High-Dimensional Graphical Model Selection

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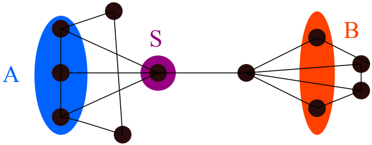
U.C. Irvine

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

Graphical Models: Definition

Conditional Independence

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



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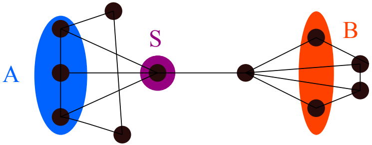

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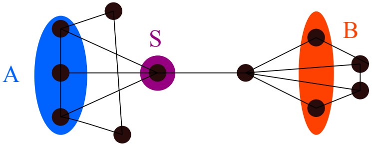

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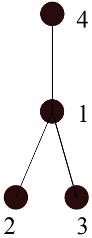
Tree-Structured Graphical Models



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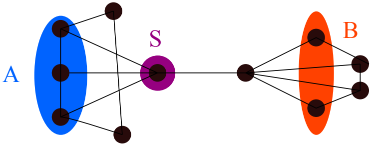

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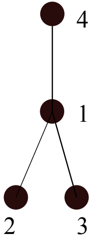
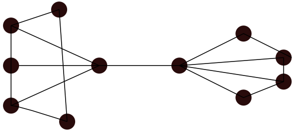
Tree-Structured Graphical Models

$$P(\mathbf{x}) = \prod_{i\in V} P_i(x_i) \prod_{(i,j)\in E} \frac{P_{i,j}(x_i, x_j)}{P_i(x_i)P_j(x_j)}$$

$$= P_1(x_1)P_{2|1}(x_2|x_1)P_{3|1}(x_3|x_1)P_{4|1}(x_4|x_1).$$



Structure Learning of Graphical Models



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

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

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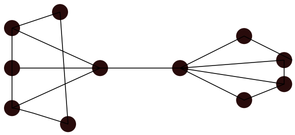

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Challenge: High Dimensionality ("Data-Poor" Regime)

- 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

Tree Graphical Models: Tractable Learning

Maximum likelihood learning of tree structure

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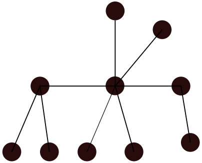
- Max. weight spanning tree



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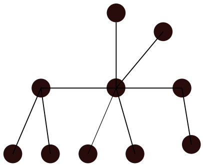

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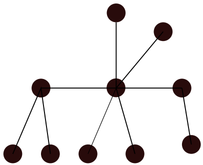

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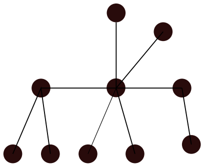

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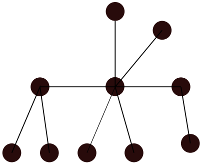

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What other classes of graphical models are tractable for learning?

Learning Graphical Models Beyond Trees

Challenges

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

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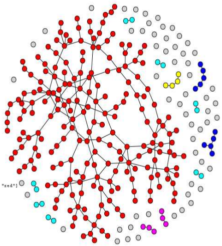

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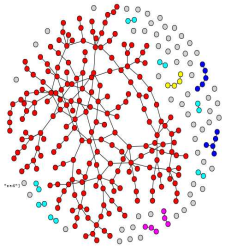

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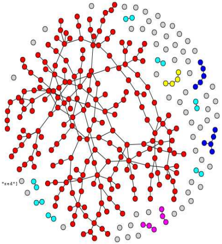

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Can we provide learning guarantees under above conditions?

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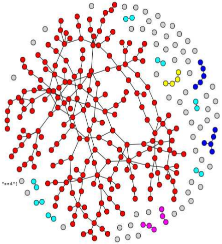

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Our Perspective: Tractable Graph Families

- 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) ...

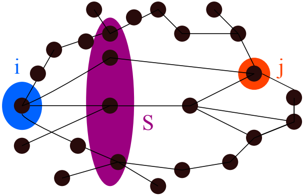
Approaches Employed

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

Outline

Intuitions: Conditional Mutual Information Test

Separators in Graphical Models



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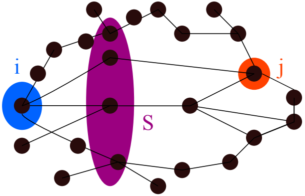

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Observations

- Δ-separator for graphs with maximum degree Δ
  - Brute-force search for the separator: $\boxed{\underset{|S| \leq \Delta}{\text{argmin}} \; I(X_i; X_j | \mathbf{X}_S)}$
  - Computational complexity scales as $O(p^{\Delta})$

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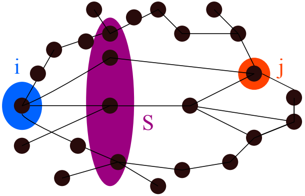

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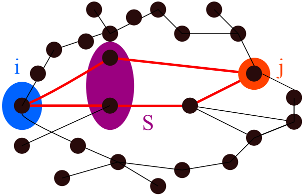

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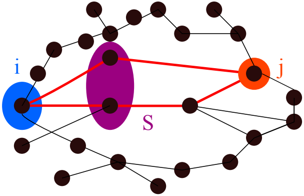

$$\boxed{X_i \not\perp\!\!\!\perp X_j|\mathbf{X}_S \overset{?}{\Longrightarrow} I(X_i;X_j|\mathbf{X}_S) \approx 0}$$

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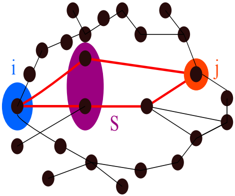
Tractable Graph Families: Local Separation

γ-Local Separator $S_\gamma(i, j)$

Minimal vertex separator with respect to paths of length less than γ

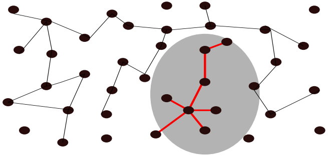


(η, γ)-Local Separation Property for Graph G

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

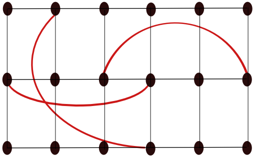
Locally tree-like

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



Small-world Graphs

- Watts-Strogatz model
- Hybrid/augmented graphs



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

Regime of Tractable Learning

Efficient Learning Under Approximate Separation

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Tractable Parameter Regime for Structure Learning

Tractable Graph Families and Regimes

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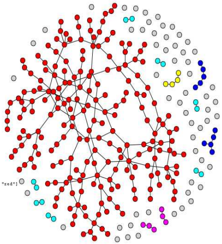

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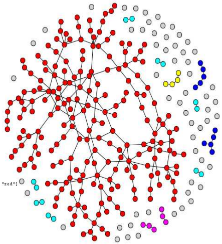

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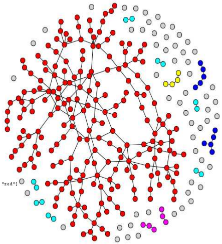

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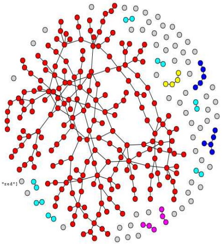
- Edge potentials are generic.



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

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

- Tradeoff: The minimum edge potential satisfies

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

For example, when

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

Learnability regime involves a tradeoff between degree and girth.

Outline

Algorithm for Structure Learning

Conditional Mutual Information Thresholding (CMIT)

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

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

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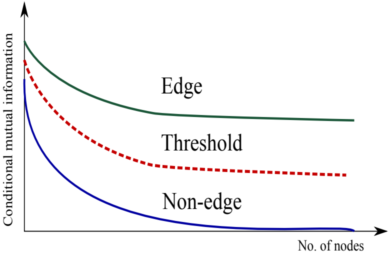

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- Depends only on # of samples n and # of nodes p

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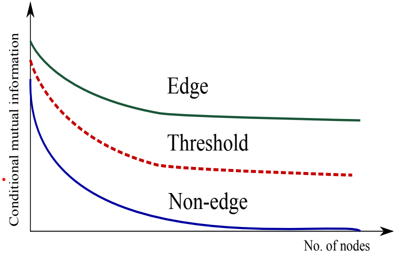

Local Test Using Low-order Statistics

Guarantees on Conditional Mutual Information Test

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

- 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

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

- Probability measure on both graph and samples

Improved Guarantees via Total Variation Distances

$$\boxed{\nu_{i|j;S} := 0.5\|P(X_i, \mathbf{X}_S|X_j = +) - P(X_i, \mathbf{X}_S|X_j = -)\|_1.}$$

- Sample complexity for graph estimation improves to $\Omega(J_{\min}^{-2} \log p)$.
- Bound for non-neighbors: $\nu_{\max}(p;\eta) := \max_{(i,j)\notin G_p} \min_{\substack{|S|\leq\eta \\ S\subset V\setminus\{i,j\}}} \nu_{i|j;S}$.
- Choose threshold $\xi_{n,p}$ as $\xi_{n,p} = \nu_{\max}(p;\eta) + \delta$.
- Min. node marginal $P_{\min} := \min_{\substack{x_j=\pm 1, \\ j\in V}} P(X_j = x_j)$.

Theorem: PAC Learning Guarantees

All edges with $\nu_{i|j;S} > \nu_{\max}(p;\eta) + 2\delta$ of a graph with η-local separators are recovered with probability at least $1-\epsilon$, when the number of samples is

$$n > \frac{(\delta+2)^2}{2\delta^2 P_{\min}^2}\left[\log\left(\frac{1}{\epsilon}\right) + (\eta+2)\log p + (\eta+4)\log 2\right].$$

Non-asymptotic Bounds on $\nu_{\max}(p)$

$$\nu_{\max}(p;\eta) := \max_{(i,j)\notin G_p} \min_{\substack{|S|\leq\eta \\ S\subset V\setminus\{i,j\}}} \nu_{i|j;S}, \qquad \alpha := \frac{\tanh J_{\max}}{\tanh J^*} < 1.$$

Bounds on $\nu_{\max}(p;\eta)$ for Graph Families

1. For degree-bounded ensemble, $\nu_{\max}(p;\Delta) = 0$.
2. For girth-bounded ensemble $\nu_{\max}(p;1) \leq \alpha^g$.
3. For Δ-random regular graphs , choose any $l \in \mathbb{N}$ such that $l < 0.5(0.25p\Delta + 0.5 - \Delta^2)$: with prob. at least $1 - \Delta^{8l-2}(p\Delta - 4\Delta^2 - 8l)^{-(4l-1)}$,
$$\nu_{\max}(p;2) \leq \alpha^l.$$
4. For Erdős-Rényi ensemble with average degree $c > 1$, choose any $l \in \mathbb{N}$ such that $l < \frac{\log p}{4\log c}$: with prob. at least $1 - le^{\sqrt{125}}p^{-2.5} - l!c^{4l-1}p^{-1}$,
$$\nu_{\max}(p;2) \leq 4l^3\alpha^l \log p.$$

Lower Bound on Sample Complexity

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

Theorem

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

- Discrete distribution over $\mathcal{X}$: $n \geq \dfrac{c \log_2 p}{2 \log_2 |\mathcal{X}|}$
- Gaussian with α-walk summability: $n \geq \dfrac{c \log_2 p}{\log_2 \left[2\pi e \left(\frac{1}{1-\alpha} + 1\right)\right]}$

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

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

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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.

Proof Ideas

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

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

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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

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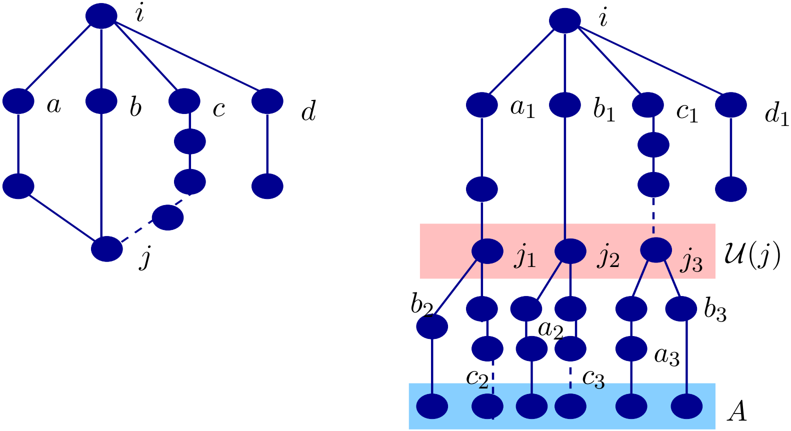
Self-Avoiding Walk Analysis



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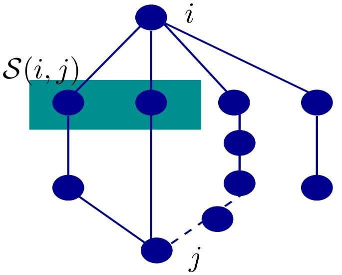

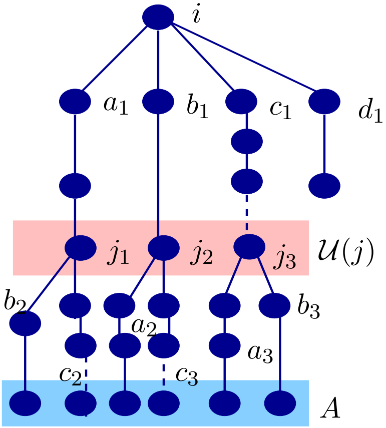

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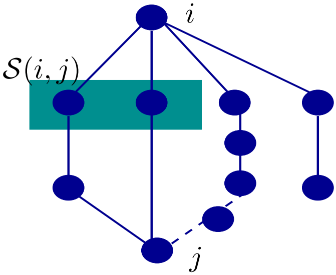

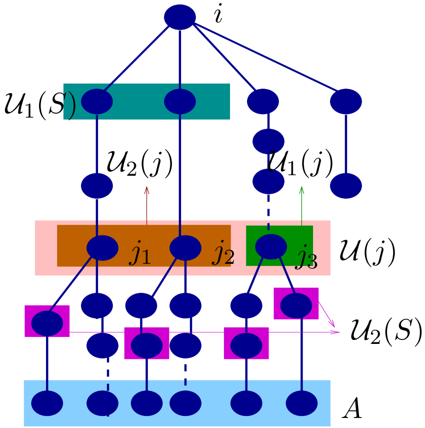

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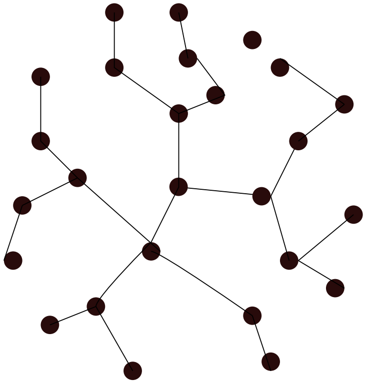
Conditional Uniqueness Regime

Correlation Decay in Residual Self-Avoid Walk Tree upon Separation



Bounds on J^*

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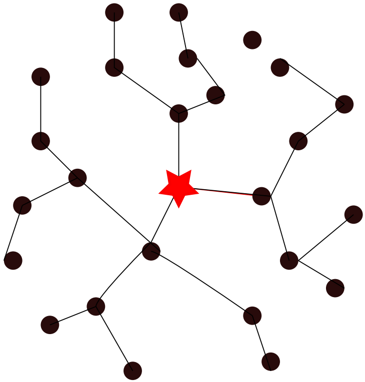

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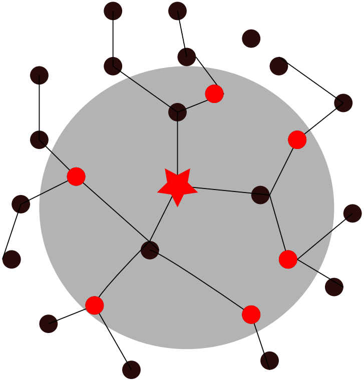

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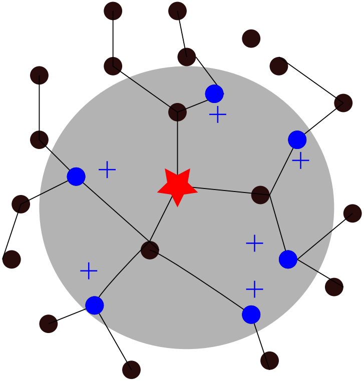

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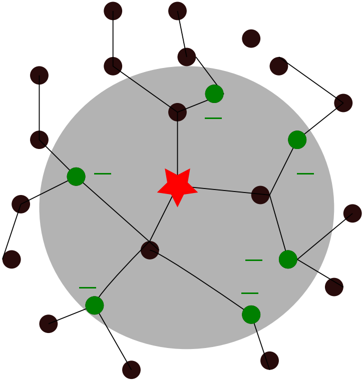

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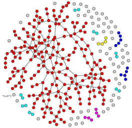
Outline

1. Introduction
2. Tractable Graph Families
3. Structure Estimation in Graphical Models
4. Method and Guarantees
5. 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.