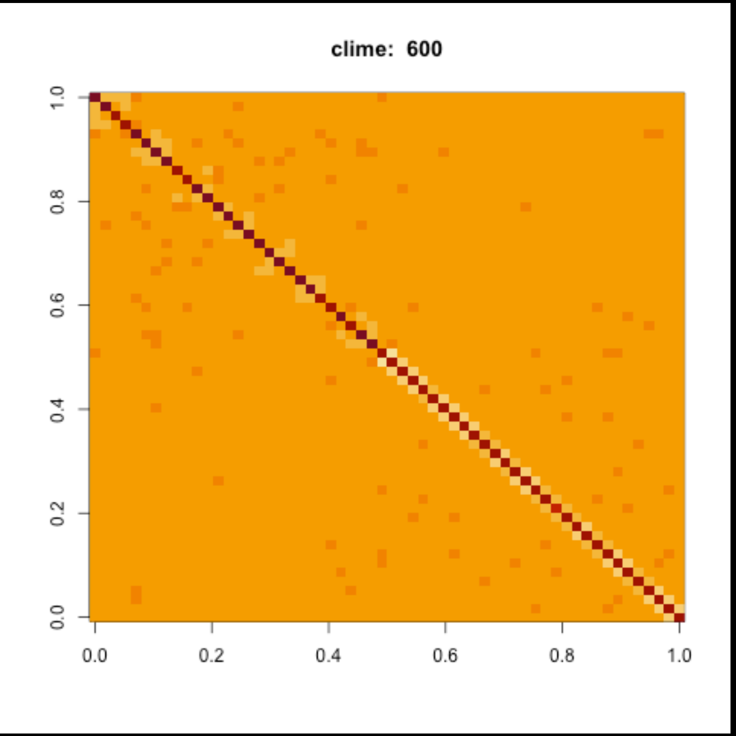
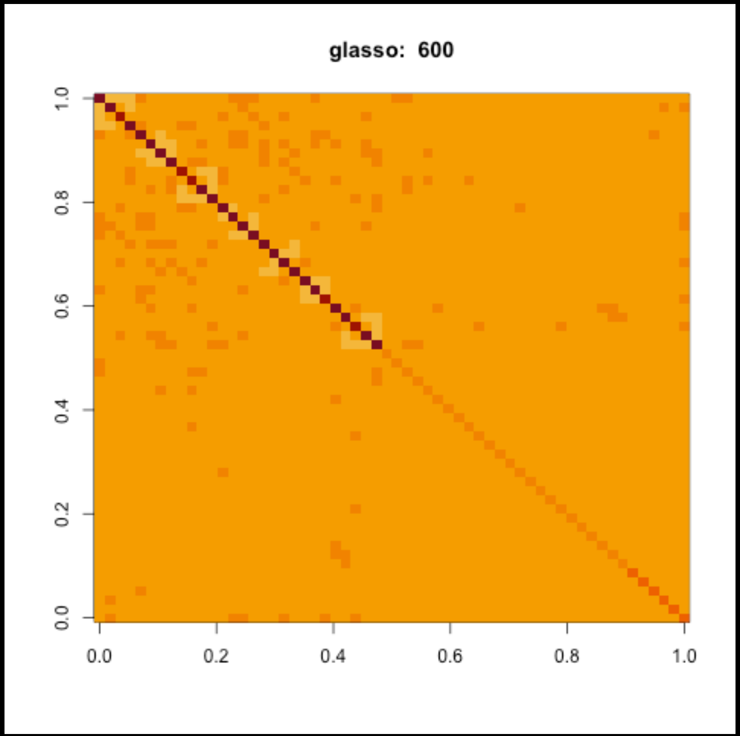
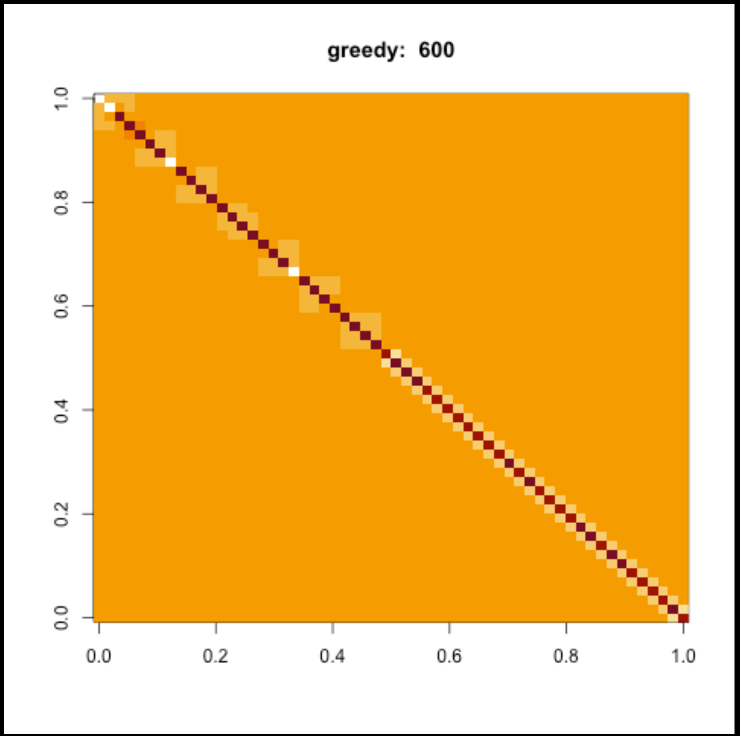


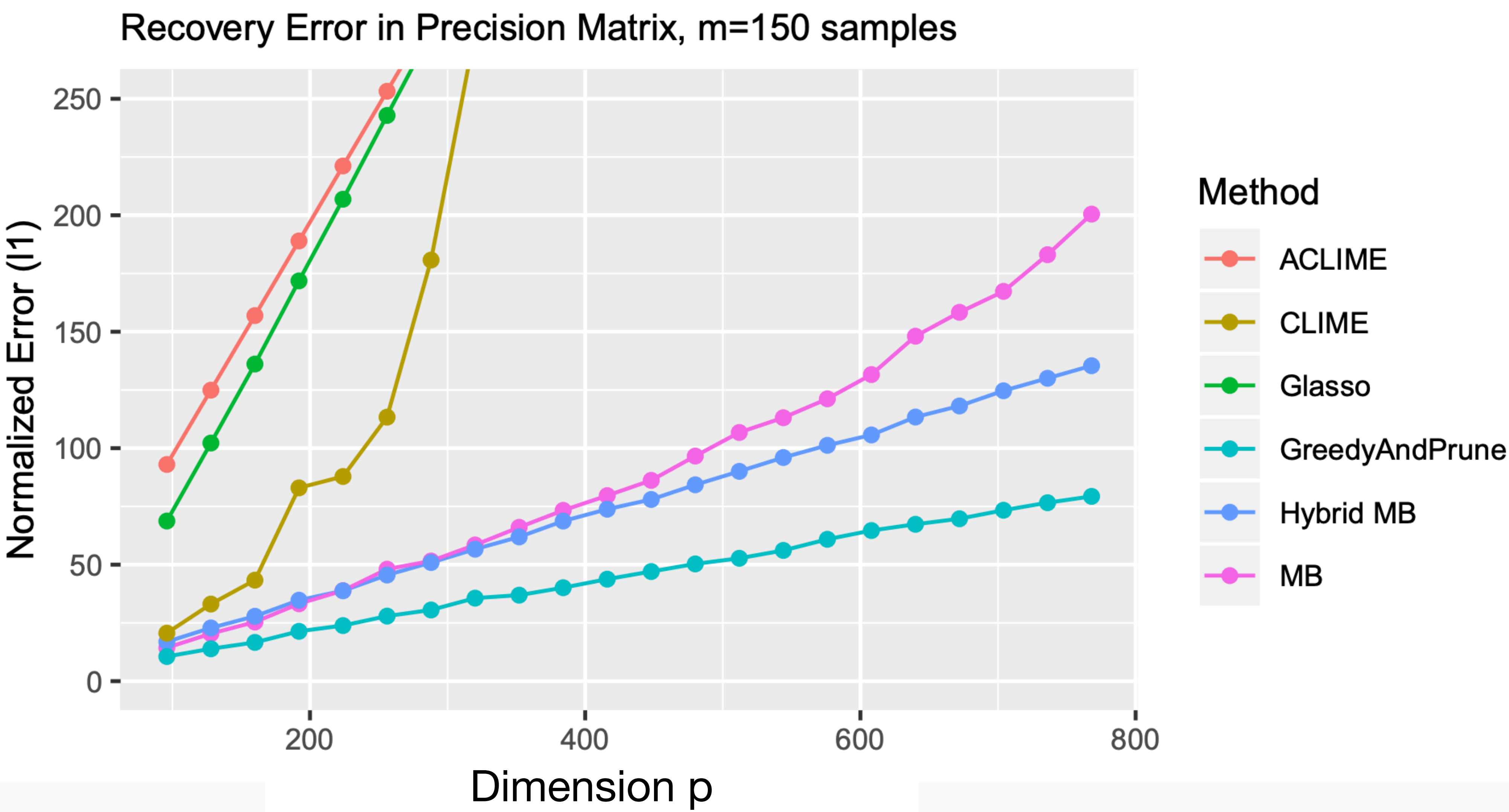


Final Outputs





A Simple Challenge: Path + Clique



GreedyPrune has best error

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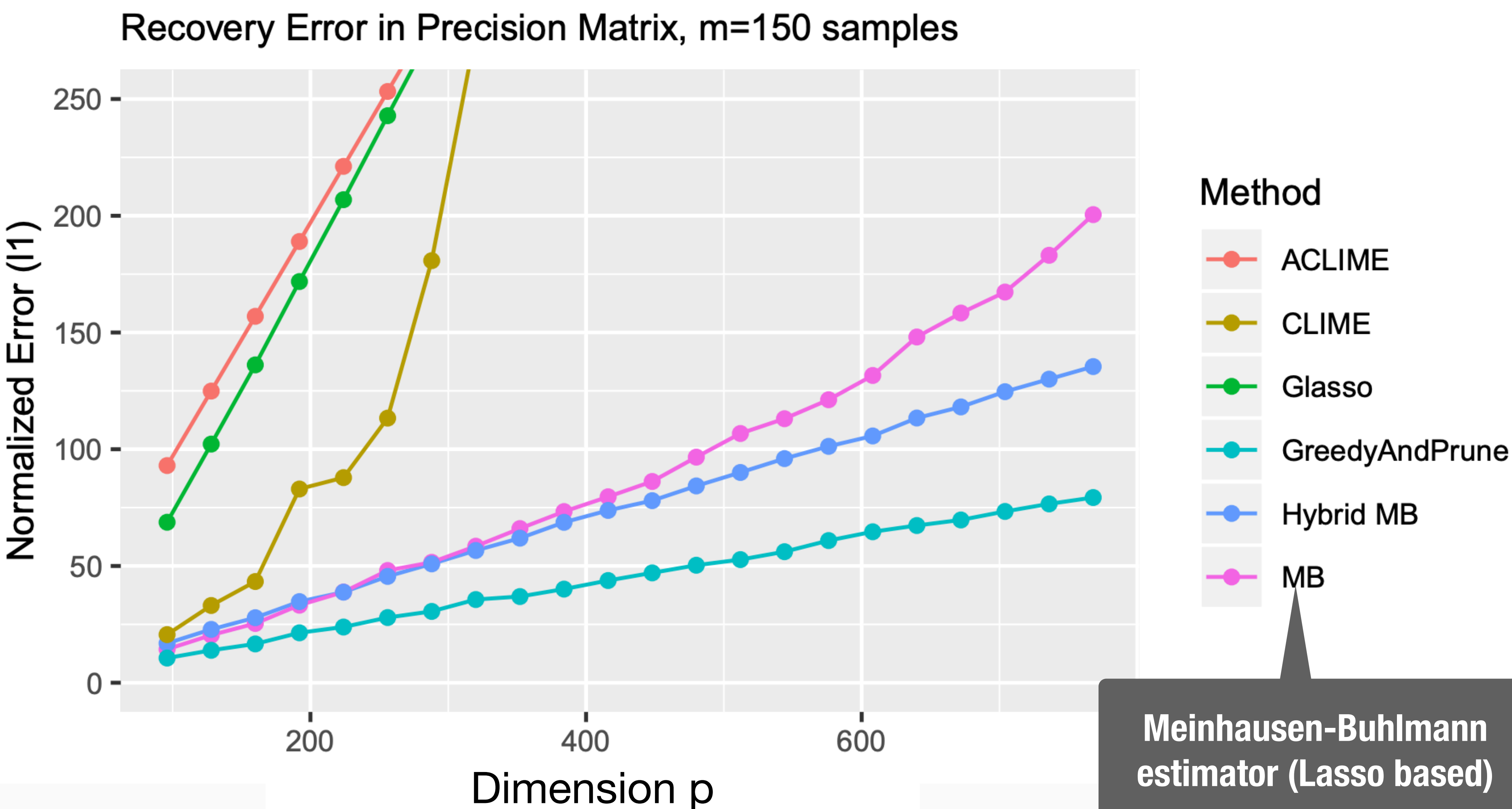

Meinhausen-Buhlmann estimator (Lasso based)

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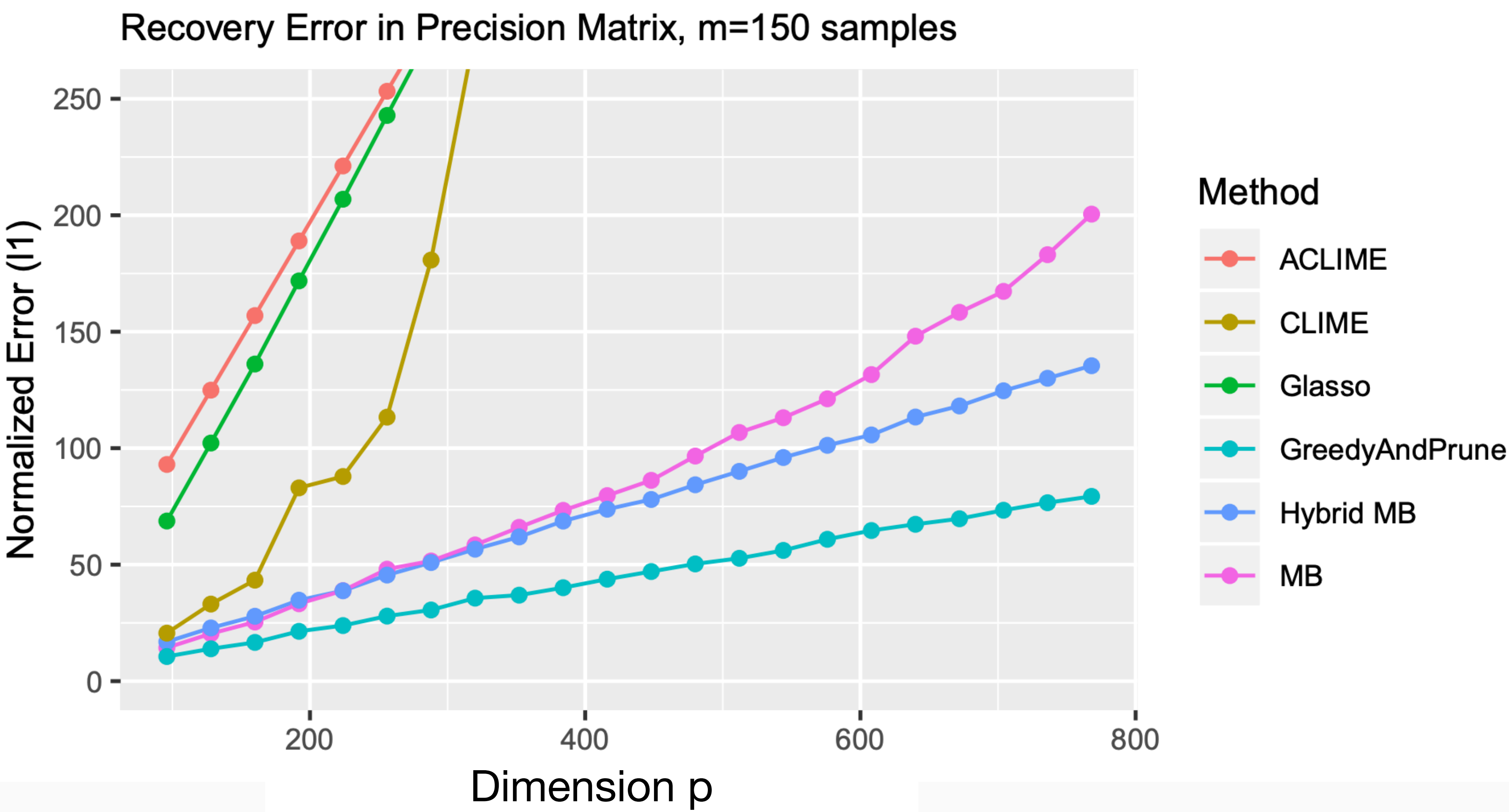

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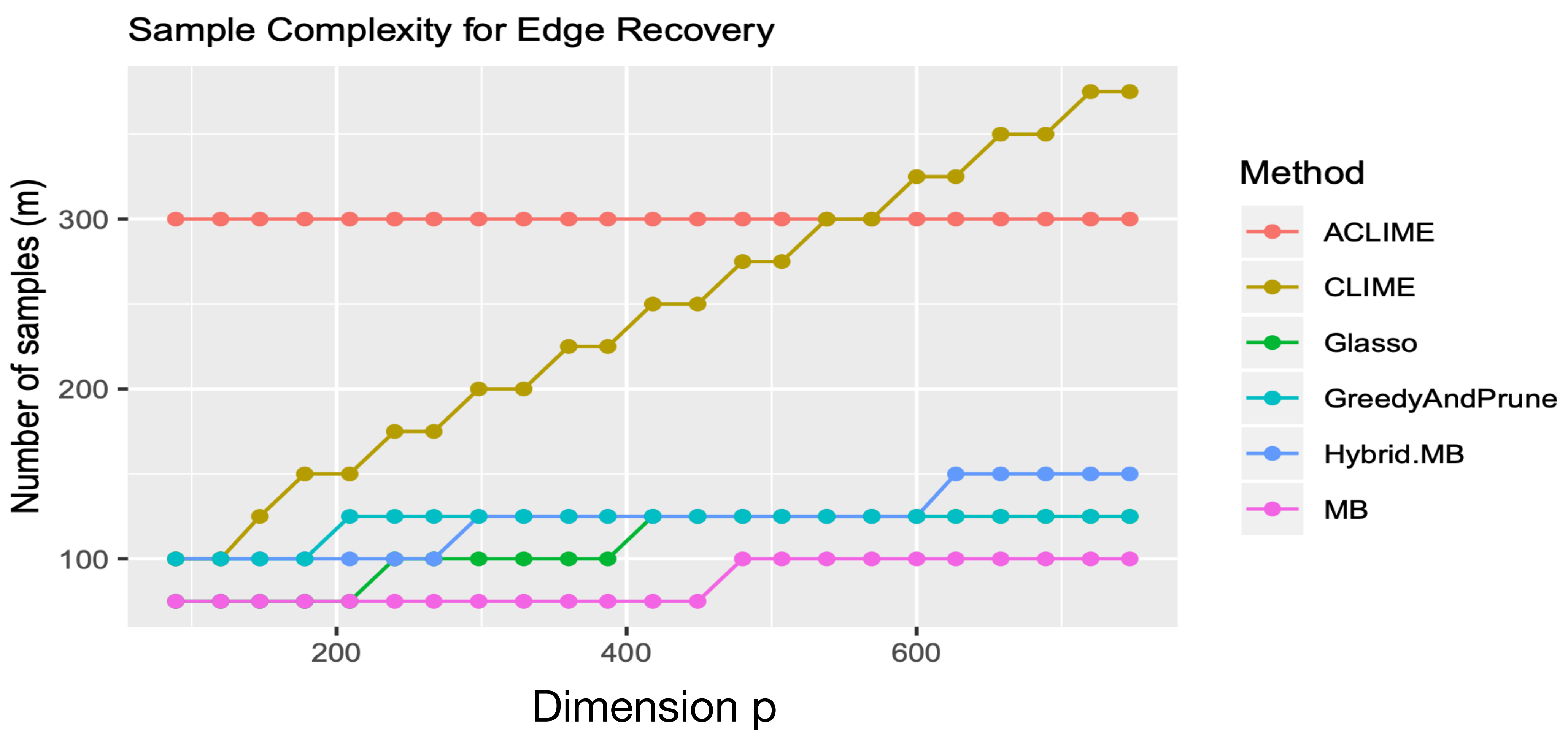

Intensity = 0.95

GreedyPrune needs very few samples.
CLIME grows nearly linearly …

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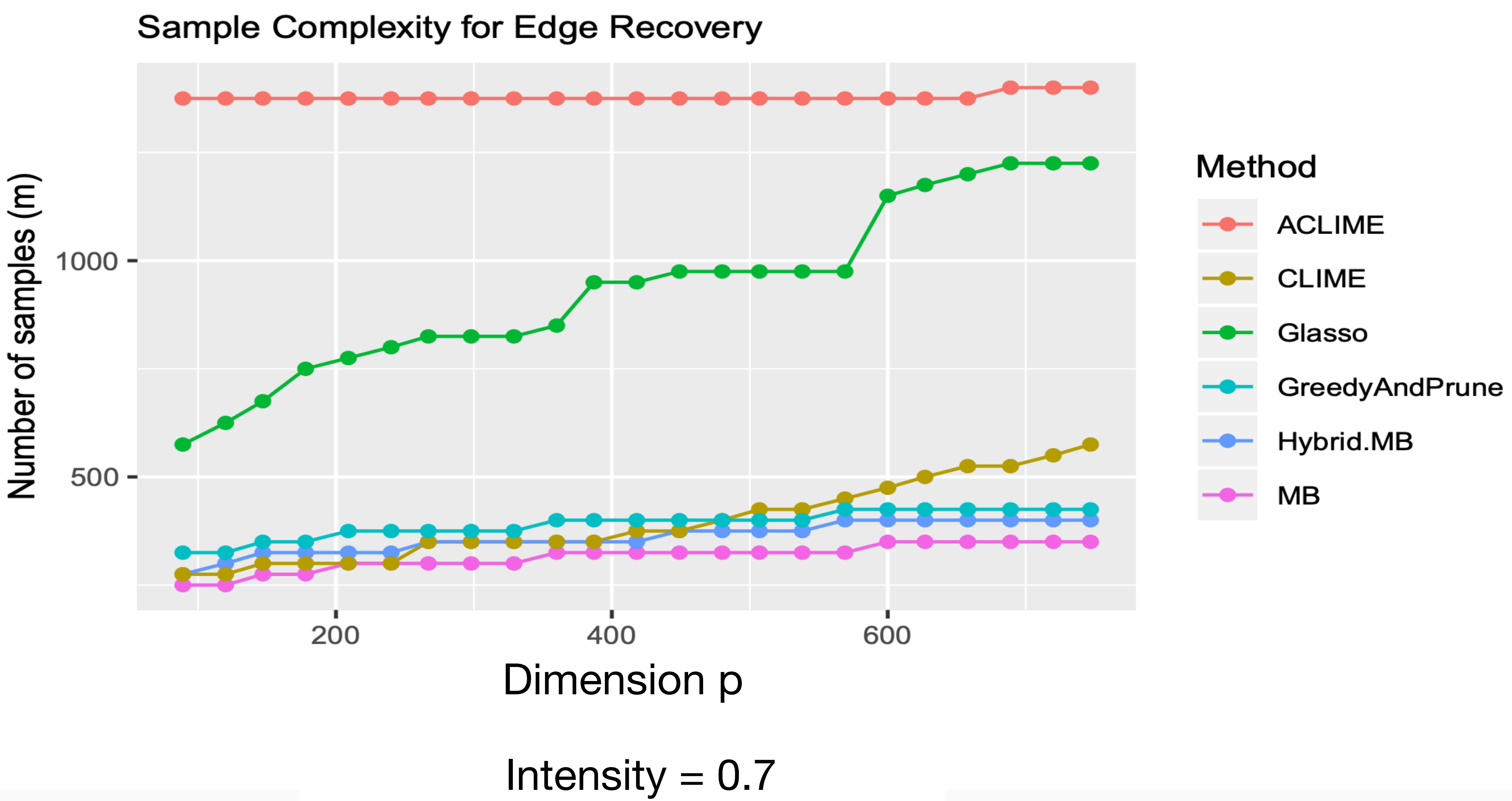

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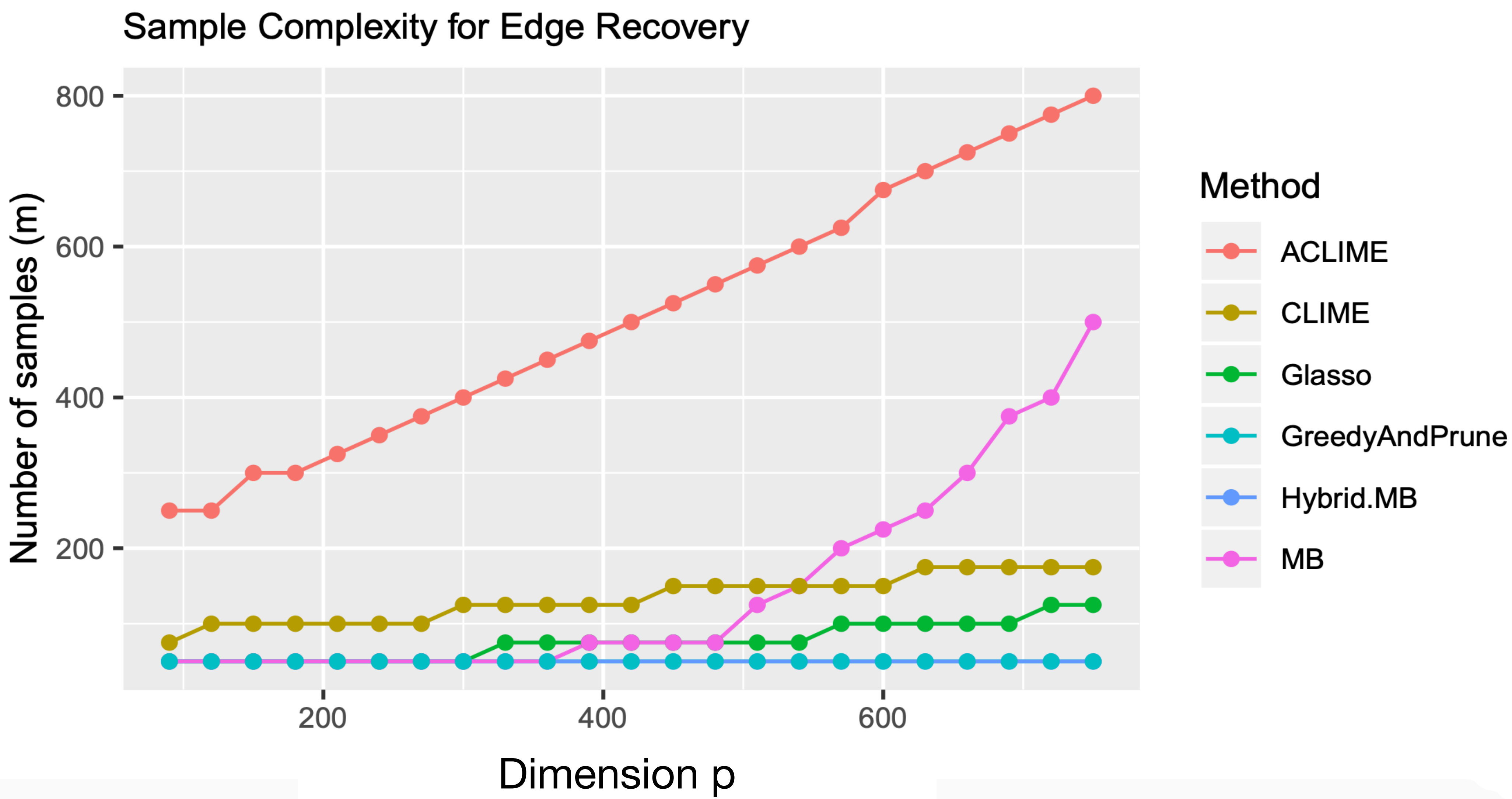
A Simple Challenge: Random walk



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GreedyPrune Summary

KKMM: **GreedyPrune** learns attractive models with $\tilde{O}(d \log p/\kappa^2)$ samples and quadratic run-time.

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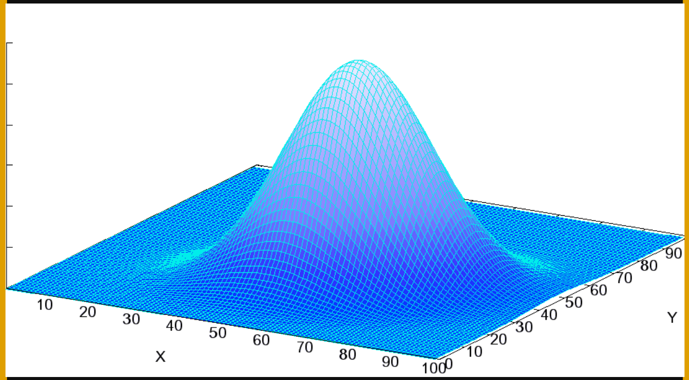
Also …

- Recovers guarantees of GLASSO, CLIME
- Empirically better
- Non-Gaussian distributions: Can learn precision matrices if good tail behaviour

GGMs



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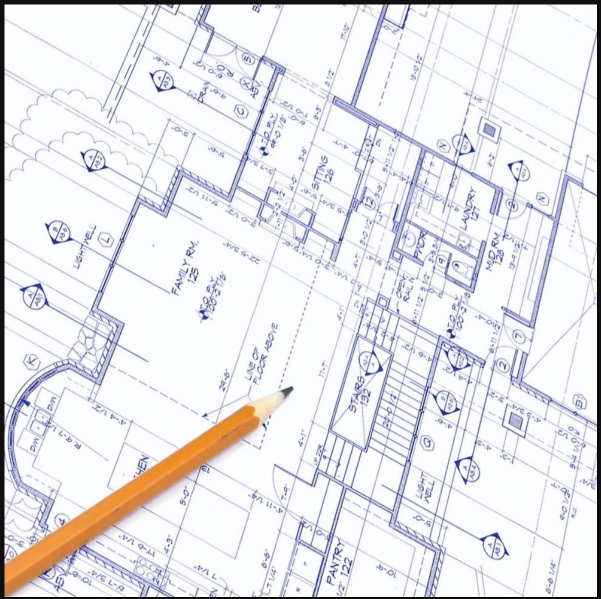
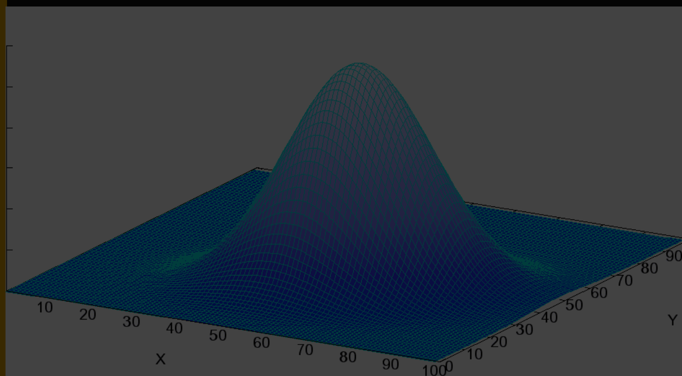


Attractive. SDD

GGMs



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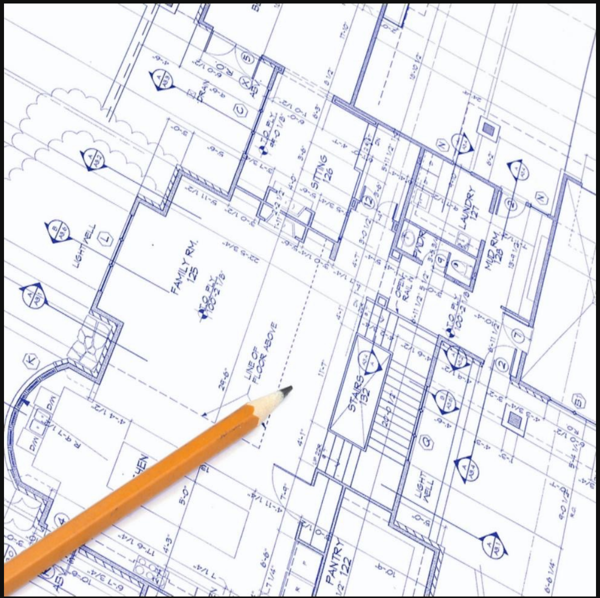

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Summary

Main Challenge: Can we recover structure of GGM of degree d, pairwise-correlation κ with run-time $p^{o(d)}$ and sample complexity $n \approx O_{d,\kappa}(poly(\log p))$?

Very well-stuided, practically important!

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Today: A simple greedy algorithm solves interesting special classes

Many Questions for GGMs …

- What other classes can we solve efficiently without condition number assumptions?
- Testing if a model is correct?
- Hidden variables?
- Computational hardness?

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Conjecture: No $p^{o(d)}$ algorithm to recover structure of general GGMs with $poly(d, 1/\kappa, \log p)$ samples.

Bigger Picture

Can we learn sparse dependency graphs from few samples?

(aka learning Markov random fields, undirected graphical models)

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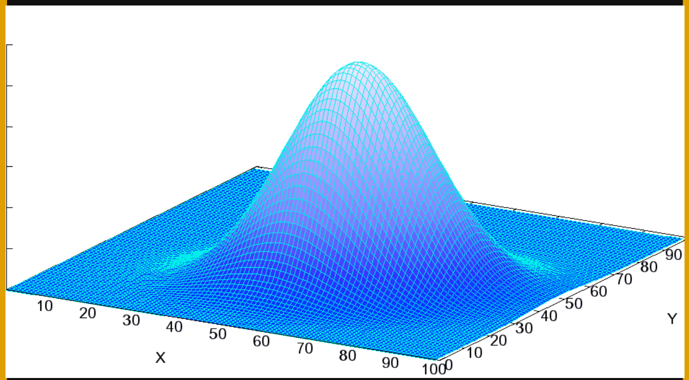
Lots of work … [Bresler10], [KM17], [HKM17], …

GGMs



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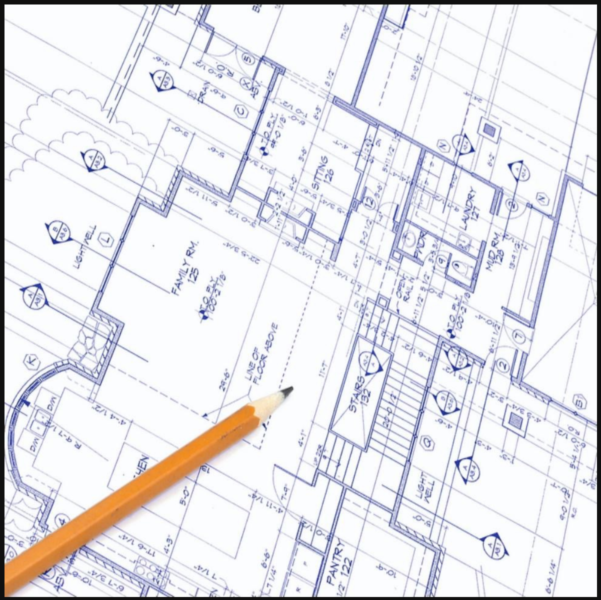

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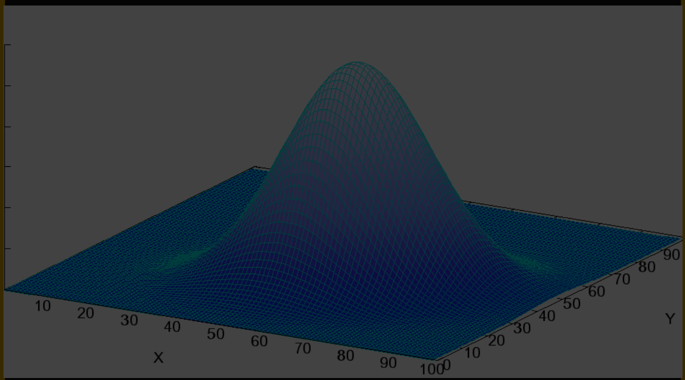

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Fix vertex 1. For $S \subseteq \{2,\ldots,n\}$, define

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Supermodular: $S \subset T$,

$$f(S) - f(S \cup \{j\}) \geq f(T) - f(T \cup \{j\})\,.$$

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Why useful?

- Optimizing supermodularity very well understood
- Greedy algorithm finds minimizer

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Almost …

- Only have estimates for f
- Crucial: missing a vertex means noticeably away from optimum

Analysis for Attractive: Supermodularity

Fix vertex 1. For $S \subseteq \{2, \ldots, n\}$, define
$f(S) = Var(X_1 \,|\, X_S)\,.$

Claim [MS, MJW]: X is attractive GGM. Then, $f(\quad)$ is monotonically decreasing and a supermodular function.

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Proof: …

- **Assume $\Theta_{ii} = 1$.**
- **Linear algebra:**

$$Var(X_1 \,|\, X_S) = \sum_{i_1, i_2, \ldots, i_k \notin S} (-\Theta_{ii_1})(-\Theta_{i_1 i_2}) \cdots (-\Theta_{i_k i})$$

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Product over cycles not touching S …

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Supermodular: $S \subset T$,
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- Thus: $f(S) - f(S \cup \{j\})$ is sum on cycles that touch j but don't touch S.
- Is decreasing with S, so f is supermodular.

Analysis for Walk-Summable

Fix vertex 1. For $S \subseteq \{2, \ldots, n\}$, define

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No longer supermodular!

(Not even weakly-supermodular …)

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- Walk-summable = Symmetric Diagonally Dominant (SDD)
- SDD implies neighbors have noticeable effect

Analysis for Walk-Summable

Def: Θ **is SDD if for all i**

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Suffices to show greedy works for SDD!

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- SDD implies neighbors have noticeable effect

Analysis: Bounded Conditional Variances

Lemma: If Θ is SDD, then for any vertex i, there exists a neighbor j such that $Var(X_i \mid X_j) \leq 4Var(X_i \mid X_{-i})/\kappa^2$.

Analysis: Bounded Conditional Variances

There exists a neighbor, that is comparable to the entire neighborhood in conditioning …

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Analysis: Bounded Conditional Variances

Why useful …

- $Var(X_i)$ can be very large!
- But conditioning on one neighbor brings the variance down.
- We can detect it with few samples.

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Analysis: Bounded Conditional Variances

Proof …

- Triangle inequality of **effective resistance** metric on graphs
- Properties of conditional variance …

Lemma: If Θ is SDD, then for any vertex i, there exists a neighbor j such that $Var(X_i | X_j) \leq 4Var(X_i | X_{-i})/\kappa^2$.

Analysis: Bounded Conditional Variances

For intuition: Assume $\Theta_{ii} = 1, \forall i$.

Recall: $\kappa(\Theta) = \min\limits_{i,j:\Theta_{ij}\neq 0} \dfrac{|\Theta_{ij}|}{\sqrt{\Theta_{ii}\Theta_{jj}}}$.

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Example: In random walk model

$Var(X_{i+1} | X_i) = 1; \quad Var(X_{i+1}) = i + 1!$

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Not true for general sparse precison matrices …

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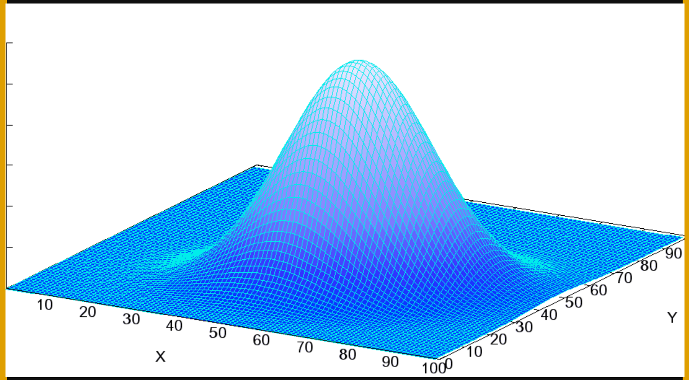
"Proof …":

- **If Laplacian …**

$$Var(X_i | X_j) = \frac{1}{2} R_{eff}(i, j) \leq \frac{1}{|\Theta_{ij}|} \leq 1/\kappa .$$

GGMs



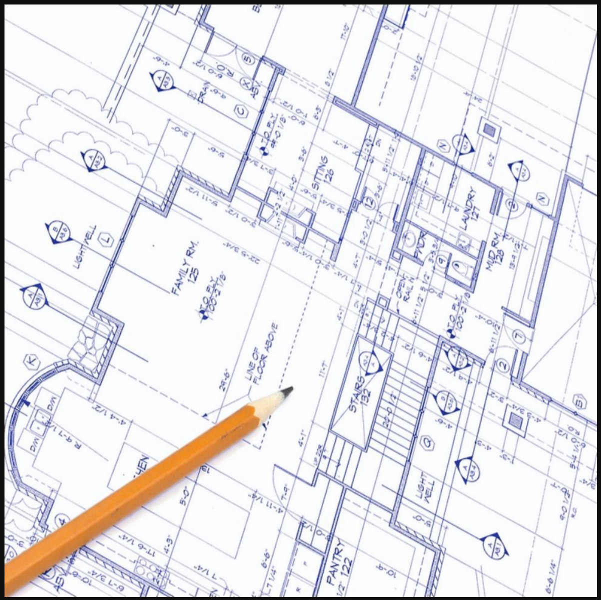
Motivation

Algorithm

While $|S| < t$:
Add $\arg\min_j Var(X_i | X_{S \cup j})$.

Special Models

Analysis



Attractive. SDD