High-Dimensional Graphical Model Selection

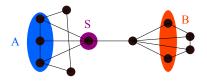
Anima Anandkumar

U.C. Irvine

Joint work with Vincent Tan (U. Wisc.) and Alan Willsky (MIT).

Conditional Independence

$$\mathbf{X}_A \perp \mathbf{X}_B | \mathbf{X}_S$$

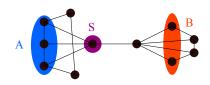


Conditional Independence

$$\mathbf{X}_A \perp \!\!\! \perp \mathbf{X}_B | \mathbf{X}_S$$

Factorization

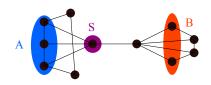
$$P(\mathbf{x}) \propto \exp \left[\sum_{(i,j) \in G} \Psi_{i,j}(x_i, x_j) \right].$$



Conditional Independence

$$\mathbf{X}_A \perp \mathbf{X}_B | \mathbf{X}_S$$

Factorization



$$P(\mathbf{x}) \propto \exp \left[\sum_{(i,j) \in G} \Psi_{i,j}(x_i, x_j) \right].$$

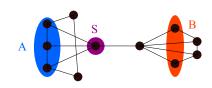
Tree-Structured Graphical Models



Conditional Independence

$$\mathbf{X}_A \perp \mathbf{X}_B | \mathbf{X}_S$$

Factorization



$$P(\mathbf{x}) \propto \exp \left[\sum_{(i,j) \in G} \Psi_{i,j}(x_i, x_j) \right].$$

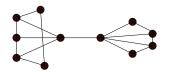
Tree-Structured Graphical Models

$$P(\mathbf{x}) = \prod_{i \in V} P_i(x_i) \prod_{(i,j) \in E} \frac{P_{i,j}(x_i, x_j)}{P_i(x_i)P_j(x_j)}$$
$$= P_1(x_1)P_{2|1}(x_2|x_1)P_{3|1}(x_3|x_1)P_{4|1}(x_4|x_1).$$



Structure Learning of Graphical Models

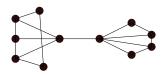
- Graphical model on p nodes
- n i.i.d. samples from multivariate distribution
- ullet Output estimated structure \widehat{G}^n



Structural Consistency:
$$\lim_{n\to\infty} P\left[\widehat{G}^n \neq G\right] = 0.$$

Structure Learning of Graphical Models

- ullet Graphical model on p nodes
- n i.i.d. samples from multivariate distribution
- ullet Output estimated structure \widehat{G}^n



Structural Consistency:
$$\lim_{n\to\infty} P\left[\widehat{G}^n \neq G\right] = 0.$$

Challenge: High Dimensionality ("Data-Poor" Regime)

- Large p, small n regime $(p \gg n)$
- Sample Complexity: Required # of samples to achieve consistency

Challenge: Computational Complexity

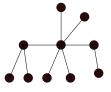
Goal: Address above challenges and provide provable guarantees



Maximum likelihood learning of tree structure

- Proposed by Chow and Liu (68)
- Max. weight spanning tree

$$\hat{T}_{\text{ML}} = \arg\max_{T} \sum_{k=1}^{n} \log P(\mathbf{x}_{V}).$$

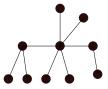


Maximum likelihood learning of tree structure

- Proposed by Chow and Liu (68)
- Max. weight spanning tree

$$\hat{T}_{\text{ML}} = \arg \max_{T} \sum_{k=1}^{n} \log P(\mathbf{x}_{V}).$$

$$\hat{T}_{\mathrm{ML}} = \arg\max_{T} \sum_{(i,j) \in T} \hat{I}^{n}(X_{i}; X_{j}).$$



Maximum likelihood learning of tree structure

- Proposed by Chow and Liu (68)
- Max. weight spanning tree

$$\hat{T}_{\mathrm{ML}} = \arg\max_{T} \sum_{k=1}^{n} \log P(\mathbf{x}_{V}).$$

$$\hat{T}_{\mathrm{ML}} = \arg \max_{T} \sum_{(i,j) \in T} \hat{I}^{n}(X_{i}; X_{j}).$$

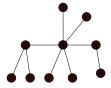
Pairwise statistics suffice for ML

Maximum likelihood learning of tree structure

- Proposed by Chow and Liu (68)
- Max. weight spanning tree

$$\hat{T}_{\mathrm{ML}} = \arg\max_{T} \sum_{k=1}^{n} \log P(\mathbf{x}_{V}).$$

$$\hat{T}_{\mathrm{ML}} = \arg\max_{T} \sum_{(i,j) \in T} \hat{I}^{n}(X_{i}; X_{j}).$$



- Pairwise statistics suffice for ML
- n samples and p nodes: Sample complexity: $\frac{\log p}{n} = O(1)$.

Maximum likelihood learning of tree structure

- Proposed by Chow and Liu (68)
- Max. weight spanning tree

$$\hat{T}_{\text{ML}} = \arg\max_{T} \sum_{k=1}^{n} \log P(\mathbf{x}_{V}).$$

$$\hat{T}_{\mathrm{ML}} = \arg\max_{T} \sum_{(i,j) \in T} \hat{I}^{n}(X_{i}; X_{j}).$$

- Pairwise statistics suffice for ML
- n samples and p nodes: Sample complexity: $\frac{\log p}{n} = O(1)$.

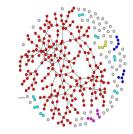
What other classes of graphical models are tractable for learning?



Challenges

- Presence of cycles
 - Pairwise statistics no longer suffice
 - Likelihood function not tractable

$$P(\mathbf{x}) = \frac{1}{Z} \exp \left[\sum_{(i,j) \in G} \Psi_{i,j}(x_i, x_j) \right].$$

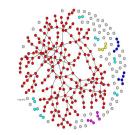


Challenges

- Presence of cycles
 - Pairwise statistics no longer suffice
 - Likelihood function not tractable

$$P(\mathbf{x}) = \frac{1}{Z} \exp \left[\sum_{(i,j) \in G} \Psi_{i,j}(x_i, x_j) \right].$$

- Presence of high-degree nodes
 - ▶ Brute-force search not tractable



Challenges

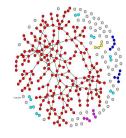
- Presence of cycles
 - Pairwise statistics no longer suffice
 - Likelihood function not tractable

$$P(\mathbf{x}) = \frac{1}{Z} \exp \left[\sum_{(i,j) \in G} \Psi_{i,j}(x_i, x_j) \right].$$



▶ Brute-force search not tractable

Can we provide learning guarantees under above conditions?



Challenges

- Presence of cycles
 - Pairwise statistics no longer suffice
 - Likelihood function not tractable

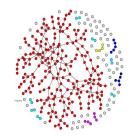
$$P(\mathbf{x}) = \frac{1}{Z} \exp \left[\sum_{(i,j) \in G} \Psi_{i,j}(x_i, x_j) \right].$$

- Presence of high-degree nodes
 - ▶ Brute-force search not tractable

Can we provide learning guarantees under above conditions?

Our Perspective: Tractable Graph Families

- Characterize the class of tractable families
- Incorporate all the above challenges
- Relevant for real datasets, e.g., social-network data



Related Work in Structure Learning

Algorithms for Structure Learning

- Chow and Liu (68)
- Meinshausen and Buehlmann (06)
- Bresler, Mossel and Sly (09)
- Ravikumar, Wainwright and Lafferty (10) ...

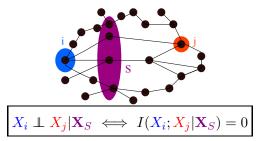
Approaches Employed

- EM/Search approaches
- Combinatorial/Greedy approach
- Convex relaxation, ...

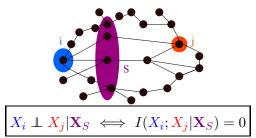
Outline

- Introduction
- Tractable Graph Families
- 3 Structure Estimation in Graphical Models
- 4 Method and Guarantees
- Conclusion

Separators in Graphical Models



Separators in Graphical Models



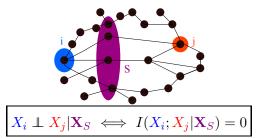
Observations

- Δ -separator for graphs with maximum degree Δ
 - lacktriangle Brute-force search for the separator: $\left| \operatorname{argmin} \ I(X_i; X_j | \mathbf{X}_S) \right|$

$$\underset{|S| \le \Delta}{\operatorname{argmin}} \ I(X_i; X_j | \mathbf{X}_S)$$

Computational complexity scales as $O(p^{\Delta})$

Separators in Graphical Models



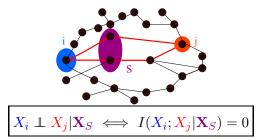
Observations

- Δ -separator for graphs with maximum degree Δ
 - lacktriangle Brute-force search for the separator: $\left| \operatorname{argmin} \ I(X_i; X_j | \mathbf{X}_S) \right|$

$$\underset{|S| \le \Delta}{\operatorname{argmin}} \ I(X_i; X_j | \mathbf{X}_S)$$

- ightharpoonup Computational complexity scales as $O(p^{\Delta})$
- Approximate separators in general graphs?

Separators in Graphical Models



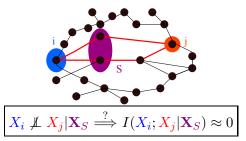
Observations

- Δ -separator for graphs with maximum degree Δ
 - lacktriangle Brute-force search for the separator: $\left| \operatorname{argmin} \ I(X_i; X_j | \mathbf{X}_S) \right|$

$$\underset{|S| \le \Delta}{\operatorname{argmin}} \ I(X_i; X_j | \mathbf{X}_S)$$

- ightharpoonup Computational complexity scales as $O(p^{\Delta})$
- Approximate separators in general graphs?

Separators in Graphical Models



Observations

- Δ -separator for graphs with maximum degree Δ
 - ▶ Brute-force search for the separator: $| \underset{\text{argmin }}{\operatorname{argmin}} I(X_i; X_j | \mathbf{X}_S) |$

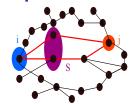
$$\underset{|S| \le \Delta}{\operatorname{argmin}} \ I(X_i; X_j | \mathbf{X}_S)$$

- ightharpoonup Computational complexity scales as $O(p^{\Delta})$
- Approximate separators in general graphs?

Tractable Graph Families: Local Separation

$$\gamma$$
-Local Separator $S_{\gamma}(i,j)$

Minimal vertex separator with respect to paths of length less than $\boldsymbol{\gamma}$

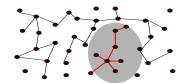


 $(\eta,\gamma)\text{-Local Separation Property for Graph }G$

$$|S_{\gamma}(i,j)| \leq \eta$$
 for all $(i,j) \notin G$

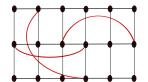
Locally tree-like

- Erdős-Rényi graphs
- Power-law/scale-free graphs



Small-world Graphs

- Watts-Strogatz model
- Hybrid/augmented graphs



Outline

- Introduction
- Tractable Graph Families
- 3 Structure Estimation in Graphical Models
- 4 Method and Guarantees
- Conclusion

 \bullet *n* i.i.d. samples available for structure estimation

- \bullet *n* i.i.d. samples available for structure estimation
- Ising and Gaussian Graphical Models

$$P(\mathbf{x}) \propto \exp\left[\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \{-1, 1\}^p.$$

$$f(\mathbf{x}) \propto \exp\left[-\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \mathbb{R}^p.$$

- \bullet *n* i.i.d. samples available for structure estimation
- Ising and Gaussian Graphical Models

$$P(\mathbf{x}) \propto \exp\left[\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \{-1, 1\}^p.$$

$$f(\mathbf{x}) \propto \exp\left[-\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \mathbb{R}^p.$$

• For $(i,j) \in G$, $J_{\min} \leq |J_{i,j}| \leq J_{\max}$

- \bullet *n* i.i.d. samples available for structure estimation
- Ising and Gaussian Graphical Models

$$P(\mathbf{x}) \propto \exp\left[\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \{-1, 1\}^p.$$

$$f(\mathbf{x}) \propto \exp\left[-\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \mathbb{R}^p.$$

- For $(i,j) \in G$, $J_{\min} \leq |J_{i,j}| \leq J_{\max}$
- Graph G satisfies (η, γ) local separation property

- \bullet *n* i.i.d. samples available for structure estimation
- Ising and Gaussian Graphical Models

$$P(\mathbf{x}) \propto \exp\left[\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \{-1, 1\}^p.$$
$$f(\mathbf{x}) \propto \exp\left[-\frac{1}{2}\mathbf{x}^T\mathbf{J}_G\mathbf{x} + \mathbf{h}^T\mathbf{x}\right], \quad \mathbf{x} \in \mathbb{R}^p.$$

- For $(i,j) \in G$, $J_{\min} \leq |J_{i,j}| \leq J_{\max}$
- Graph G satisfies (η, γ) local separation property

Tradeoff between $\eta, \gamma, J_{\min}, J_{\max}$ for tractable learning



Regime of Tractable Learning

Efficient Learning Under Approximate Separation

ullet Maximum edge potential $J_{
m max}$ of Ising model satisfies

$$J_{\text{max}} < J^*$$
.

 J^* is threshold for phase transition for conditional uniqueness.

Regime of Tractable Learning

Efficient Learning Under Approximate Separation

ullet Maximum edge potential $J_{
m max}$ of Ising model satisfies

$$J_{\text{max}} < J^*$$
.

 J^* is threshold for phase transition for conditional uniqueness.

• Gaussian model is α -walk summable

$$\|\overline{\mathbf{R}}_G\| \le \alpha < 1.$$

 $\overline{\mathbf{R}}_G$ is absolute partial correlation matrix.

$$\mathbf{J}_G = \mathbf{I} - \mathbf{R}_G.$$

Regime of Tractable Learning

Efficient Learning Under Approximate Separation

ullet Maximum edge potential $J_{
m max}$ of Ising model satisfies

$$J_{\text{max}} < J^*$$
.

 J^* is threshold for phase transition for conditional uniqueness.

• Gaussian model is α -walk summable

$$\|\overline{\mathbf{R}}_G\| \le \alpha < 1.$$

 $\overline{\mathbf{R}}_G$ is absolute partial correlation matrix.

$$\mathbf{J}_G = \mathbf{I} - \mathbf{R}_G.$$

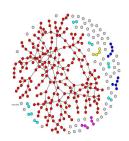
Tractable Parameter Regime for Structure Learning



Tractable Graph Families and Regimes

• Graph G satisfies (η, γ) -local separation property where

$$\eta = O(1)$$
.



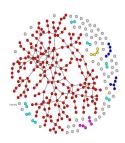
Tractable Graph Families and Regimes

• Graph G satisfies (η, γ) -local separation property where

$$\eta = O(1)$$
.

ullet Maximum edge potential $J_{
m max}$ satisfies

$$\alpha := \frac{\tanh J_{\max}}{\tanh J^*} < 1 \text{ or } \|\overline{\mathbf{R}}_G\| \le \alpha < 1.$$



Tractable Graph Families and Regimes

• Graph G satisfies (η, γ) -local separation property where

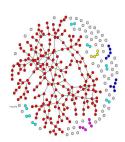
$$\eta = O(1)$$
.

ullet Maximum edge potential $J_{
m max}$ satisfies

$$\alpha := \frac{\tanh J_{\max}}{\tanh J^*} < 1 \text{ or } \|\overline{\mathbf{R}}_G\| \le \alpha < 1.$$

ullet Minimum edge potential J_{\min} is sufficiently strong

$$\frac{J_{\min}}{\alpha^{\gamma}} = \widetilde{\omega}(1).$$



Tractable Graph Families and Regimes

• Graph G satisfies (η, γ) -local separation property where

$$\eta = O(1)$$
.

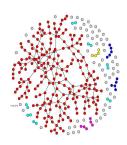
ullet Maximum edge potential $J_{
m max}$ satisfies

$$\alpha := \frac{\tanh J_{\max}}{\tanh J^*} < 1 \text{ or } \|\overline{\mathbf{R}}_G\| \le \alpha < 1.$$

ullet Minimum edge potential J_{\min} is sufficiently strong

$$\frac{J_{\min}}{\alpha^{\gamma}} = \widetilde{\omega}(1).$$

• Edge potentials are generic.



Example: girth g, maximum degree Δ

• Structural criteria: (η, γ) -local separation property is satisfied

$$\eta = 1, \quad \gamma = g.$$

• Parameter criteria: The maximum edge potential satisfies

$$J_{\text{max}} < J^* = \operatorname{atanh}(\Delta^{-1}), \quad \alpha := \frac{\tanh J_{\text{max}}}{\tanh J^*}.$$

• Tradeoff: The minimum edge potential satisfies

$$J_{\min}\alpha^g = \omega(1).$$

For example, when

$$J_{\min} = \Theta(\Delta^{-1}) \implies \Delta \alpha^g = o(1).$$

Learnability regime involves a tradeoff between degree and girth.



Outline

- Introduction
- Tractable Graph Families
- 3 Structure Estimation in Graphical Models
- 4 Method and Guarantees
- Conclusion

Algorithm for Structure Learning

Conditional Mutual Information Thresholding (CMIT)

- Empirical Conditional Mutual Information from samples
- ullet Attempt to search for approx. separator of size η

$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \leq \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

Algorithm for Structure Learning

Conditional Mutual Information Thresholding (CMIT)

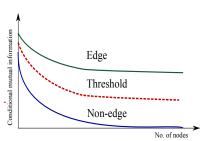
- Empirical Conditional Mutual Information from samples
- Attempt to search for approx. separator of size η

$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \le \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

Threshold $\xi_{n,n}$

• Depends only on # of samples n

Depends only on
$$\#$$
 of samples n and $\#$ of nodes p
$$\xi_{n,p} = O(J_{\min}^2) \cap \omega(\alpha^{2\gamma}) \cap \Omega\left(\frac{\log p}{n}\right).$$



Algorithm for Structure Learning

Conditional Mutual Information Thresholding (CMIT)

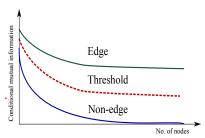
- Empirical Conditional Mutual Information from samples
- Attempt to search for approx. separator of size η

$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \le \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

Threshold $\xi_{n,n}$

• Depends only on # of samples n

Depends only on
$$\#$$
 of samples n and $\#$ of nodes p
$$\xi_{n,p} = O(J_{\min}^2) \cap \omega(\alpha^{2\gamma}) \cap \Omega\left(\frac{\log p}{n}\right).$$



Local Test Using Low-order Statistics

Guarantees on Conditional Mutual Information Test

$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \le \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

- Ising/Gaussian graphical model on p nodes
- No. of samples n such that

$$n = \Omega(J_{\min}^{-4} \log p).$$

Theorem

CMIT is structurally consistent

$$\lim_{\substack{p,n\to\infty\\n=\Omega(J^{-4}\log p)}} P\left[\widehat{G}_p^n \neq G_p\right] = 0.$$

Probability measure on both graph and samples

Lower Bound on Sample Complexity

• Erdős-Rényi random graph $G \sim \mathfrak{G}(p,c/p)$

Theorem

For any estimator \widehat{G}_{n}^{n} , it is necessary that

- Discrete distribution over \mathcal{X} : $n \geq \frac{c \log_2 p}{2 \log_2 |\mathcal{X}|}$
- Gaussian with α -walk summability: $n \geq \frac{c \log_2 p}{\log_2 \left[2\pi e \left(\frac{1}{1-\alpha} + 1 \right) \right]}$ $\lim_{n \to \infty} P \left[\widehat{G}_p^n \neq G_p \right] = 0.$

Lower Bound on Sample Complexity

• Erdős-Rényi random graph $G \sim \Im(p,c/p)$

Theorem

For any estimator \widehat{G}_{n}^{n} , it is necessary that

- Discrete distribution over \mathcal{X} : $n \geq \frac{c \log_2 p}{2 \log_2 |\mathcal{X}|}$
- Gaussian with α -walk summability: $n \geq \frac{c \log_2 p}{\log_2 \left[2\pi e \left(\frac{1}{1-\alpha} + 1 \right) \right]}$ $\lim_{n \to \infty} P \left[\widehat{G}_p^n \neq G_p \right] = 0.$

Proof Techniques

- Fano's inequality over typical graphs
- Characterize typical graphs for Erdős-Rényi ensemble

 $\Omega(c\log p)$ samples needed for random graph structure estimation.



$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \le \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

- Correctness of algorithm under exact statistics
- Consistency under prescribed sample complexity
 - Concentration bounds for empirical quantities

$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \le \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

- Correctness of algorithm under exact statistics
- Consistency under prescribed sample complexity
 - Concentration bounds for empirical quantities

Analysis for non-neighbors

- Conditional mutual information upon conditioning by local separator
- Derive rate of decay for conditional mutual information
 Self-avoiding walk tree analysis for Ising models
 Walk-sum analysis for Gaussian models

$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \le \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

- Correctness of algorithm under exact statistics
- Consistency under prescribed sample complexity
 - Concentration bounds for empirical quantities

Analysis for non-neighbors

- Conditional mutual information upon conditioning by local separator
- Derive rate of decay for conditional mutual information
 Self-avoiding walk tree analysis for Ising models
 Walk-sum analysis for Gaussian models

Analysis for neighbors

Lower bound under generic edge potentials



$$(i,j) \in \widehat{G} \text{ if } \min_{\substack{S \subset V \setminus \{i,j\} \ |S| \le \eta}} \widehat{I}(X_i; X_j | \mathbf{X}_S) > \xi_{n,p}$$

- Correctness of algorithm under exact statistics
- Consistency under prescribed sample complexity
 - Concentration bounds for empirical quantities

Analysis for non-neighbors

- Conditional mutual information upon conditioning by local separator
- Derive rate of decay for conditional mutual information
 Self-avoiding walk tree analysis for Ising models
 Walk-sum analysis for Gaussian models

Analysis for neighbors

Lower bound under generic edge potentials



Outline

- Introduction
- 2 Tractable Graph Families
- 3 Structure Estimation in Graphical Models
- 4 Method and Guarantees
- Conclusion

Summary and Outlook

Summary

- Local algorithm based on low-order statistics
- Transparent assumptions
- Logarithmic sample complexity



Outlook

- Is structure learning beyond this regime hard?
- Connections with incoherence conditions
- Structure learning with latent variables

A. Anandkumar, V. Tan and Alan Willsky, "High-Dimensional Structure Learning of Ising Models: Tractable Graph Families" ArXiv 1107.1736.

A. Anandkumar, V. Tan and Alan Willsky, "High-Dimensional Gaussian Graphical Model Selection: Tractable Graph Families" ArXiv 1107.1270.