LECTURE 17

Today

→ What are graphical Models ?

→ Bayesian Networks : Definition, Example,
learning challenges, Chow-Liu Algorithm.

1. The class on 05/25/2022 will be remote on zoom.
2. Final exam:
   - Covers all topics until the exam
   - Easier than assignments.
   - In-person exam as per university schedule
   - MSOL students online.

Unsupervised Learning: Given a dataset, we want to build a "model" for the dataset.

PROBABILISTIC MODELS OF DATA

→ Graphical models are probabilistic models for generating data

→ Precursors for modern "deep" generative models

↘ Core issues : ① Succinct representations of distributions

② Modeling dependencies.

Applications : ⓐ "Generate" new examples.

ⓑ "In-Painting"

ⓒ Applied Sciences useful in identifying relations.

Independence: (X, Y) random variables (joint dist.)

$$X \perp Y \iff Pr[X=x \wedge Y=y] = Pr[X=x] \cdot Pr[Y=y]$$
$$\iff Pr[Y=y \mid X=x] = Pr[Y=y].$$

Weather today is independent of Stock market.

	Heart Problems	Wake up time	Age
P_1	NO	11AM	19
P_2	YES	6:30AM	45
P_3	YES	7:AM	40
P_4	NO	12PM	24
P_5	NO	10AM	25
	⋮	⋮	
P_{10}	YES	6:AM	59
P_{11}	YES	6:30	62
		⋮	⋮

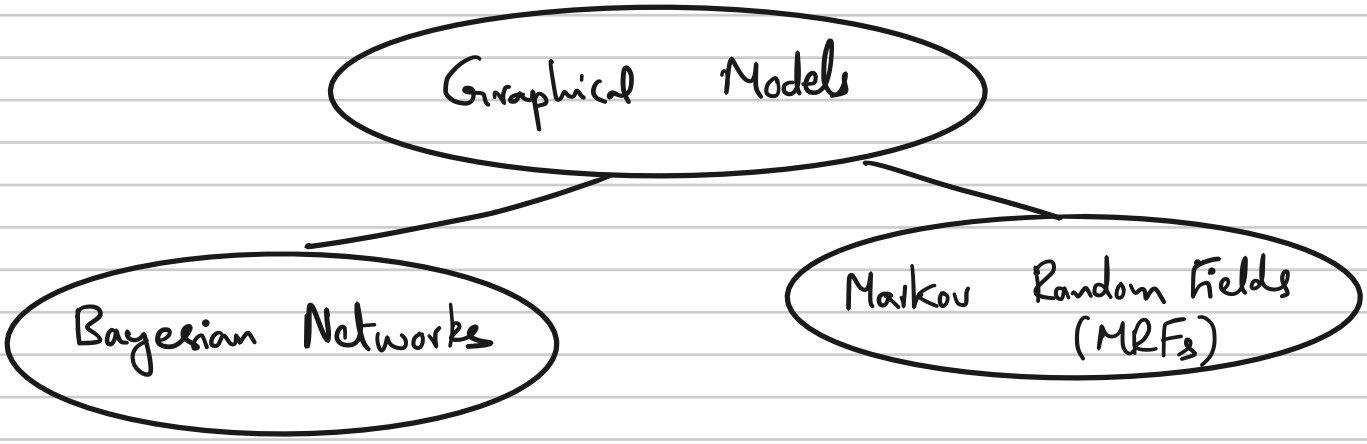
Comparing features directly:

Waking up early is bad for heart

Conditional Independence: X, Y, Z random variables

$$X \perp Y \mid Z \iff \Pr[X=x, Y=y \mid Z=z]$$
$$= \Pr[X=x \mid Z=z] \cdot \Pr[Y=y \mid Z=z]$$
$$\iff \Pr[Y=y \mid X=x, Z=z] = \Pr[Y=y \mid Z=z].$$

Graphical Models are distributions with "constrained" conditional independence ("CI") relations.



"Directed" Graphical Models

"Undirected" Graphical Models.

Bayesian Networks

$X \in \Sigma^d$ $\qquad (X_1, X_2, \ldots, X_d)$

A Directed Acyclic Graph (DAG) on $[d]$ vertices. G

A distribution D is a Bayes Net with graph G if

$$D(x_1, x_2, \ldots, x_d) = \prod_{i=1}^{d} P[x_i = x_i \mid X_{\text{parents}(i)} = z_{\text{parents}(i)}]$$

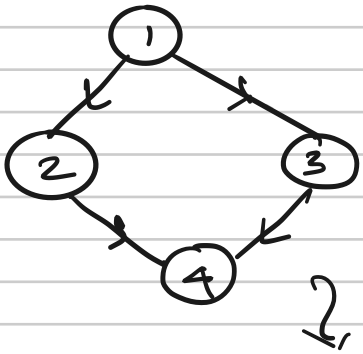
$P(X = x_1, x_2, \ldots, x_d) = \prod_{i=1}^{d} P[X = x_i \mid X_{Pa(i)} = x_{Pa(i)}]$

$Pa(1) = \phi$

$Pa(2) = \{1\}$

$Pa(3) = \{1\}$

$Pa(4) = \{2, 3\}$



$pa(i)$ = the parents of i.

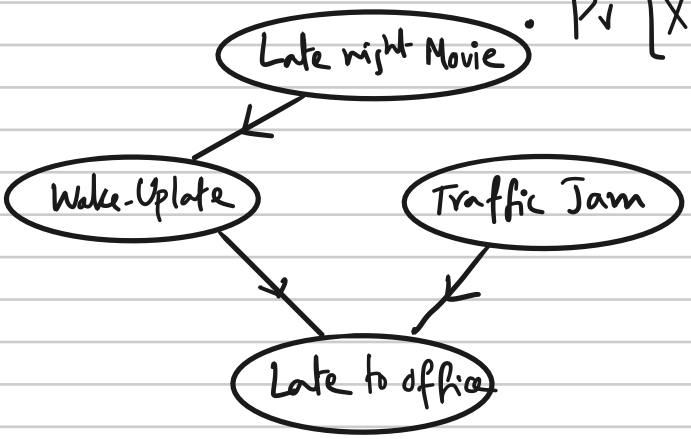
Example: $P(X = x_1, x_2, x_3, x_4)$

$= P_r[X_1 = x_1] \cdot P_r[X_2 = x_2 \mid X_1 = x_1]$

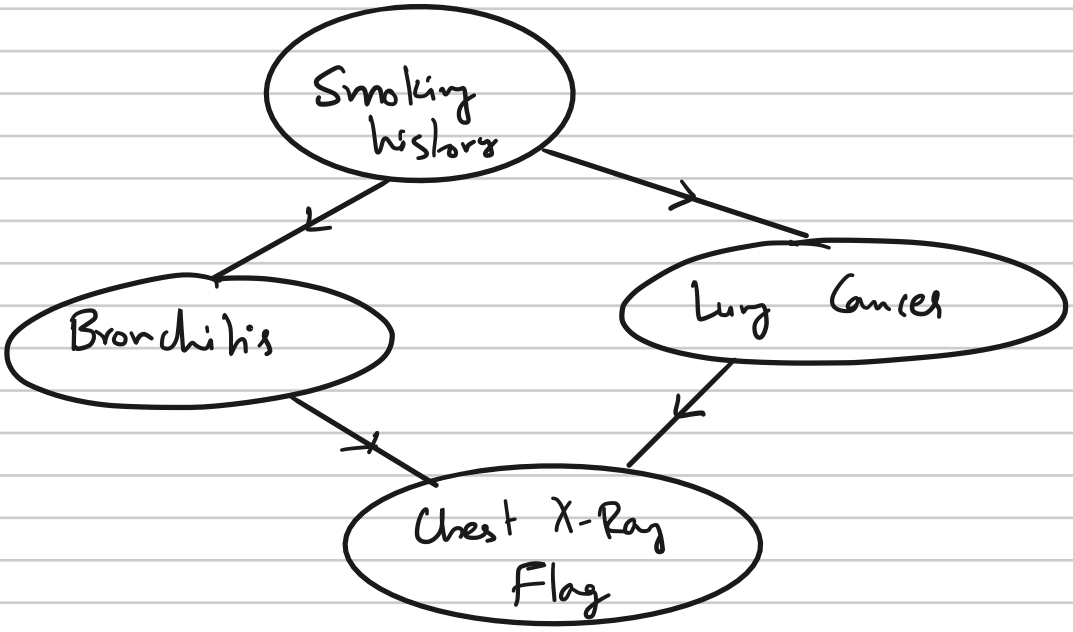
$\cdot P_r[X_3 = x_3 \mid X_1 = x_1]$

$\cdot P_r[X_4 = x_4 \mid X_2 = x_2, X_3 = x_3]$

Example:



Examples:



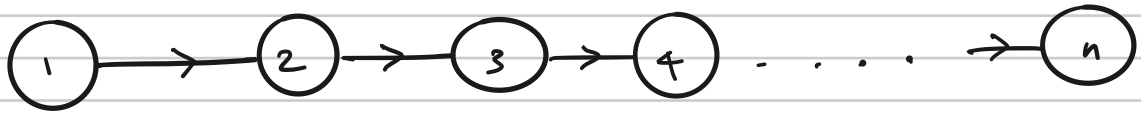
Learn the Bayes Net from

Samples

→ Given n samples $x^1, x^2, \ldots, x^n$

→ Learn the underlying directed dependency graph

Ex:



"Markov chain".

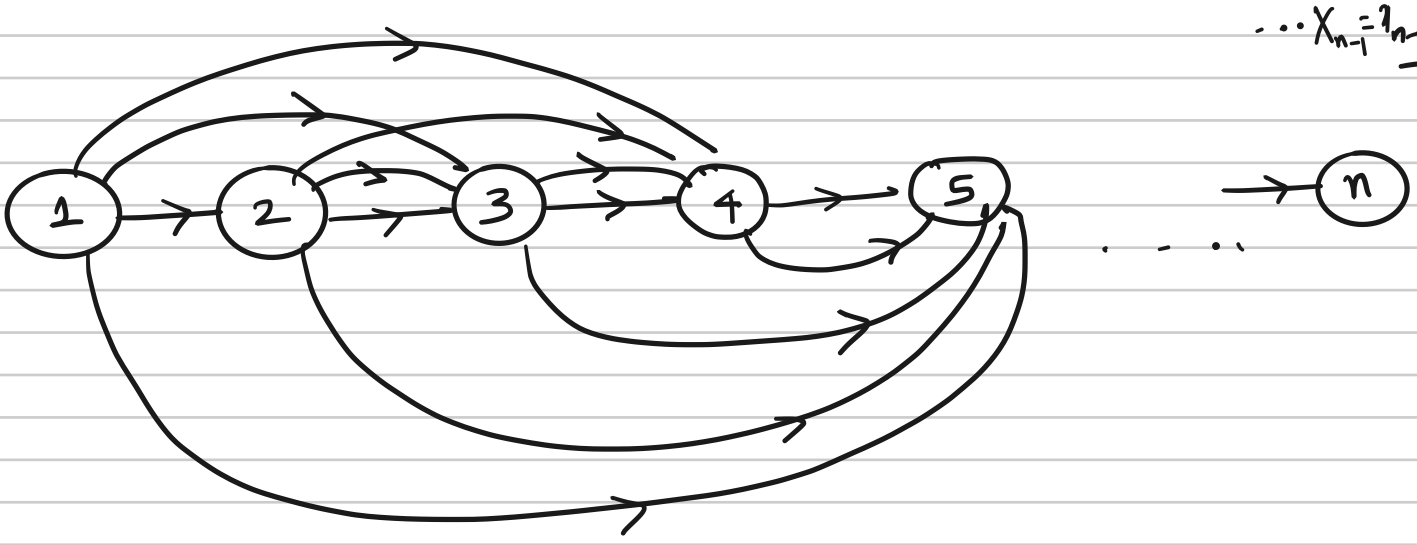
$$X_i \perp X_j \mid X_{i-1} \quad \text{for} \quad j < i-1$$

$$X_{10} \perp X_2 \mid X_9$$

$$\Pr[X = x_1, x_2, \ldots, x_n]$$

$$= \Pr[X_1 = x_1] \cdot \Pr[X_2 = x_2 \mid X_1 = x_1]$$

$$\cdot \Pr[X_3 = x_3 \mid X_1 = x_1, X_2 = x_2] \cdots \Pr[X_n = x_n \mid X_1 = x_1 \ldots X_{n-1} = x_{n-1}]$$



Make an assumption about the true "graph"

(being "simple" in some sense).

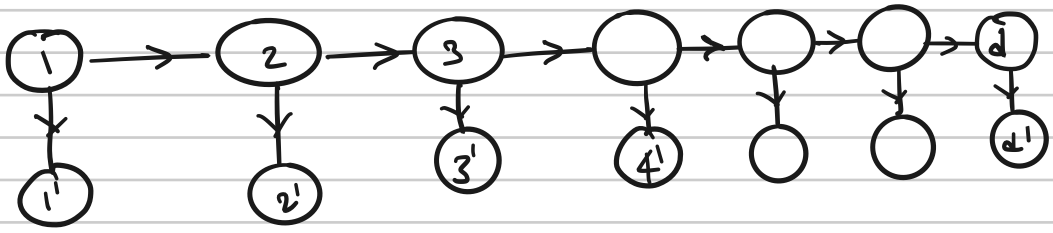
→ Degree is bounded ?

→ The "unknown" graph is a tree / path ...

→ Learn the structure graph under assumptions on the graph

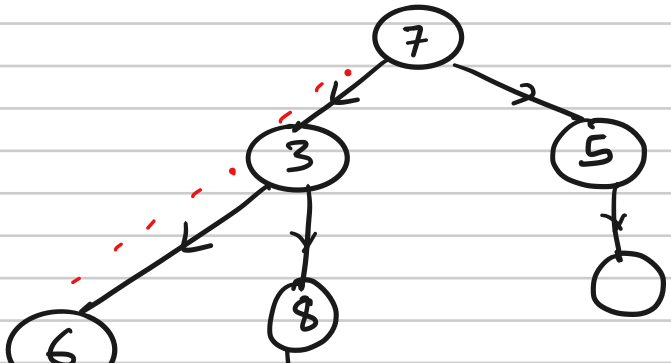
→ Learn the distribution assuming you even know the graph.

→ Some features are missing ?
(Hidden Markov Models)



Suppose we get samples from a distribution generated by a tree Bayes network.

→ Can you learn the distribution from samples?



Each node has a single parent.

CHOW-LIU Algorithm 1968:

→ We can learn tree-shaped Bayesian networks.

LECTURE 18 05/25

Last class
- → Defined Bayesian Nets
- → Structural assumptions
- → Learning Bayes nets

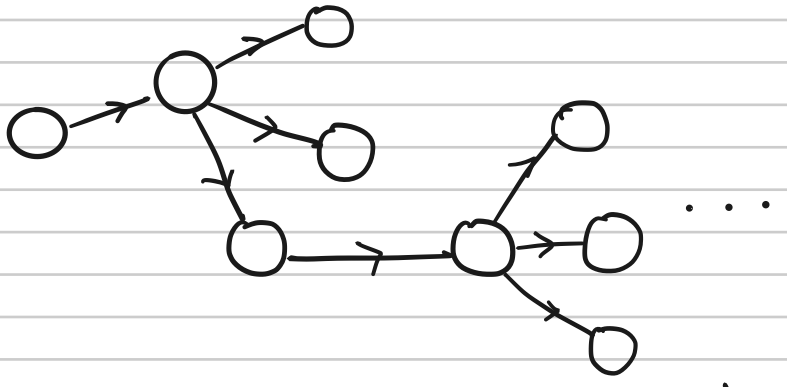
Today
- → Chow-Liu algorithm
- → Undirected graphical Models

- Assignment 4 is due today @ 10PM
- Office hours on Wednesday 06/02 @ 4-5 PM.

Learning Bayesian Networks defined by trees

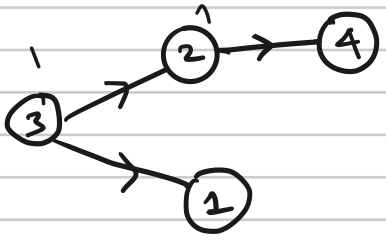
Distribution D: $(X_1, X_2, \ldots, X_d) \in \Sigma^n \quad \left(\{0,1\}^d\right)$

Assumption:



Rooted tree: Each node (except root) has exactly one parent.

Example:



$$P(X = x_1, x_2, x_3, x_4)$$

$$= P(X_3 = x_3) \cdot Pr\left[X_2 = x_2 \mid X_3 = x_3\right]$$

$$\cdot Pr\left[X_1 = x_1 \mid X_3 = x_3\right]$$

. $Pr\left[X_4 = x_4 \mid X_2 = x_2\right]$.

- Suppose we see samples from a Bayes net as above
- Can you learn the distribution?

Structure Learning
"learn the underlying graph"
learn the tree

Parameter learning
Learn the conditional distributions.

Goal: Let us try to learn a distribution D' such that $dist(D, D')$ is small.

KL-Divergence: "Measures distance between distributions"
We have two dist P, Q over some space Ω.
(Cross entropy).

$$KL(P\|Q) = \sum_{s \in \Omega} P(s) \log \frac{P(s)}{Q(s)}$$

$P(s)$: Probability s happens under P.
$Q(s)$: Probability s happens under Q

Example: $\Omega = \{0, 1\}$

$P(0) = \frac{1}{2}$, $P(1) = \frac{1}{2}$

$Q(0) = \frac{3}{4}$, $Q(1) = \frac{1}{4}$.

$$\rightarrow KL(P|q) = P(0)\cdot \log\frac{P(0)}{q(0)} + P(1)\cdot \log\frac{P(1)}{q(1)}.$$

$$= \frac{1}{2}\cdot \log\left(\frac{2}{3}\right) + \frac{1}{2}\cdot \log(2)$$

$$= \frac{1}{2}\cdot \log\left(\frac{4}{3}\right).$$

Question: What is $KL(P|P)$?

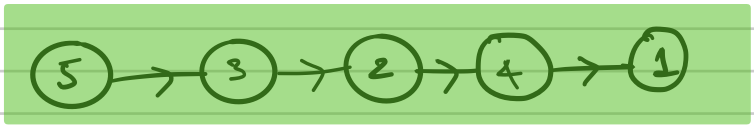
Answer: 0.

Property: $KL(P|q) \geq 0$ and is $0 \Leftrightarrow P = q$.

INPUT: Samples from a distribution P on Σ^d $(\Sigma = \{0,1\})$
(being generated by some unknown Bayes net which is a tree: T^*)

OUTPUT: Find a tree T and a corresponding Bayes net P_T such that $KL(P|P_T) \leq \varepsilon$.

Example:

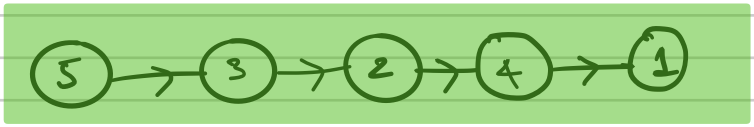


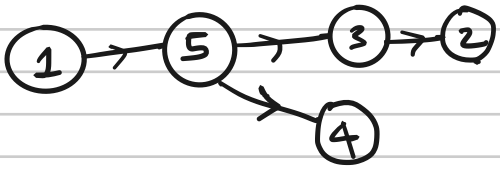
T^*.

$\rightarrow (X_1, X_2, X_3, X_4, X_5)$

If I give a tree T and ask find me the Bayes net P_T that minimizes

$KL(P|P_T)$.





$\rightarrow (X_1, X_2, X_3, X_4, X_5)$ T^*

Idea: Well, use the "empirical" conditional probabilities

1. Estimate the conditional probabilities along the tree T.
   (e.g.: Estimate $\Pr[X_1=1]$. $\Pr[X_5=1|X_1=0]$, $\Pr[X_5=1|X_1=1]$
   ⋮

INPUT: Samples from P & a tree T.

Algorithm: For each edge (i,j) in T, estimate $\Pr[X_j|X_i]$ and use these to define P_T.

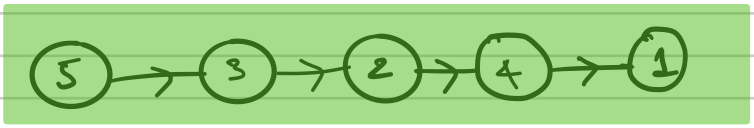
Chow-Liu Bound:

→ For any tree T,

$$KL(P|P_T) = J_P - \sum_{(i,j) \text{ is an edge in } T} I(X_i; X_j)$$

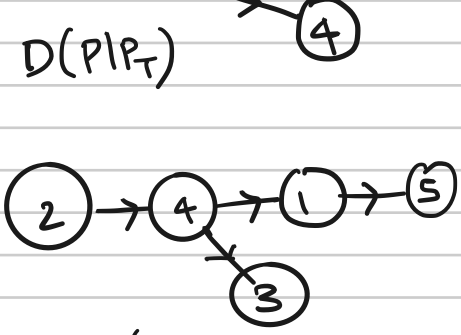
↓

Some number depending on P



$(X_1, X_2, X_3, X_4, X_5)$ T^*

$D(P|P_T)$



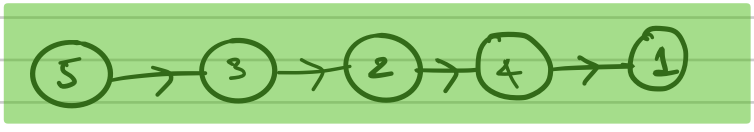
$D(P|P_-)$

$I(X_i; X_j) =$ "Measures how much information about X_j does X_i have".

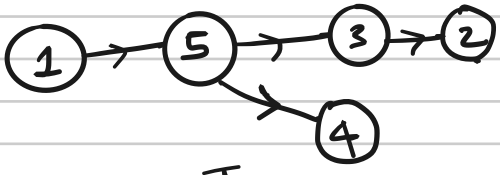
$$I(X_i; X_j) \sum_{a,b} P_1[X_i=a, X_j=b] \cdot \log \frac{P_1[X_i=a] \cdot P_1[X_j=b]}{P_1[X_i=a, X_j=b]}$$

We can estimate $I(X_i; X_j)$ from Samples.

$P[X_1 = x_1,$



$(X_1, X_2, X_3, X_4, X_5)$ T^*



T

Chow-Liu Bound (1968): $KL(P|P_T)$

$$= J_p - I(X_1; X_5) - I(X_5; X_3) - I(X_5; X_4) - I(X_3; X_2).$$

Summary: Find T that minimizes $KL(P|P_T)$. Or find

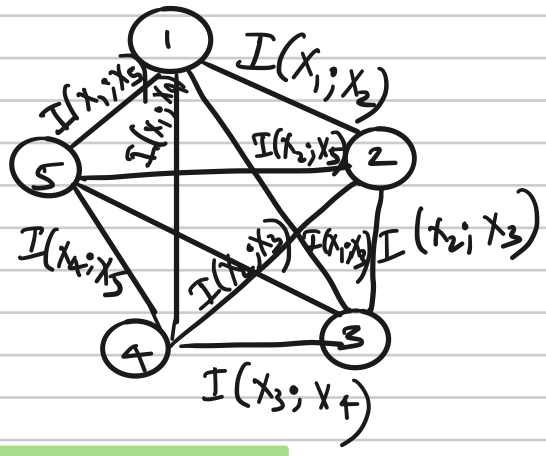
$$\operatorname{argmin}_T \; J_p - \sum_{(i,j) \in T} I(X_i; X_j)$$

$$\equiv \underset{T}{\operatorname{argmin}} \sum_{(i,j)\in T} -I(X_i; X_j)$$

$$\equiv \underset{T}{\operatorname{argmax}} \sum_{(i,j)\in T} I(X_i; X_j)$$

Idea:

We have Samples from P ⟶



CHOW-LIU ALGORITHM

→ Use samples to estimate $I(X_i;X_j)$ for all i,j.

→ Form a weighted graph where weights are exactly $I(X_i;X_j)$

→ Compute the max. spanning tree T' in G_I

→ Output $P_{T'}$.

Given a weighted graph G_I on d vertices, find tree T that has maximum total weight.

We can do this very fast!

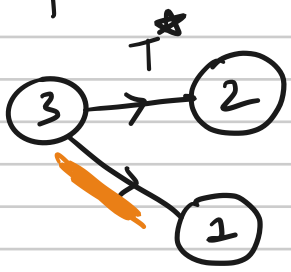
We can do this in linear time.

$(X_1, X_2, \ldots, X_5)$: ☐ → Compute $I(X_1; X_2)$

☐ → Compute $I(X_1; X_3)$

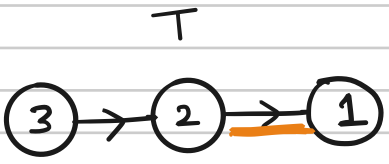
$\square \rightarrow$ Compute $I(X_1; X_f)$

Example:



$$P[X_0 = x_1, x_2, x_3] = P[X_3 = x_3] \cdot P[X_2 = x_2 | X_3 = x_3] \cdot P[X_1 = x_1 | X_3 = x_3]$$

"true distribution".



$$P_T[X = x_1, x_2, x_3] = P[X_3 = x_3] \cdot P[X_2 = x_2 | X_3 = x_3] \cdot P[X_1 = x_1 | X_2 = x_2]$$

Summary:

→ Can learn tree-structured Bayes networks

→ Active research: What are other structural assumptions Can we learn Bayes networks.

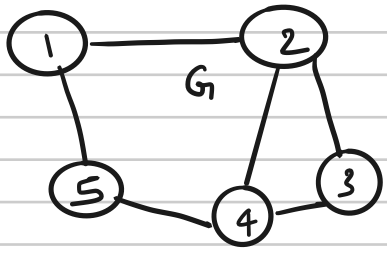
"Directed Graphical Models"

Undirected Graphical Models

- "Markov Random Fields". (MRFs).

Distribution: $D \equiv (X_1, X_2, \ldots, X_d)$

Dependency graph G for D.

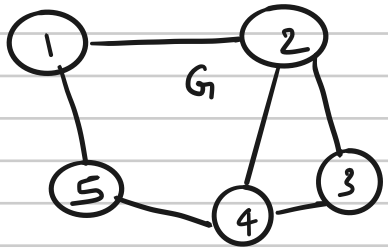


e.g: $X_1 \perp X_4 \mid X_2, X_3, X_5$

D satisfies "Pairwise Markov Property" with respect to G if

If i, j have no edge, then

$$X_i \perp X_j \mid X_{rest}$$

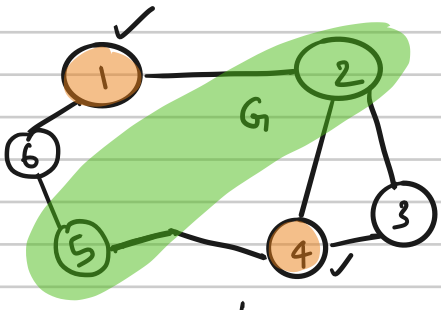


e.g: $X_1 \perp X_4 \mid X_2, X_5$

D satisfies "Local Markov Property" with respect to G if

If i, j have no edge, then

$$X_i \perp X_j \mid X_{\{\text{neighbors of } i\}}$$



e.g: $X_1 \perp X_4 \mid X_2, X_5$

D satisfies "Global Markov Property" with respect to G if

If i, j have no edge, then

$$X_i \perp X_j \mid X_{\{\text{any separating set}\}}$$

$X_1 \perp X_4 \mid X_2, X_5$

↓

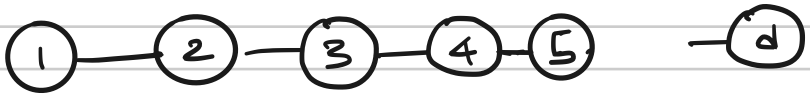
Subset of vertices removing which disconnects i and j in G.

Global MP $\Rightarrow$ Local MP $\Rightarrow$ Pairwise MP

For "most reasonable" distributions all three are equivalent.

Example: Markov Chain

$X_1, X_2, \ldots, X_d$ $\quad X_{i+1} \perp X_{i-1} \mid X_i$



Remark: We'll say D has dependency graph G if it satisfies Markov property with respect to G.

Main Learning Challenges:

Structure Learning: Given samples from D learn its dependency graph G.

Parametric learning: Given samples from D learn the full distribution.

Inference: You know dependency graph

MAP Want to find most likely value of $X_i \mid X_{\{\text{partial assignment}\}}$.

Goal: Structure Learning

INPUT: Samples $x^1, x^2, \ldots, x^n \sim D$

OUTPUT: Dependency graph of D.

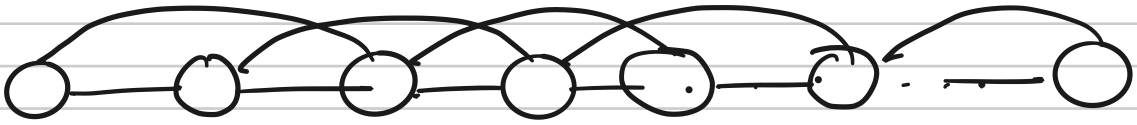
ILL-POSED: Complete graph is a dep. graph for all distributions!

"Minimal dependency graph?

Assumption: Dependency graph of D is Sparse.
- Each vertex has a bounded degree k.

INPUT: Samples $x^1, x^2, \ldots, x^n \sim D$

OUTPUT: A dependency graph for D where each vertex has degree $\leq k$.



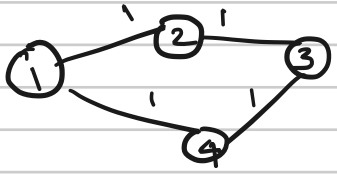
$k = 4$

→ If we know the structure, the general learning problem becomes easier.

Learning Boltzmann Machines

D on $\{1,-1\}^d$

$$Pr[X = x] \propto \exp\left(\sum_{\{i,j\} \in G} w_{ij} x_i x_j\right)$$



$$Pr[X = x] \propto \exp\left(x_1x_2 + x_2x_3 + x_3x_4 + x_4x_1\right)$$

Gaussian Graphical Models

D on $\mathbb{R}^d$

Dist D is $N(0, \Sigma)$

Σ is the covariance matrix. $X \sim N(0, \Sigma)$

$\Sigma_{ij} = \mathbb{E}[x_i x_j]$

$\Sigma_{ij} = 0 \Rightarrow x_i, x_j$ are

independent.

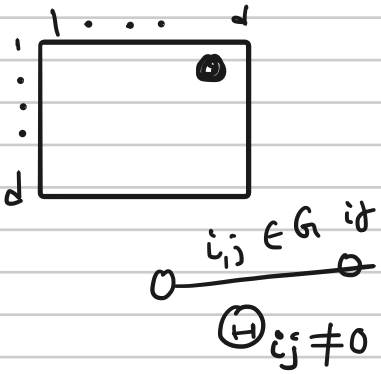
(Dempsey 1972):

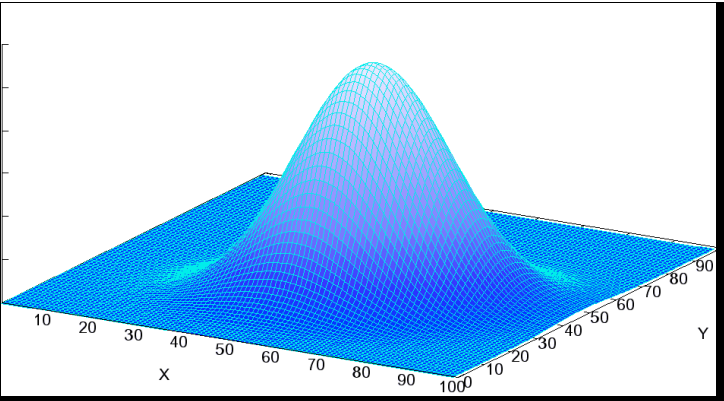
Distributions as defined above, they satisfy Markov property wrt G.

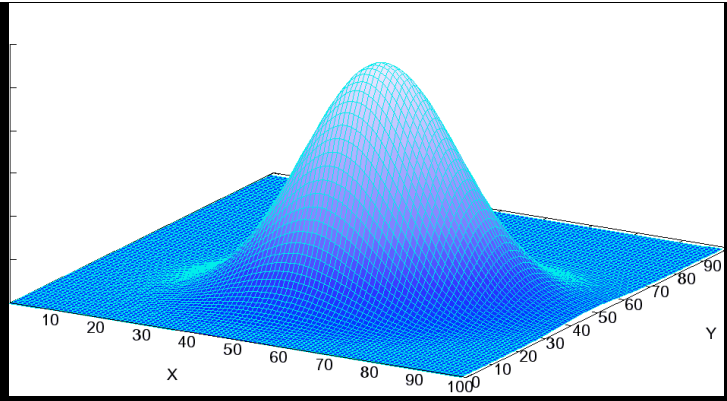
Precision Matrix:

$$\Theta = \Sigma^{-1}.$$

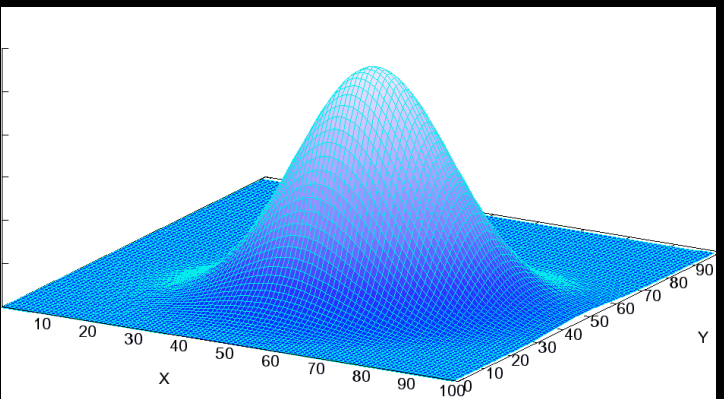
Thm: Gaussian dist has dependency graph with $\text{Supp}(\Theta)$.

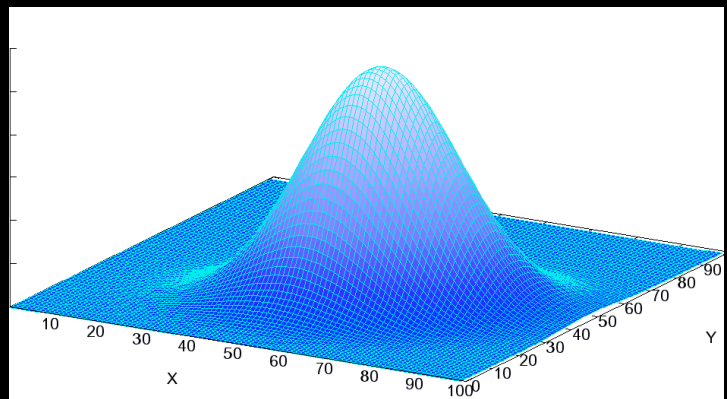




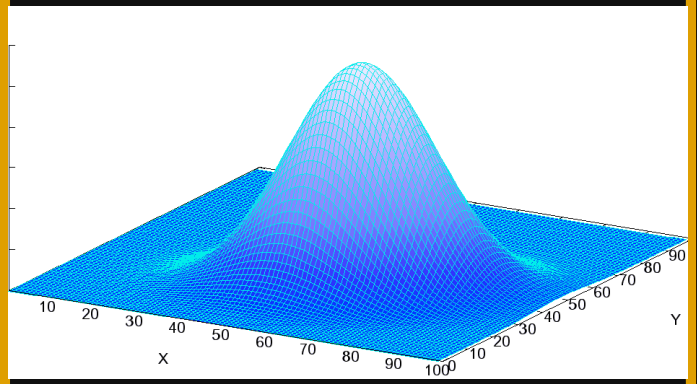


Learning Gaussian Graphical Models w/o condition number bounds





GGMs



Motivation

Algorithm

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

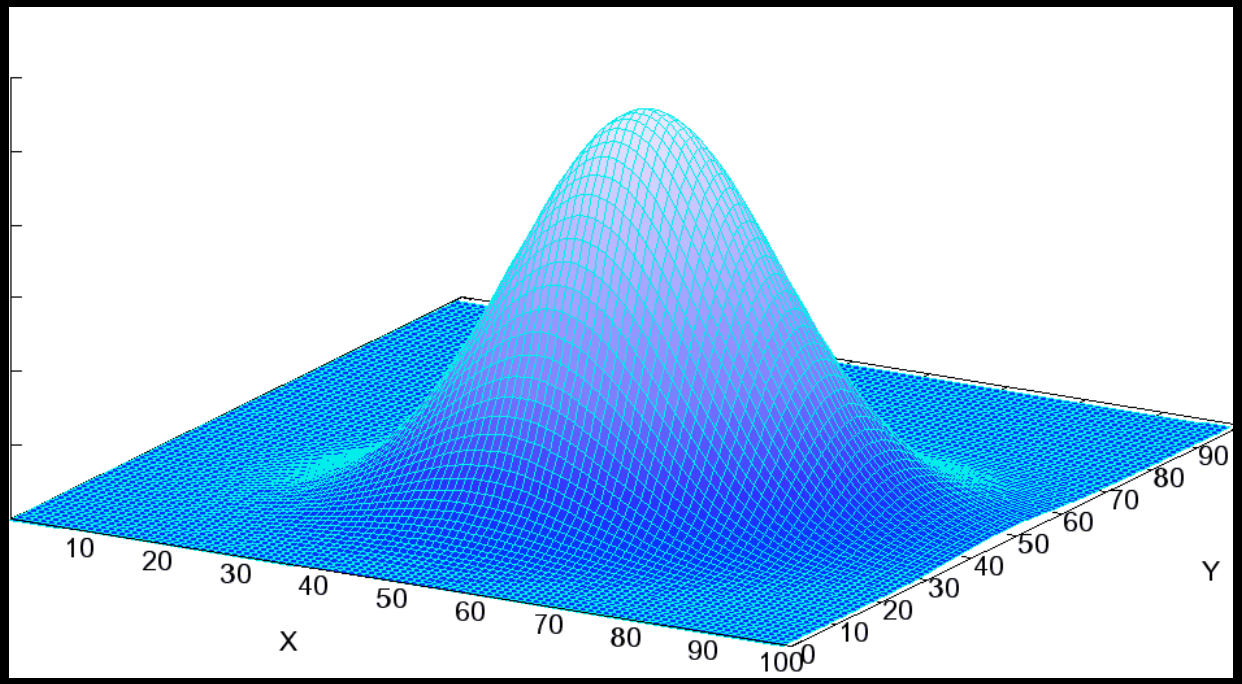
Special Models

Analysis

Attractive. SDD

Gaussian Graphical Models (GGMs)

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



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

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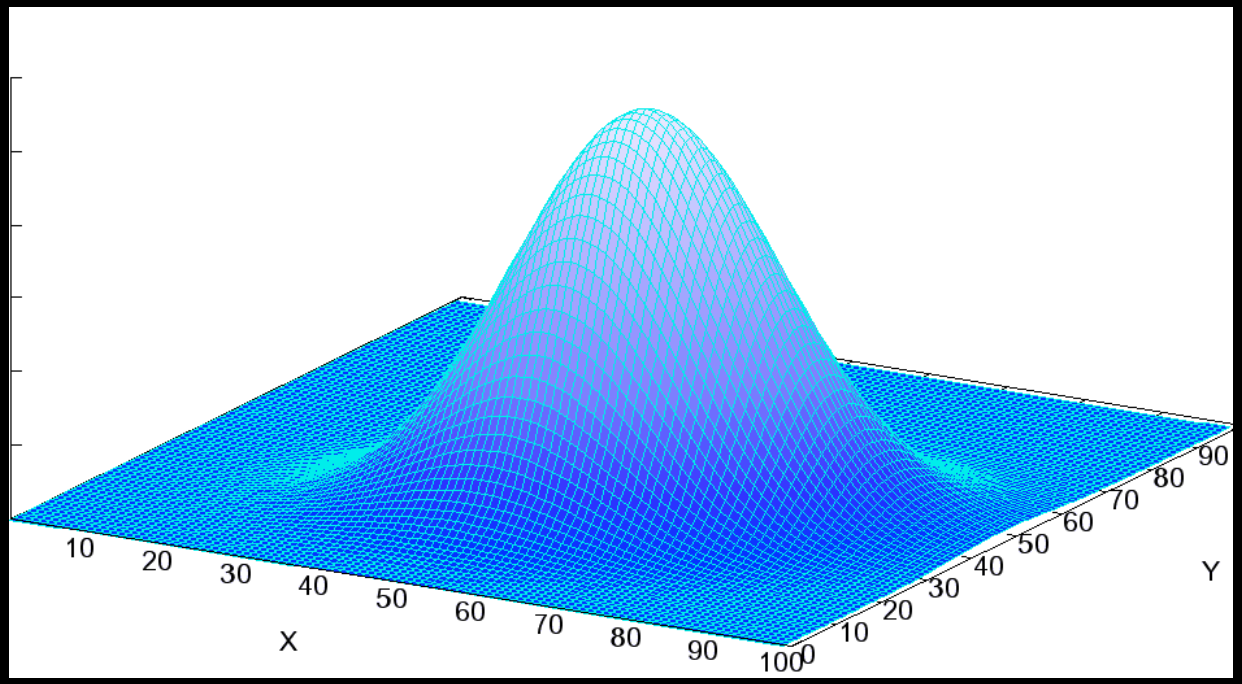

Today's Focus: Precision Matrix $\Theta = \Sigma^{-1}$.

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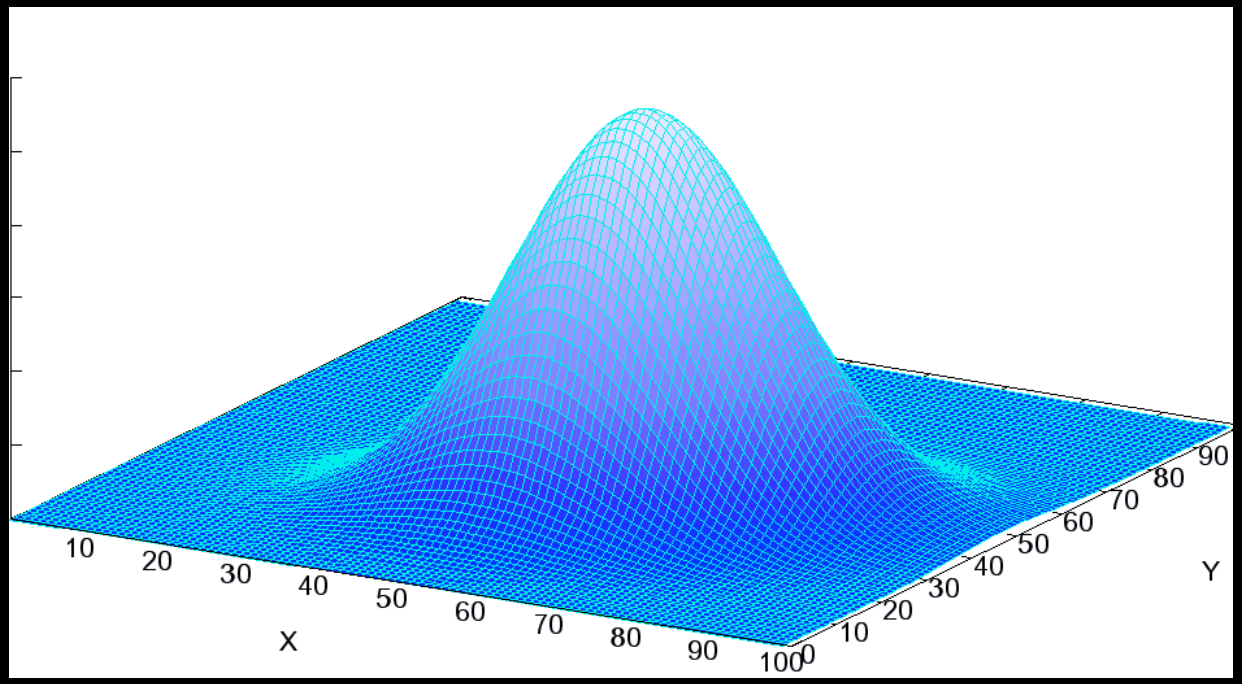

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Dempster 72: Encodes conditional independence structure

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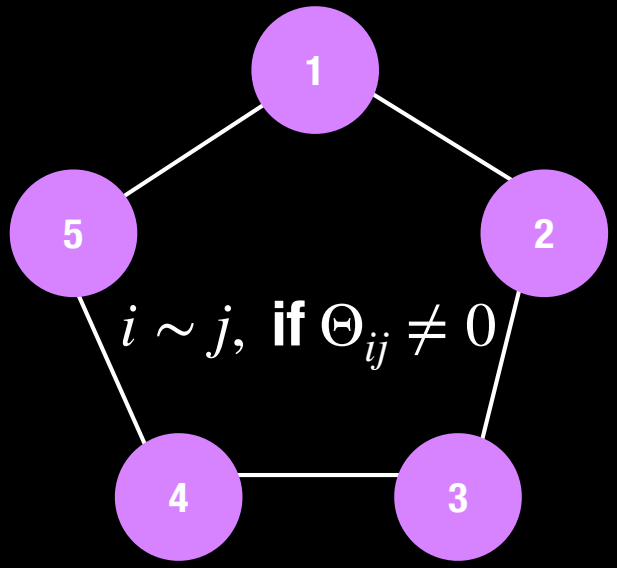

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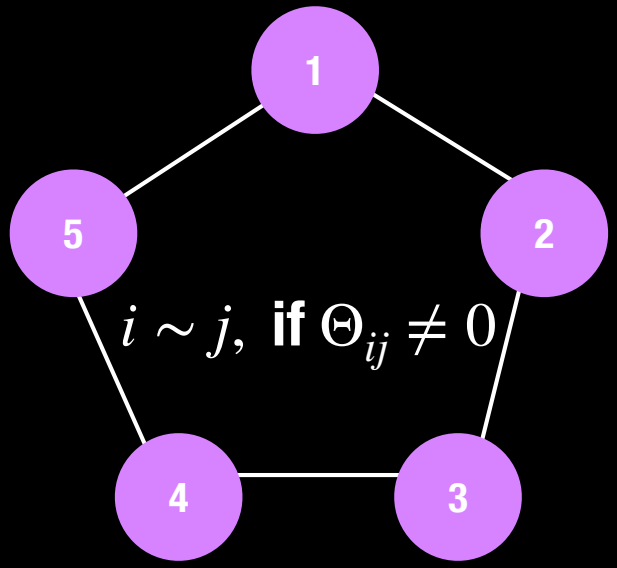

Markov property: $\Theta_{ij} = 0 \Rightarrow X_i, X_j$ **are independent conditioned on neighbors of** i**.**

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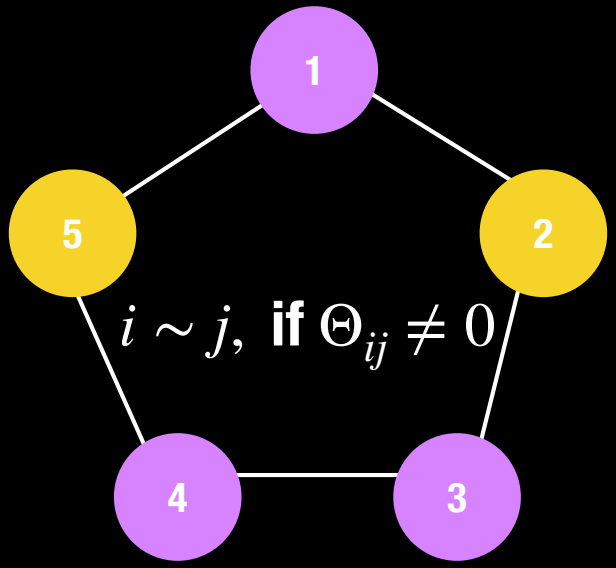

Example: $(X_1 \mid X_2, X_5)$ **independent of** $(X_3 \mid X_2, X_5)$

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Complexity of GGMs: **max-degree of G** $d \ll p$.

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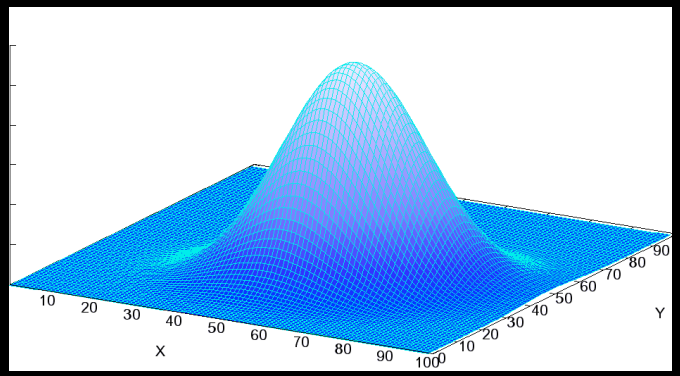
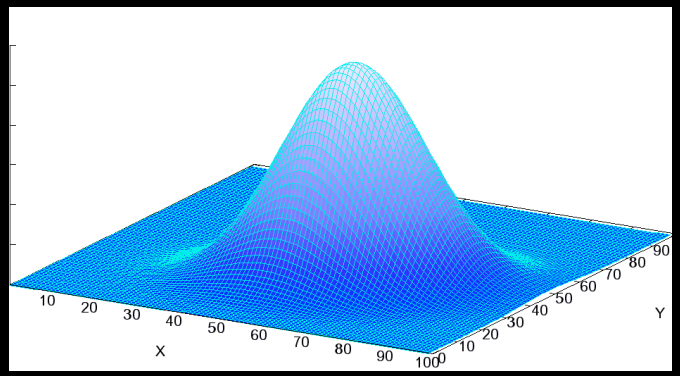
The assumption that makes the formalism non-trivial and useful …

Why?



Fundamental model for modeling statistical relations between variables



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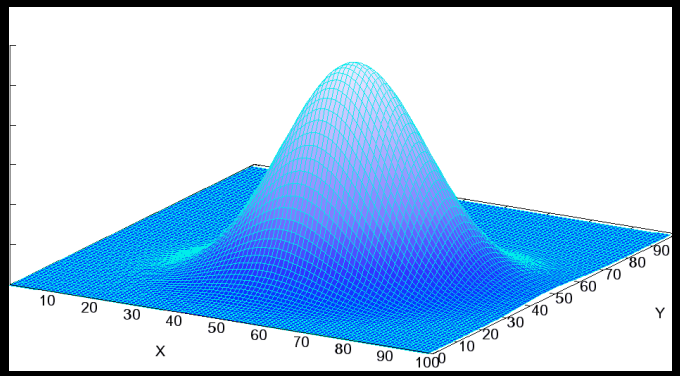

Many applications in machine learning, sciences:

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: $i \not\sim j \Rightarrow X_i, X_j$ **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
1	2	3	3	3	3	3	3	3	3
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
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Σ : Covariance Matrix

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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

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
0	0	0	0	0	0	0	0	-1	2

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1	2	3	4	5	5	5	5	5	5
1	2	3	4	5	6	6	6	6	6
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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

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
0	0	0	0	0	0	0	0	-1	2

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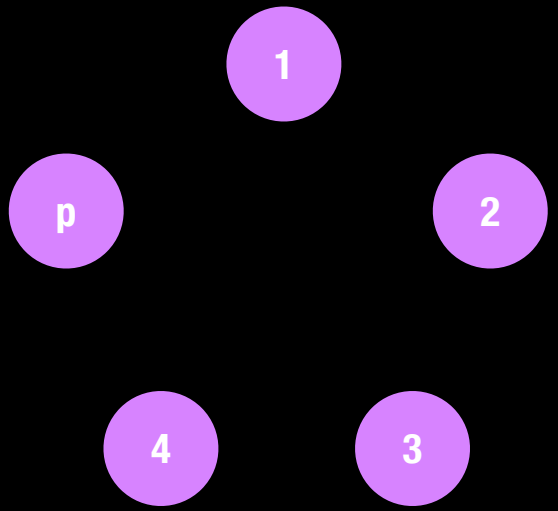
Learning Sparse GGMs

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

Structure Learning for GGMs

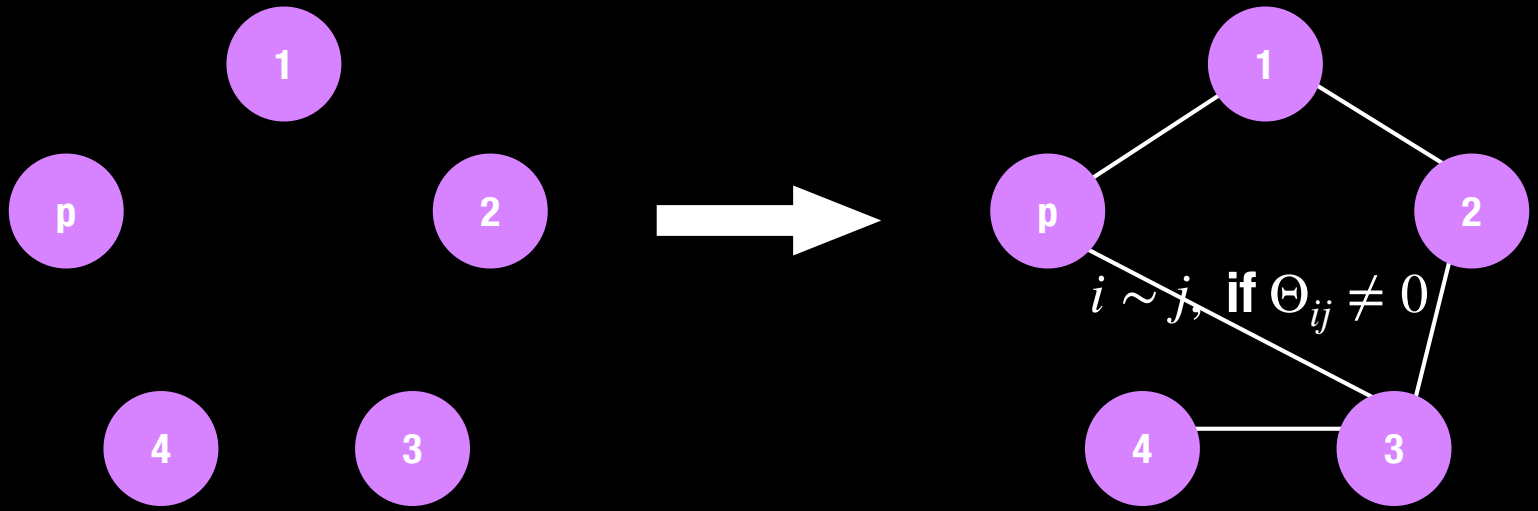
- Structure learning - learn dependency graph.



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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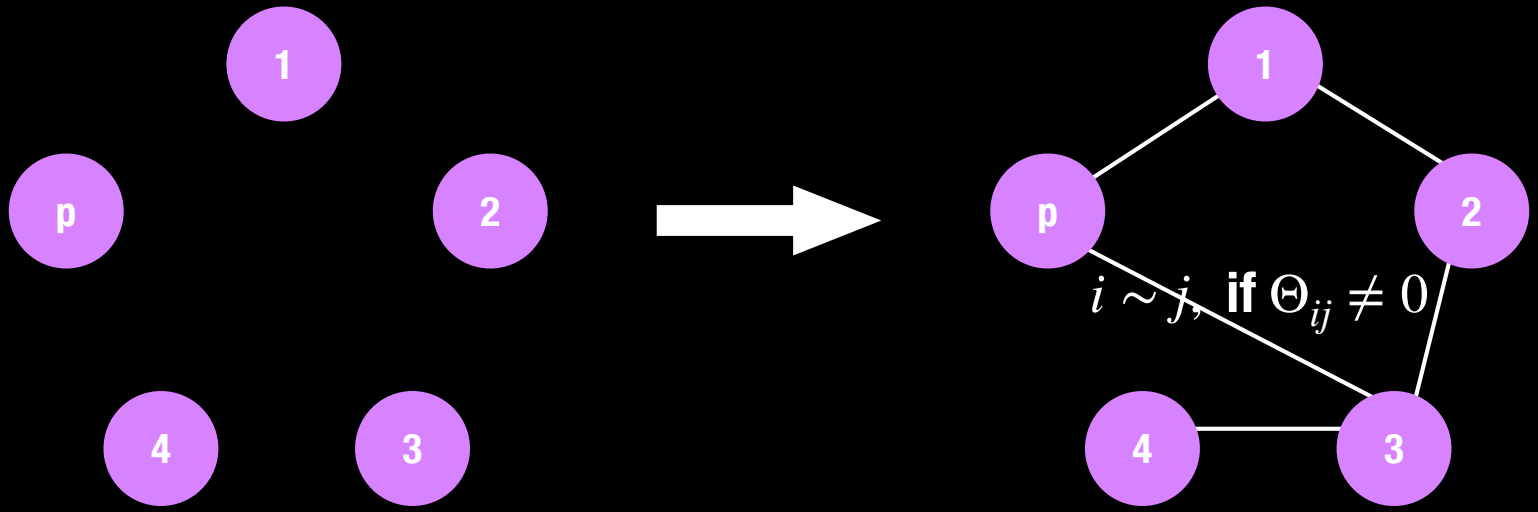
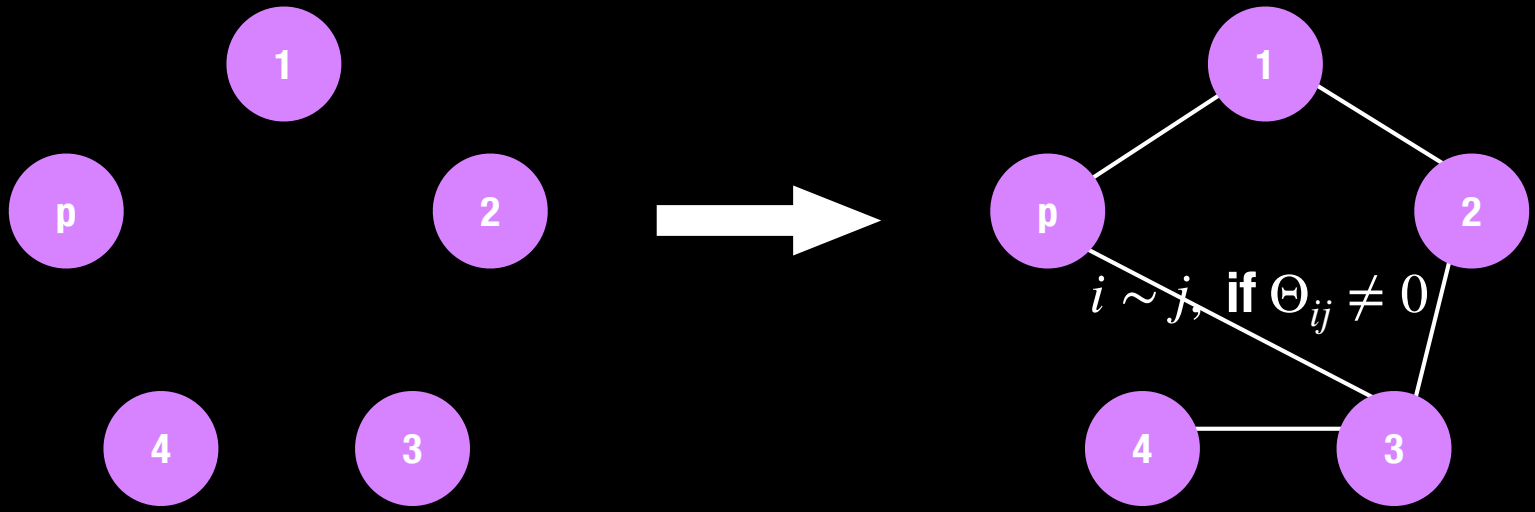


Input: Given samples $X^1, X^2, \ldots, X^n$ from a GGM
Output: Dependency graph of the GGM.

Challenge: Often $n \ll p$.

Structure Learning for GGMs

- Structure learning - learn dependency graph.



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

Core of problem. Can learn parameters easily afterward.

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

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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Σ : Covariance Matrix

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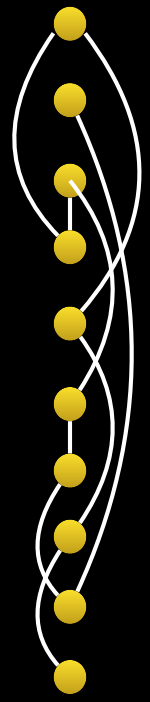

Dependency graph?

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

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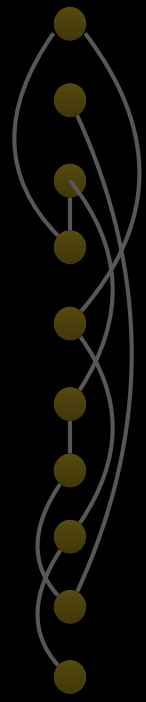

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-1	0	-1	2	0	0	0	0	0	0
-1	0	0	0	2	0	0	-1	0	0
0	0	-1	0	0	2	-1	0	0	0
0	0	0	0	0	-1	2	0	-1	0
0	0	0	0	-1	0	0	2	0	-1
0	-1	0	0	0	0	-1	0	2	0
0	0	0	0	0	0	0	-1	0	1

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

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Strong assumption: Violated by random walk …

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  Can learn with $O(M^4 \log p)$ samples where M ~ maximum ratio of entries in Σ, Θ .

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

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

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

Previous Work

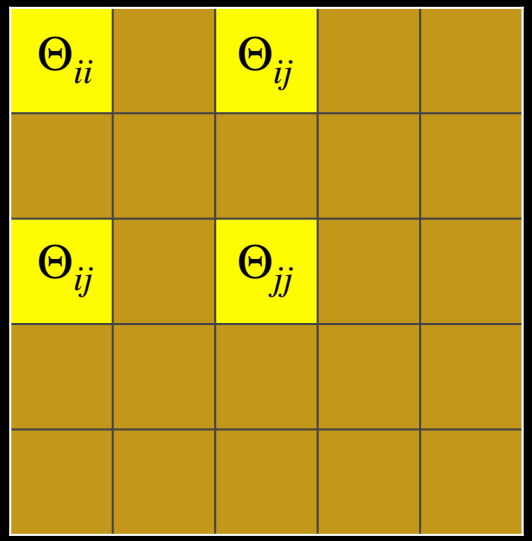
Given samples $X^1, X^2, \ldots, X^n$ from a GGM of degree $d \ll p$, can we efficiently find the dependency graph with $n \ll p$?

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 $n \ll p$?

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



Θ : Precision Matrix

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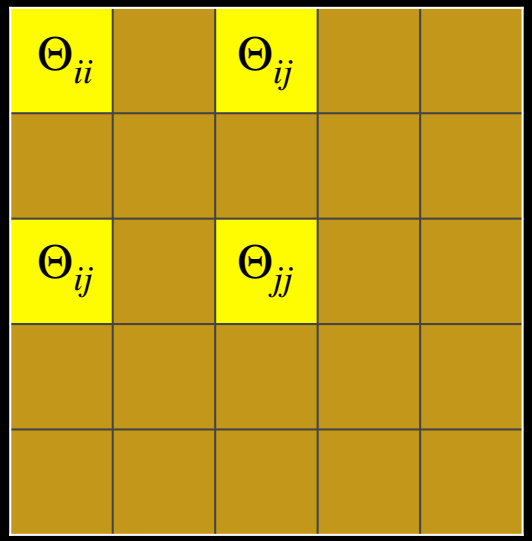

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Measures signal in 2x2 submatrices … not whole matrix.

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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 $n \ll p$?

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

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Run-time of algorithm: $p^{O(d)}$.

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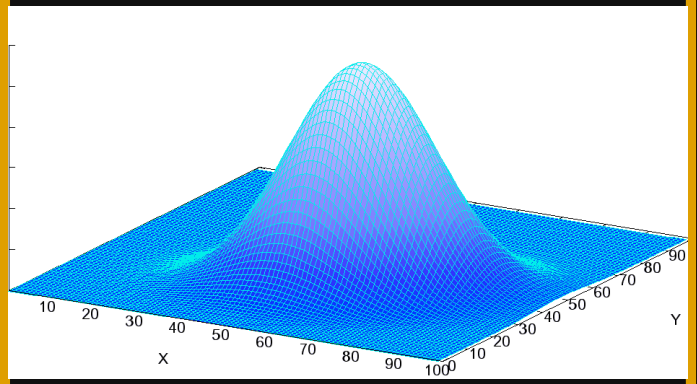
Main: A simple greedy algorithm solves above ill-conditioned cases
(and recovers guarantees of GLASSO, CLIME, …)

GGMs



Motivation

Algorithm

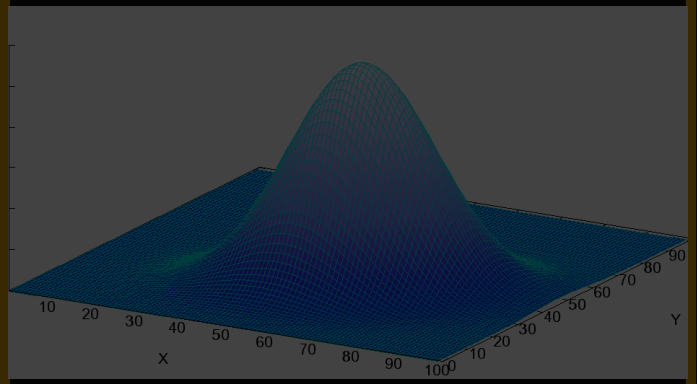
While $|S| < t$:
Add $\arg\min_j Var(X_i \mid X_{S \cup j})$.

Special Models

Analysis

Attractive. SDD.

GGMs



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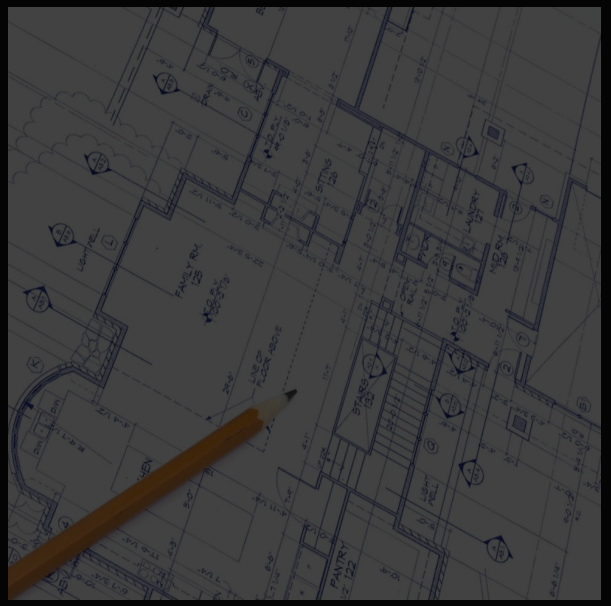
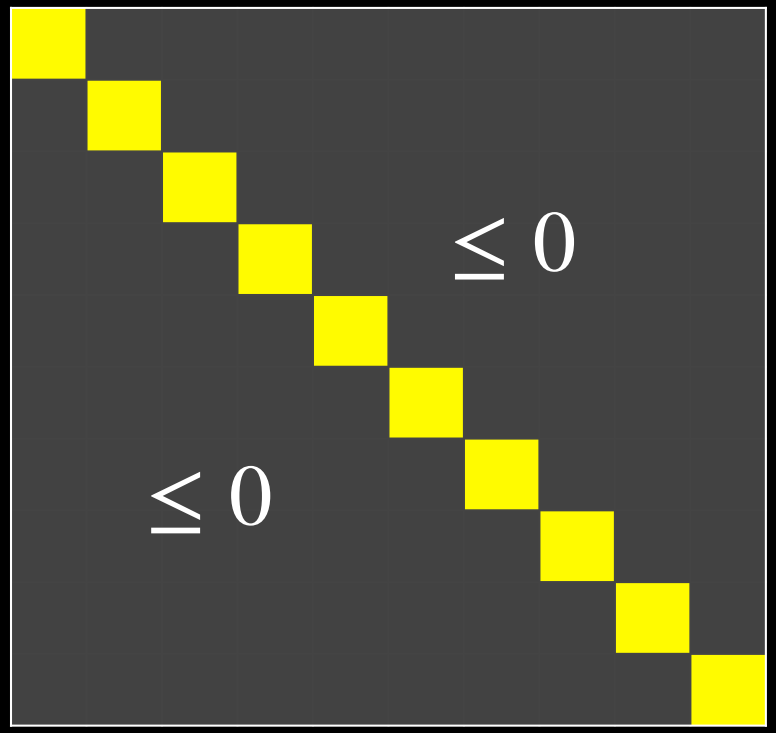


Attractive. SDD.

Attractive GGMs

GGM is attractive if all covariances are non-negative.

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



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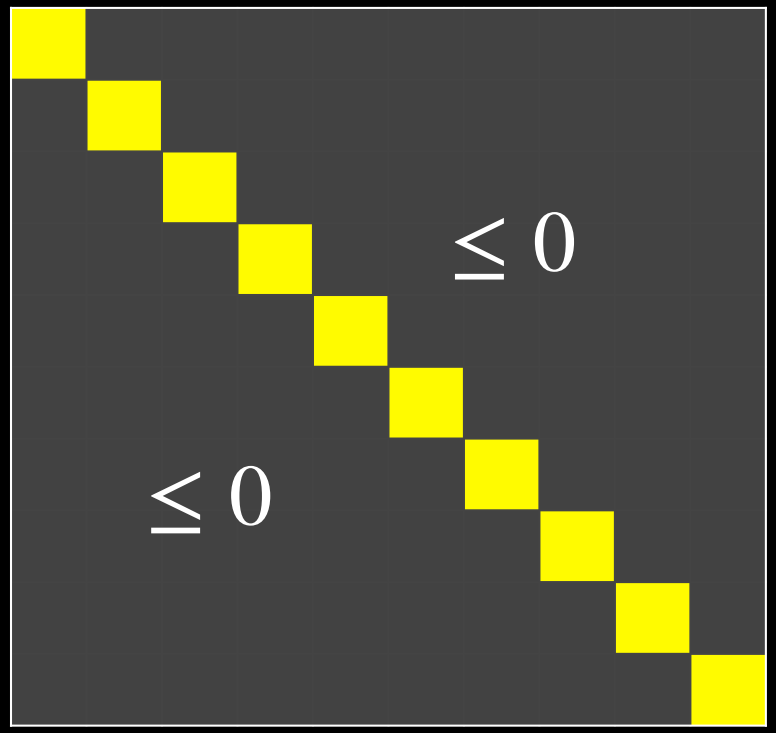

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Ex: Gaussian Free Fields

- **Many applications via Gaussian processes**

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

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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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Θ : Precision Matrix

Ex: Gaussian Free Fields

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

Attractive GGMs

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

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

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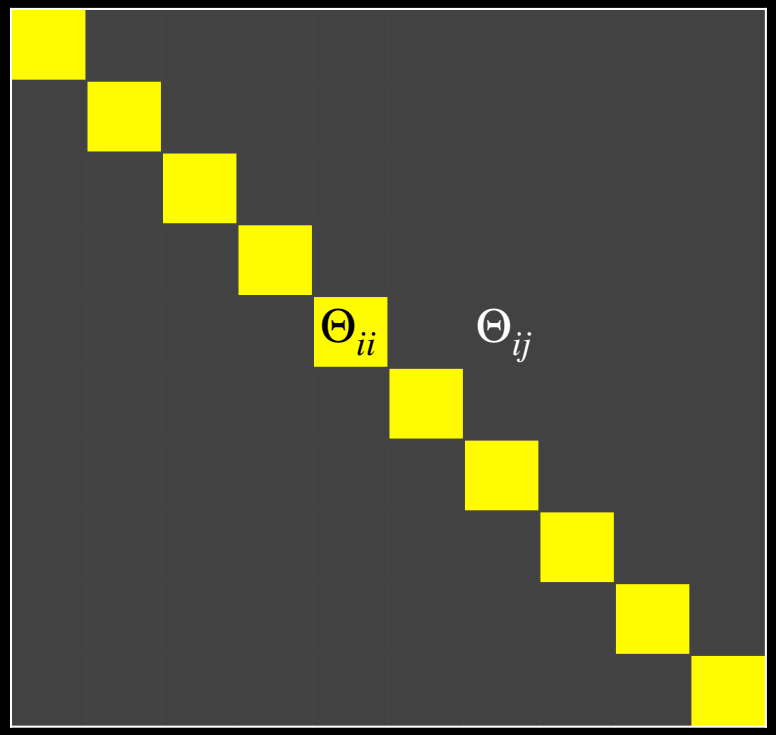
Walk-Summable GGMs

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



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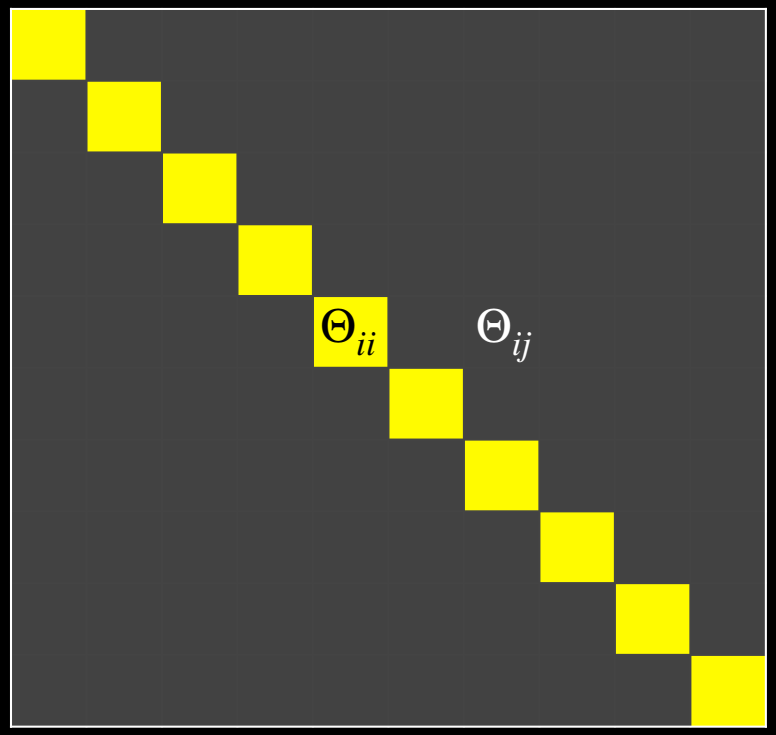

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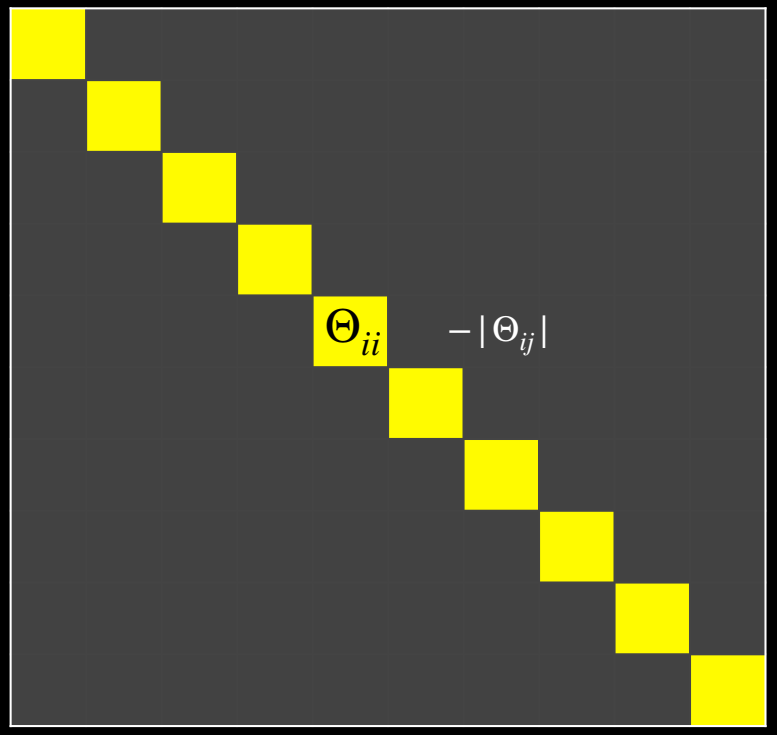

Offdiagonals negative $\succeq 0$

Walk-Summable GGMs

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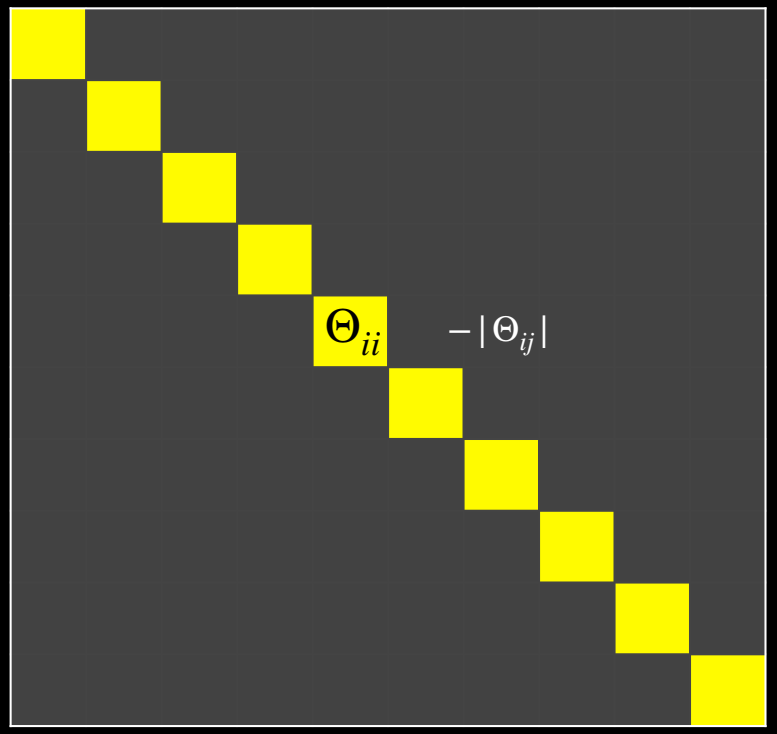
- Introduced by Maliutov, Johnson, Willsky 2006
- Generalize many classes
  - Attractive
  - Pairwise normalizable
  - Non-frustrated
  - Symmetric diagonally-dominant



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KKMM: **GreedyPrune** learns walk-summable models with $O(d^2 \log p / \kappa^6)$ samples and quadratic run-time.

Previous: ATHW12, MVL18 - $p^{O(d)}$ run-time algorithm with logarithmic samples.

Walk-Summable GGMs

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

Previous: ATHW12, MVL18 - $p^{O(d)}$ run-time algorithm with logarithmic samples.

Learning GGMs Greedily

Input: Samples from a sparse GGM ~ X.
Output: Dependency graph of X.

Similar greedy approaches for discrete GMs: [Bresler10], [HKM17], [BKM19]

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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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GREEDY-GROWING

1. **Set** $S \leftarrow \emptyset$

2. **While S is small enough:**

    1. **Find j to minimize estimate of** $Var(X_1 \mid X_{S \cup j})$.

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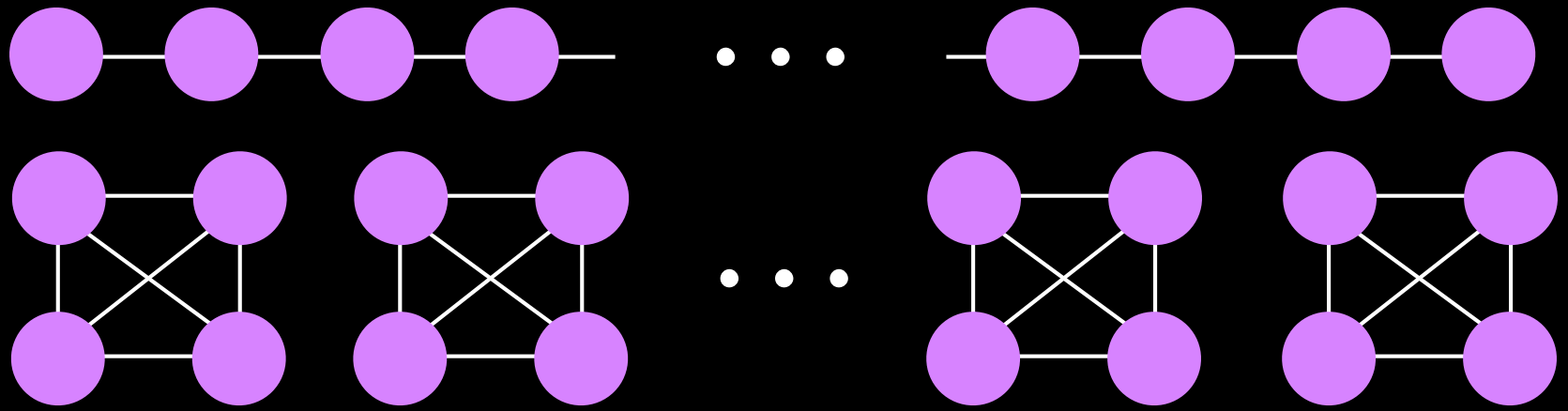
GREEDY-PRUNING

1. For each j in S:

    1. If $Var(X_1 \mid X_{S\setminus\{j\}}) < (1+\tau)Var(X_1 \mid X_S)$, 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

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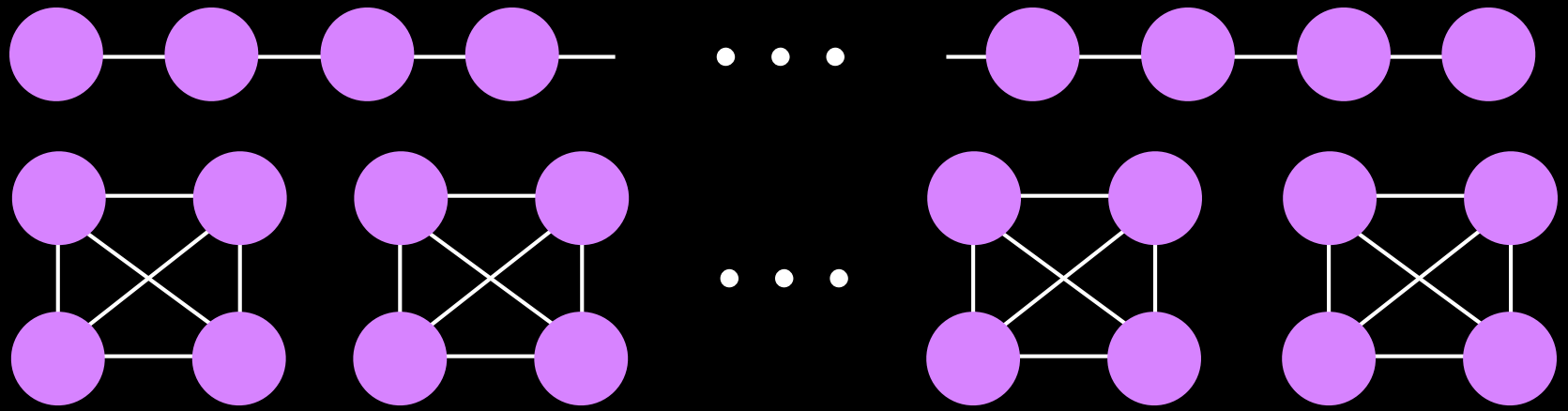

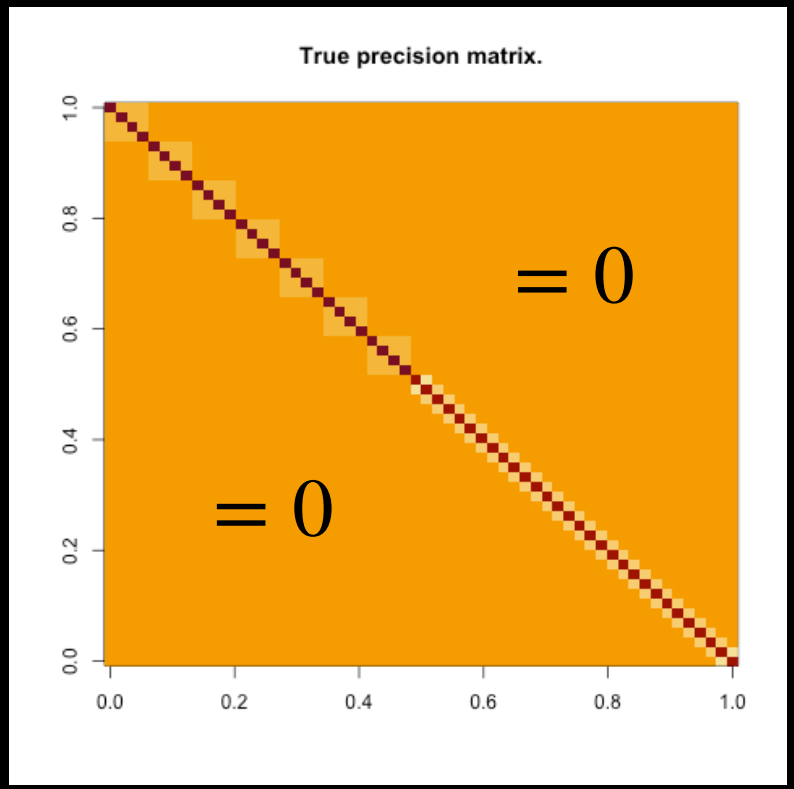

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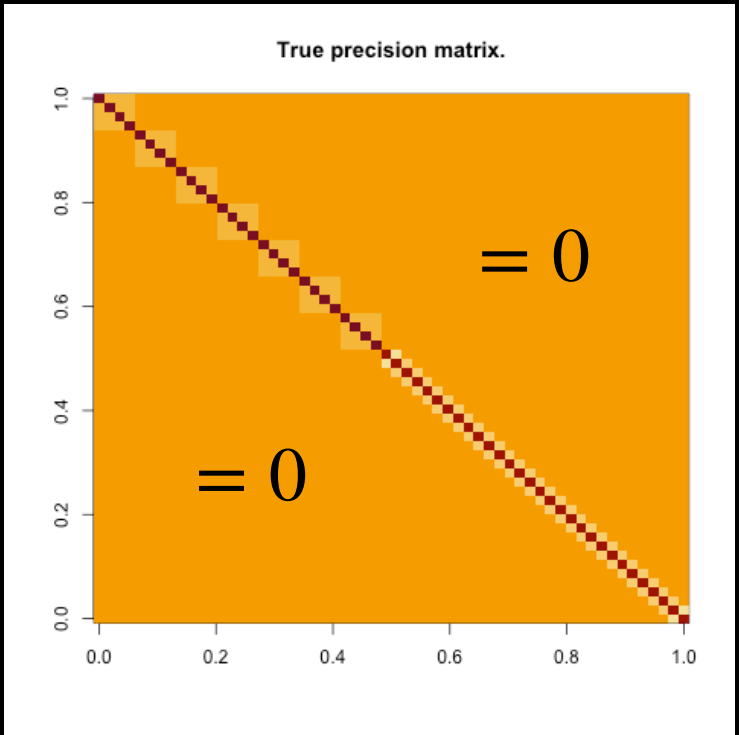
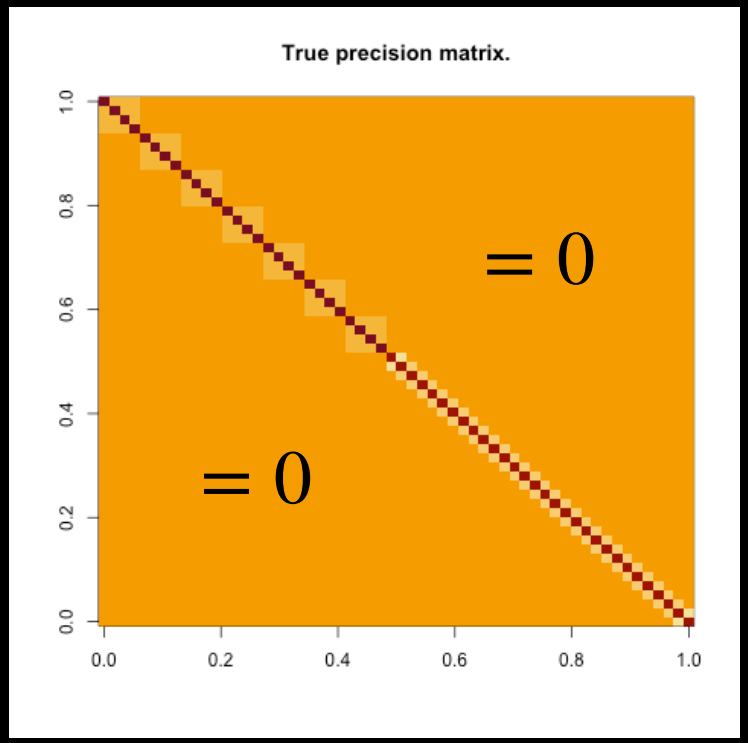

True precision matrix.
= 0
= 0
0.0
0.2
0.4
0.6
0.8
1.0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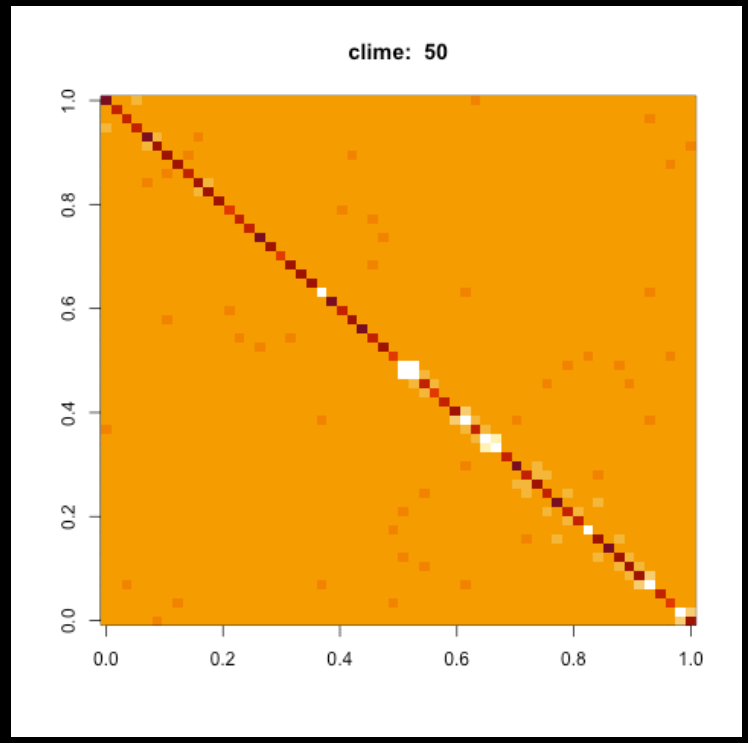
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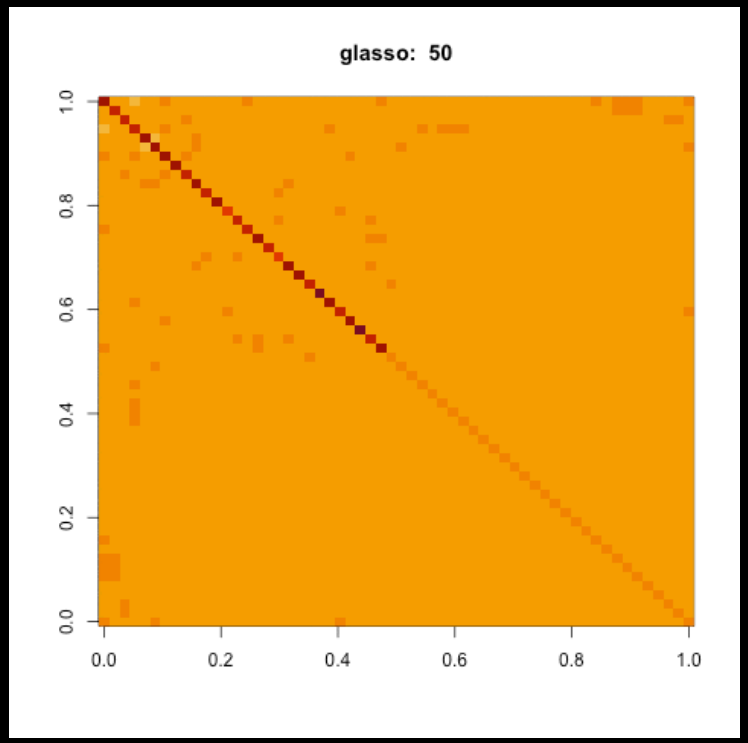
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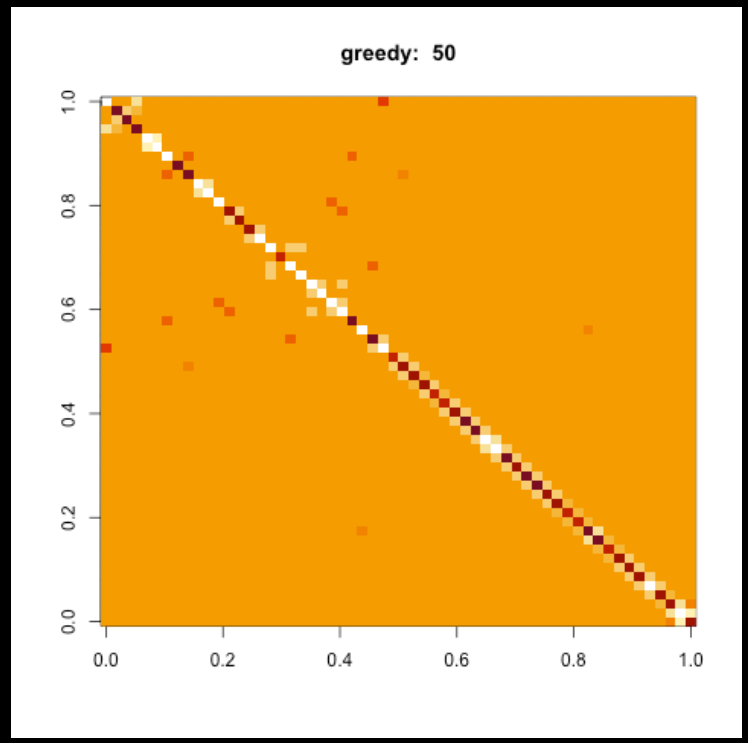
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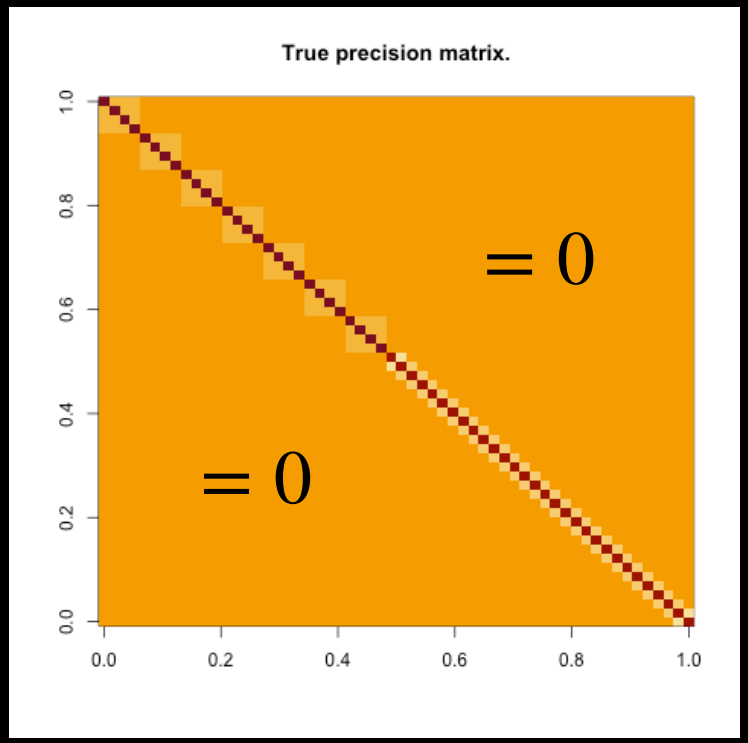
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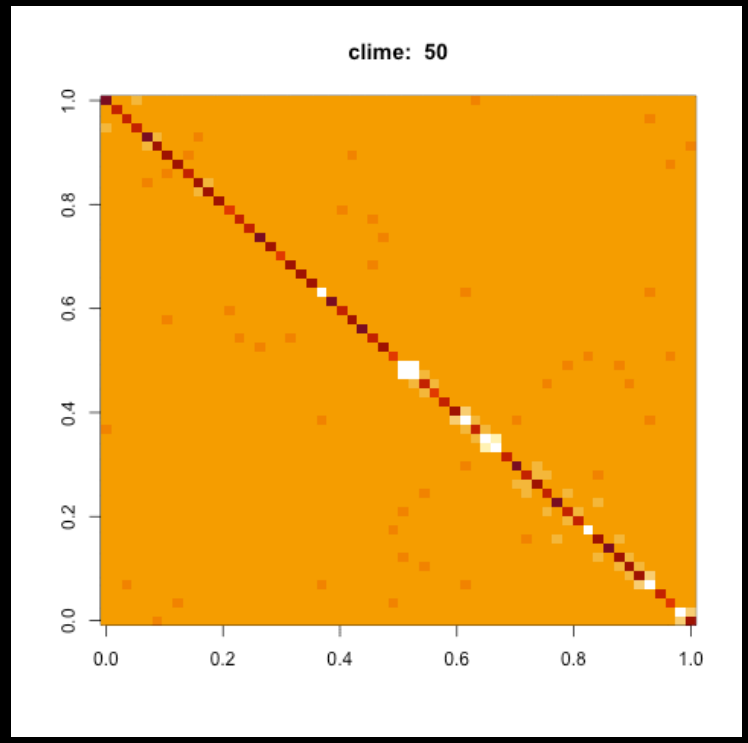
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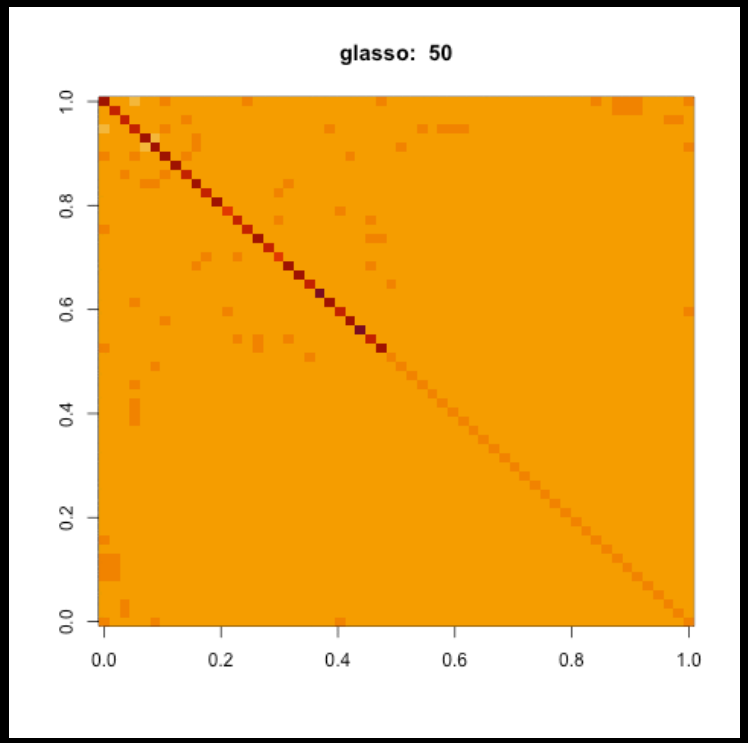
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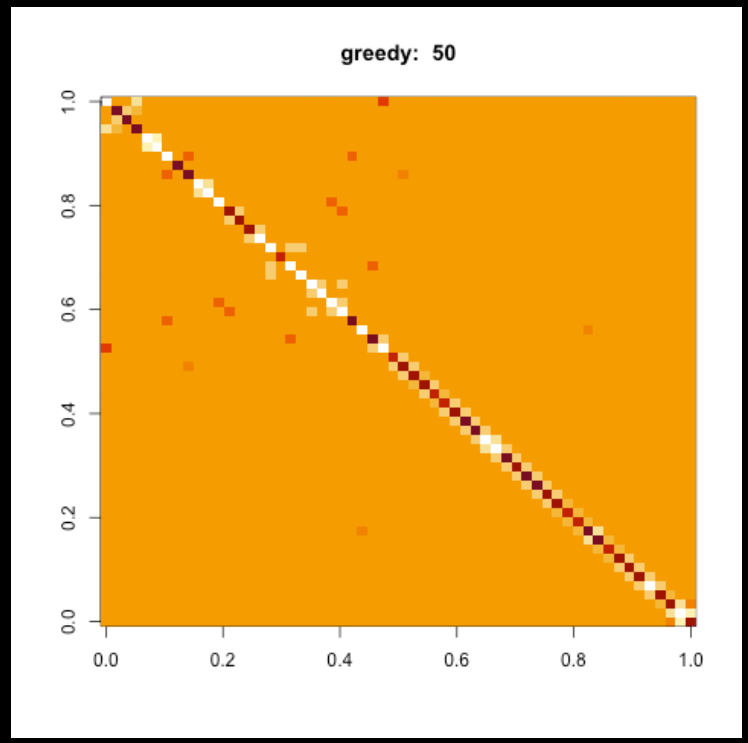
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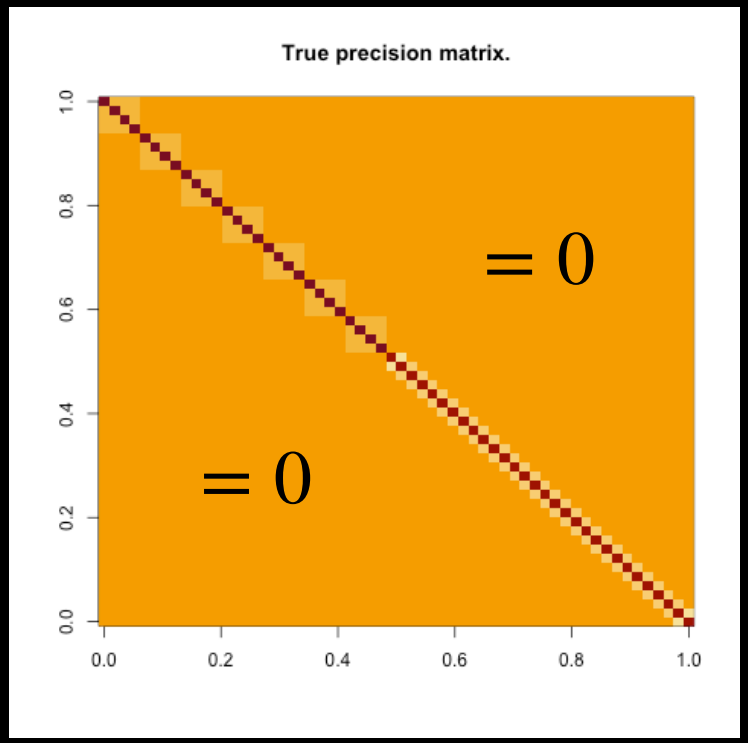
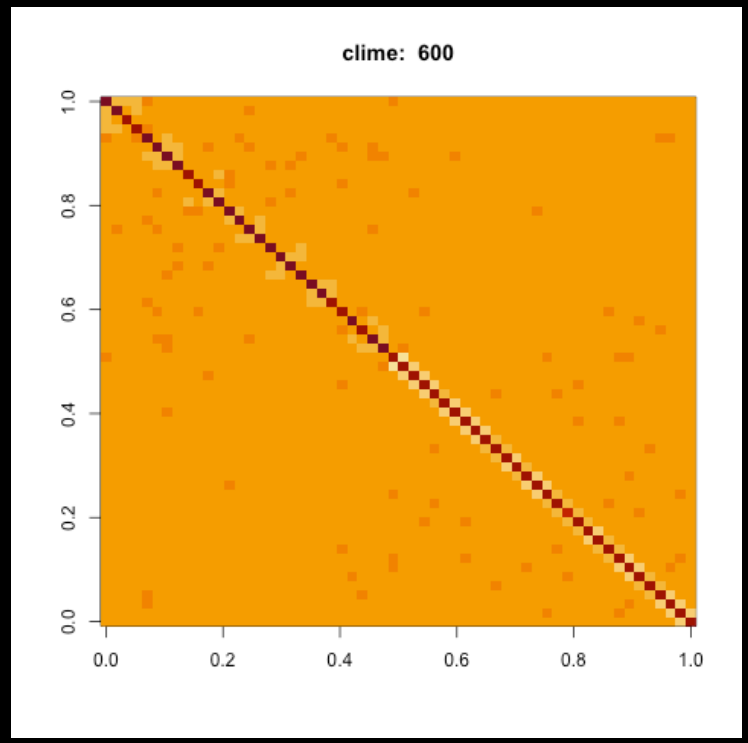
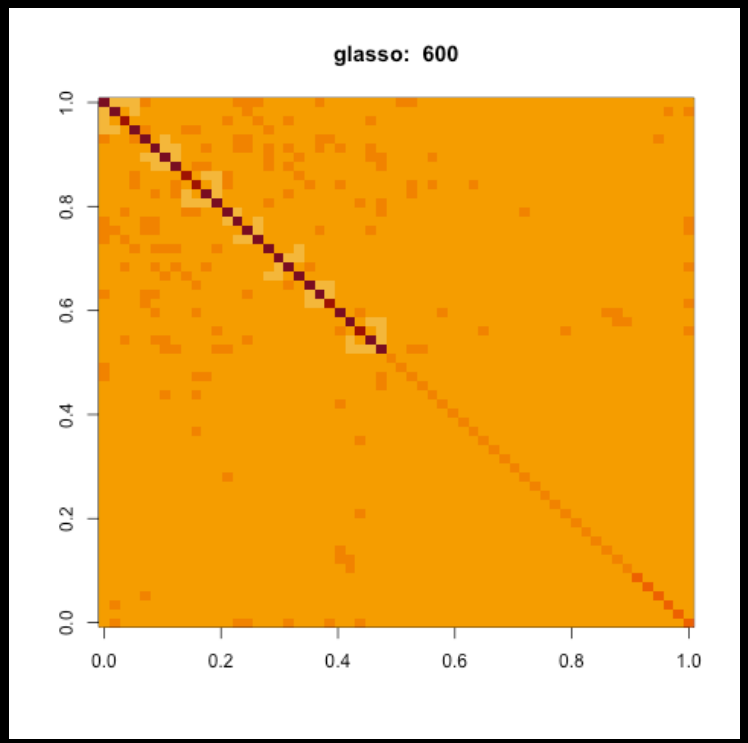
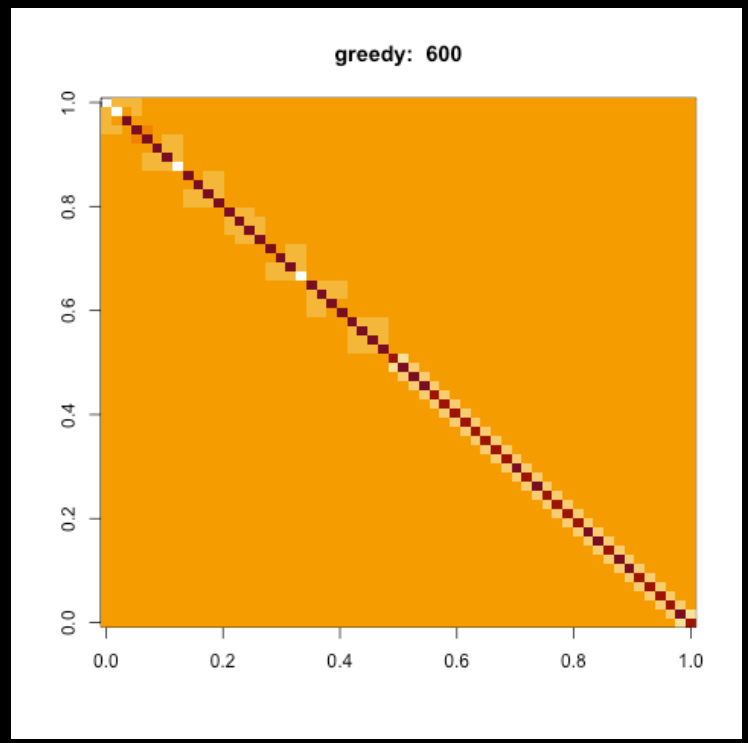


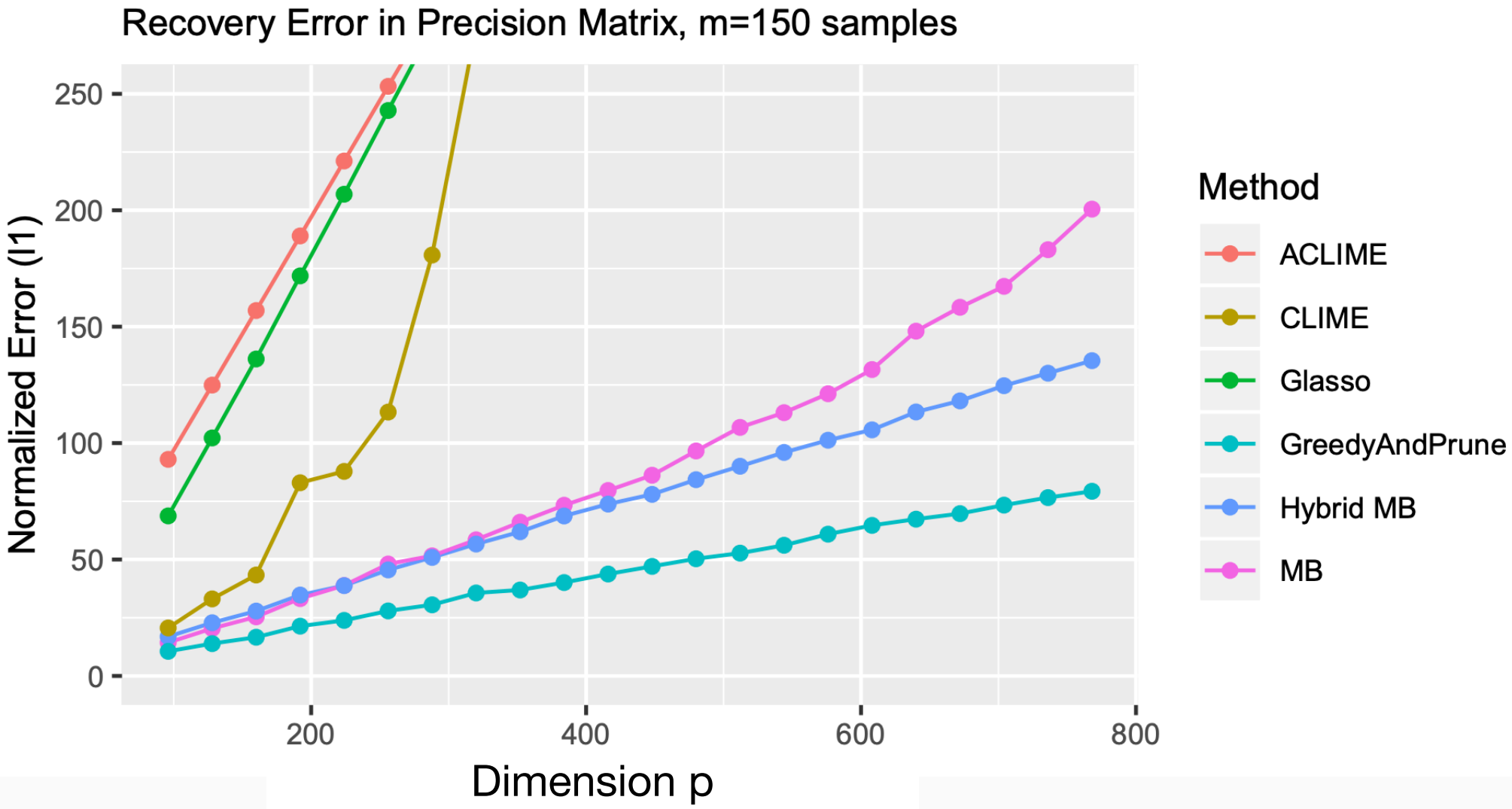
Final Outputs





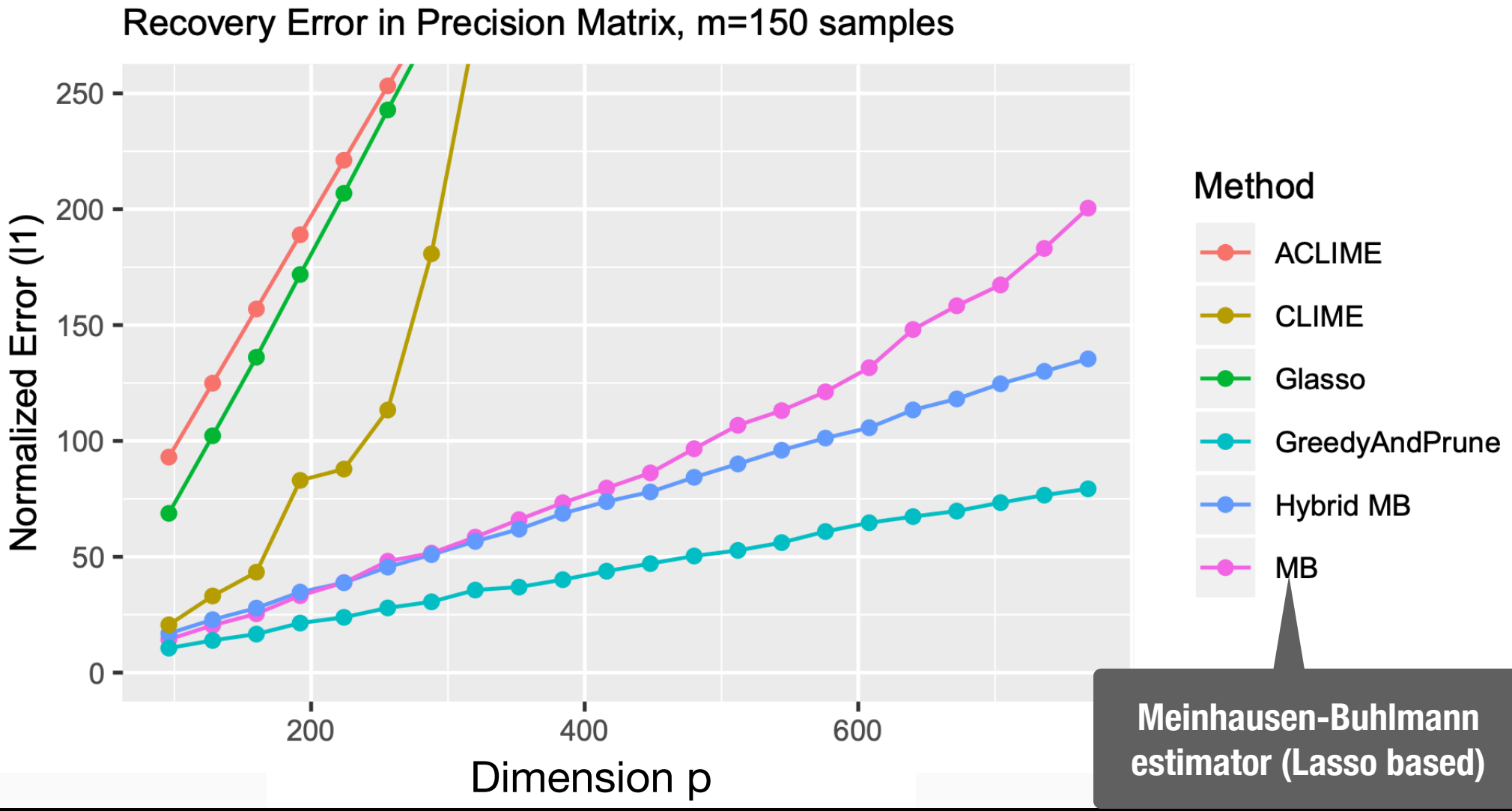


A Simple Challenge: Path + Clique



GreedyPrune has best error

A Simple Challenge: Path + Clique



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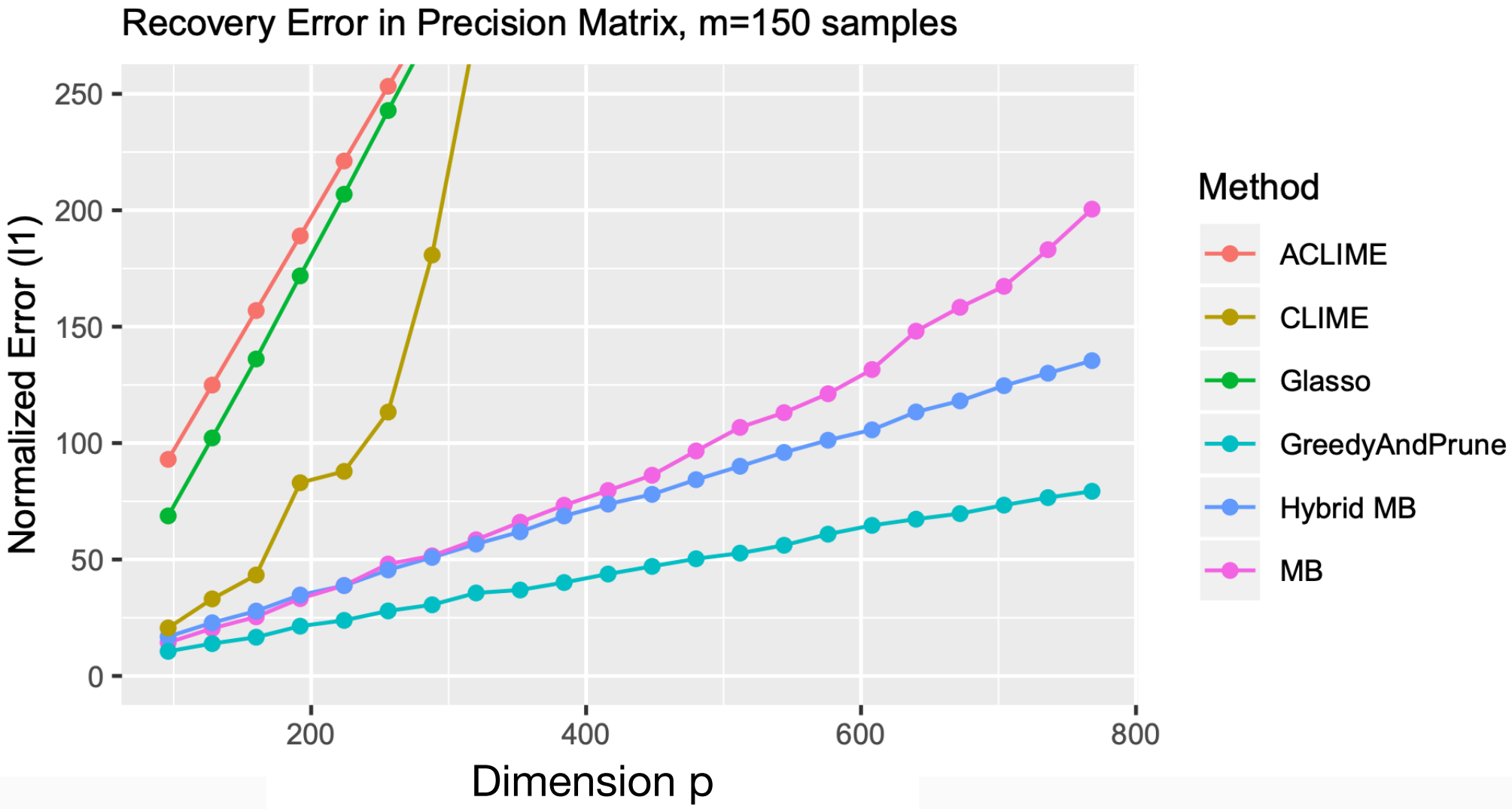
A Simple Challenge: Path + Clique



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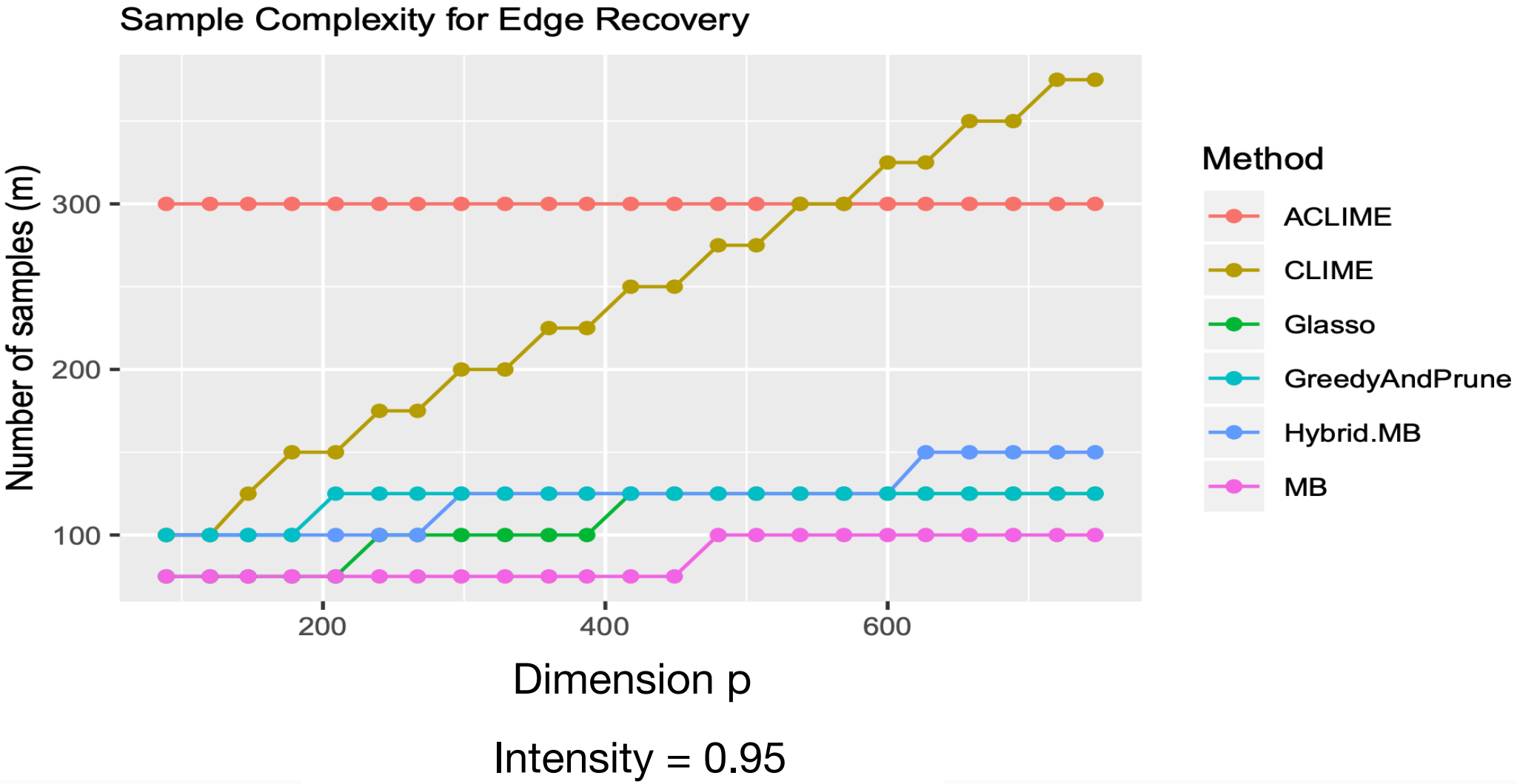

GreedyPrune needs very few samples.
CLIME grows nearly linearly …

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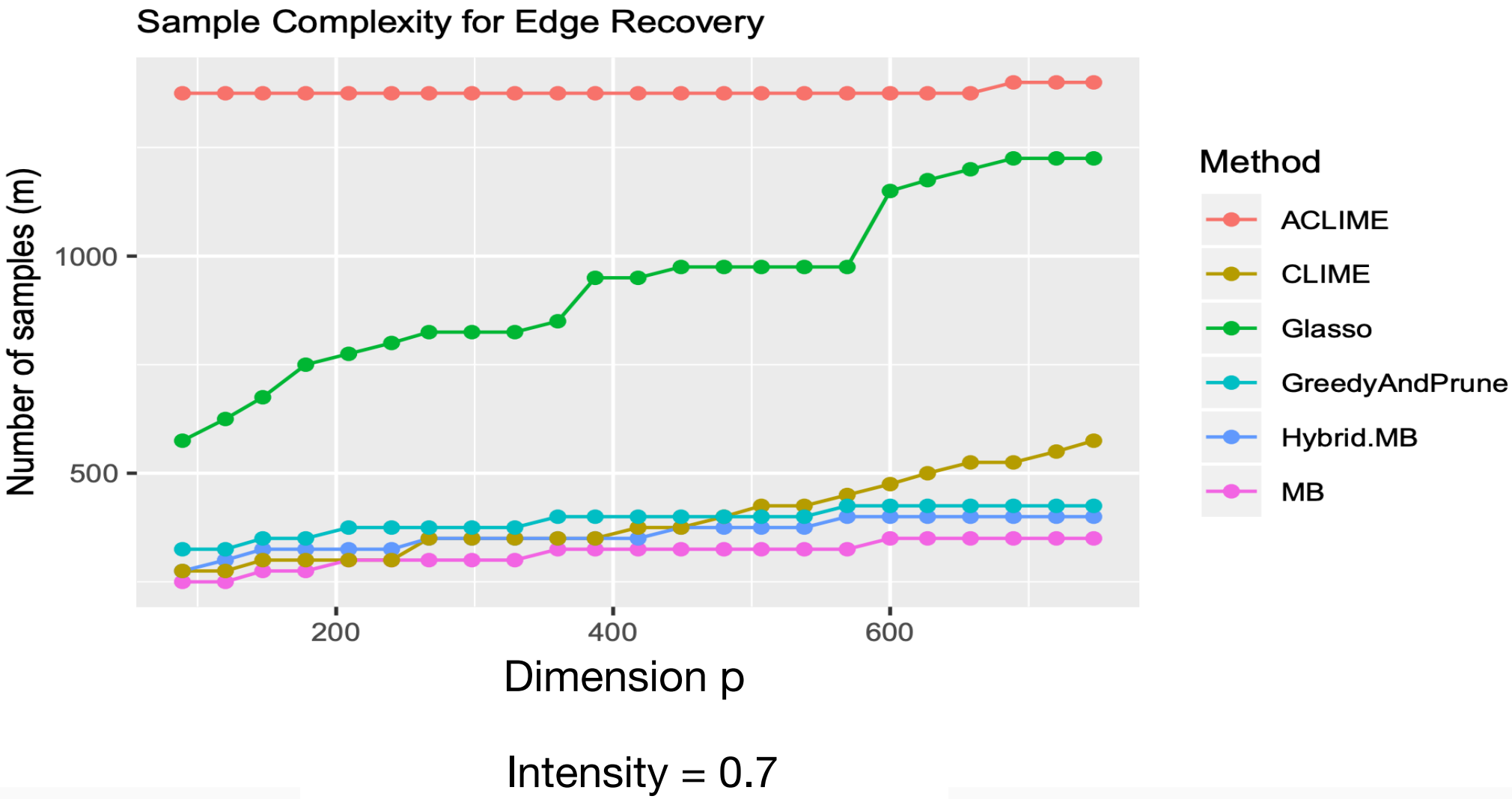
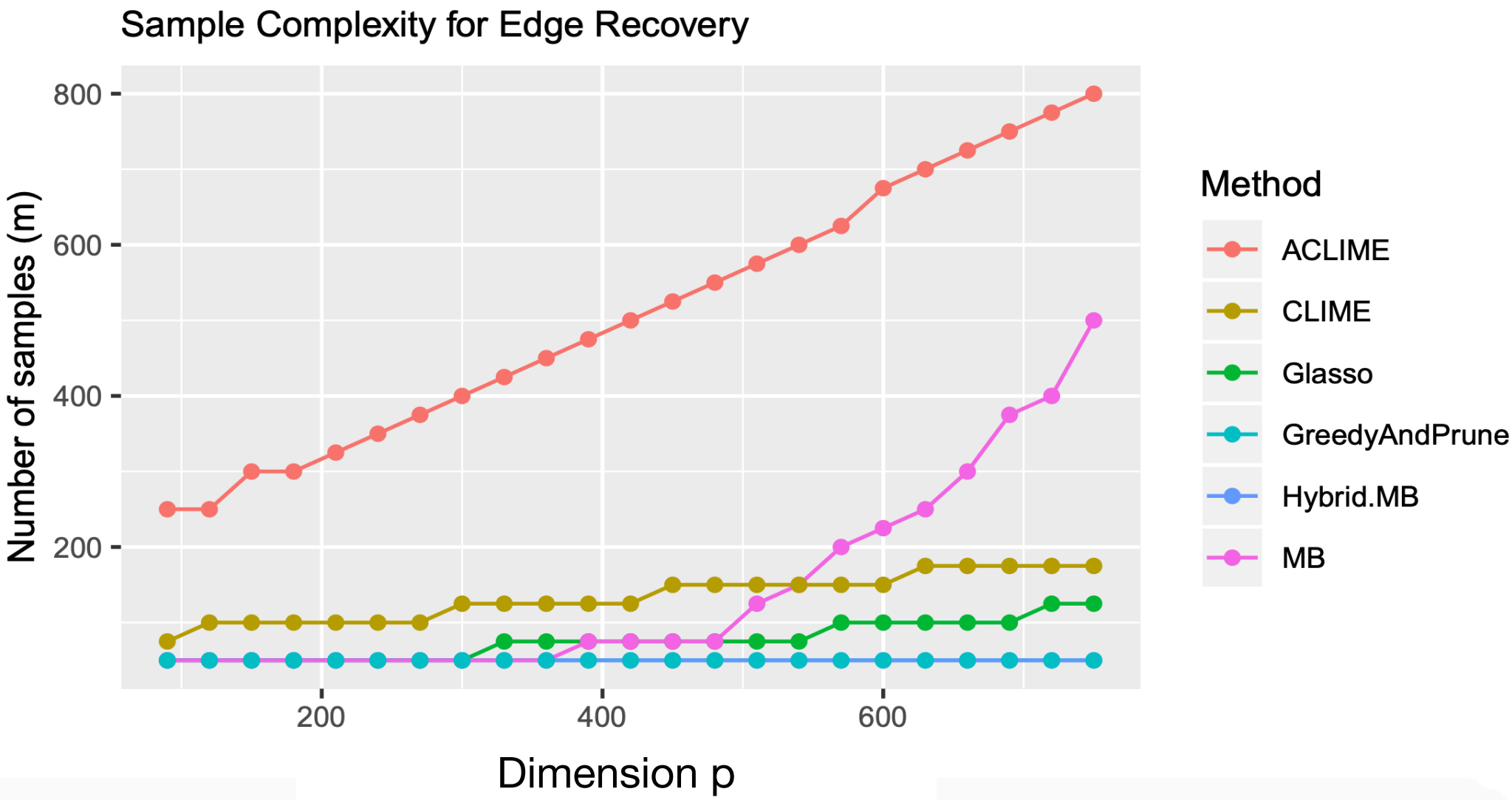


Intensity = 0.7

GreedyPrune needs very few samples.
GLASSO grows nearly linearly …

A Simple Challenge: Random walk



GreedyPrune needs very few samples.
MB grows nearly linearly …

GreedyPrune Summary

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

KKMM: **GreedyPrune** learns walk-summable models with $O(d^2 \log p/\kappa^6)$ samples and quadratic run-time.

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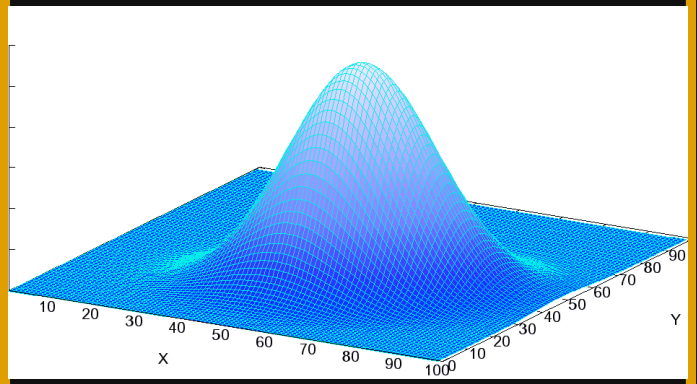
Also …

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

GGMs



Motivation

Algorithm

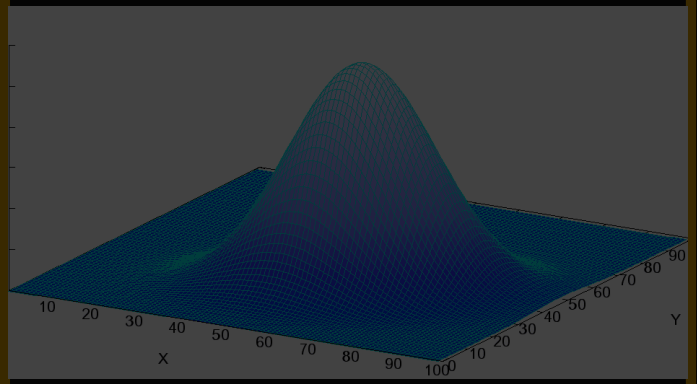
While $|S| < t$:
Add $\arg\min_j Var(X_i \mid X_{S \cup j})$.

Special Models

Analysis

Attractive. SDD

GGMs



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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!

Summary

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Very well-stuided, practically important!

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

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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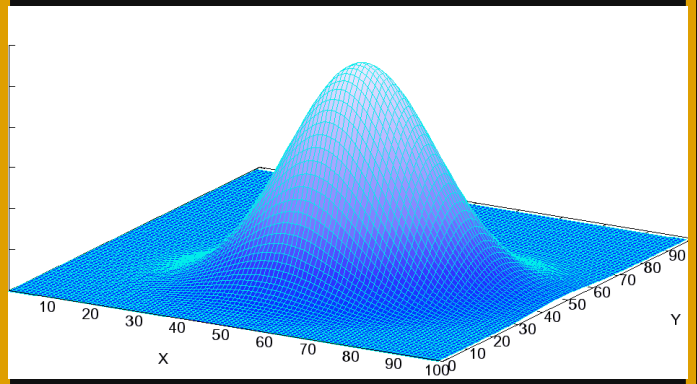
(aka learning Markov random fields, undirected graphical models)

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

GGMs



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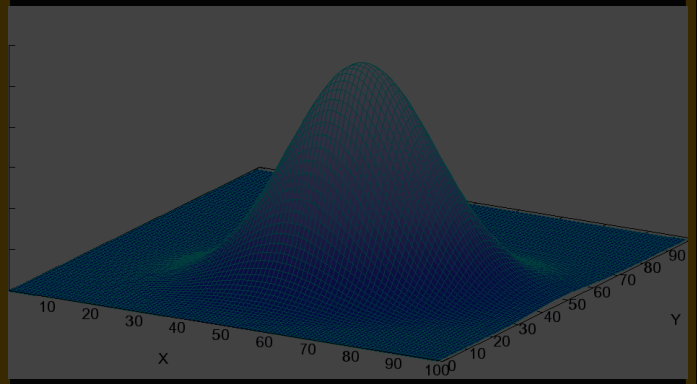

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Learning GGMs Greedily

Input: Samples from a sparse GGM ~ X.
Output: Dependency graph of X.

(d: max-degree; p: dimension;

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Thm 1: `GreedyPrune` learns attractive models with $\tilde{O}(d \log p/\kappa^2)$ samples and quadratic run-time.

Thm 2: `GreedyPrune` learns walk-summable models with $O(d^2 \log p/\kappa^6)$ samples and quadratic run-time.

Analysis for Attractive: Supermodularity

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

$$f(S) = Var(X_1 \mid X_S)\,.$$

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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**

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

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

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- **Is decreasing with S, so f is supermodular.**

Analysis for Walk-Summable

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

$$f(S) = Var(X_1 \,|\, X_S)\,.$$

No longer supermodular!

(Not even weakly-supermodular …)

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- **SDD implies neighbors have noticeable effect**

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Suffices to show greedy works for SDD!

- **Walk-summable = Symmetric Diagonally Dominant (SDD)**
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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 …

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

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

So $i \sim j \Rightarrow |\Theta_{ij}| \geq \kappa$.

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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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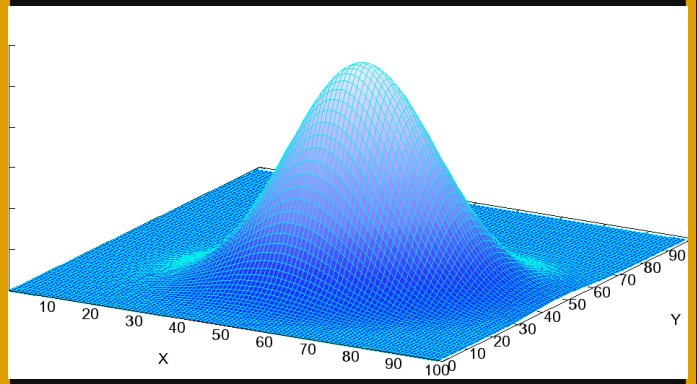
"Proof …":

- **If Laplacian …**

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

GGMs



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