Introduction to Algebraic Methods in Graphical Models

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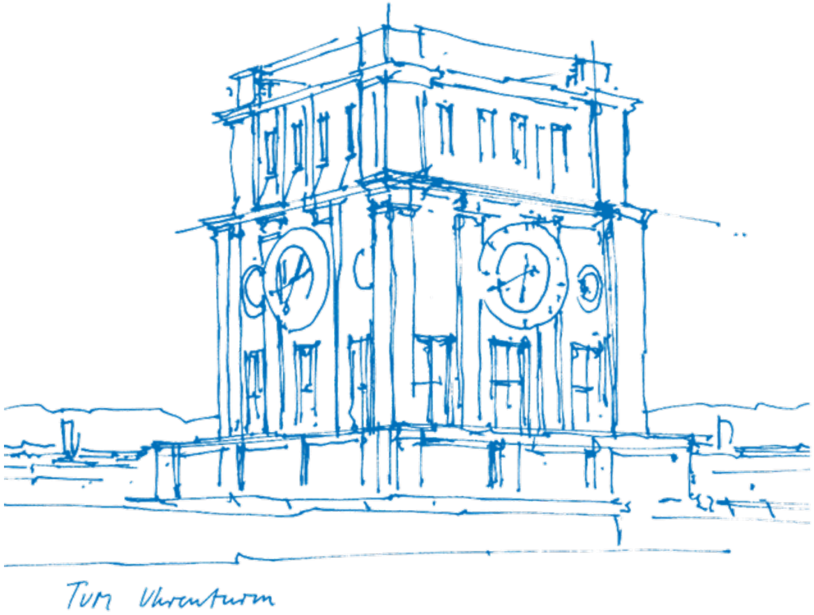


Statistical Graphical Models

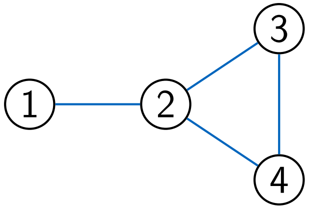
Setup: Random variables $(X_v)_{v\in V}$ and undirected/directed graph $G=(V,E)$.

$$\mathcal{M}(G) = \{\textit{probability distributions on } \mathbb{R}^{|V|} \textit{ that factorize according to } G\}$$

Undirected Graphical Models:

$$p(x) = \frac{1}{Z}\prod_{C\in\mathcal{C}} \psi_C(x_C),$$

where $\mathcal{C}$ is the collection of cliques of G.



$$p(x_1,x_2,x_3,x_4) \propto \psi_{12}(x_1,x_2)\cdot\psi_{234}(x_2,x_3,x_4)$$

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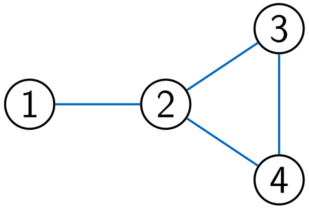

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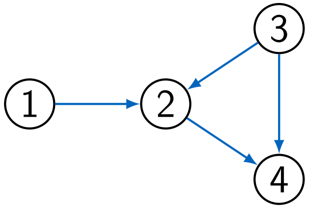
Directed Graphical Models:

$$p(x) = \prod_{v \in V} p(x_v | x_{\mathrm{pa}(v)}),$$

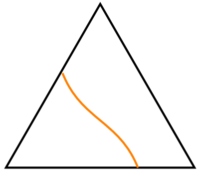
where $\mathrm{pa}(v) = \{w \in V : w \to v \in E\}$.



$$p(x_1, x_2, x_3, x_4) = p(x_1) \cdot p(x_2 | x_1, x_3) \cdot p(x_3) \cdot p(x_4 | x_2, x_3)$$

Polynomial Parameterizations in Directed Graphical Models

Discrete Distributions



- Finite state space:

$$\mathcal{I} = \times_{v \in V} [d_v].$$

- Each prob. distribution is a point in

$$\Delta_{|\mathcal{I}|-1} = \{p \in \mathbb{R}^{\mathcal{I}} : p(x) \geq 0, \sum_{i \in \mathcal{I}} p(x) = 1\}.$$

- Graphical model $\mathcal{M}(G) \subseteq \Delta_{|\mathcal{I}|-1}$ is given by

$$\mathcal{M}(G) = \{p \in \mathbb{R}^{\mathcal{I}} : p(x) = \prod_{v \in V} p(x_v | x_{\mathrm{pa}(v)})\}.$$

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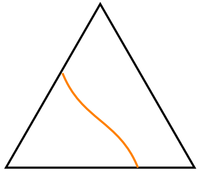

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Gaussian Distributions

- Each distribution $N(0,\Sigma)$ is given by cov. matrix

$$\Sigma \in PD(|V|) \subseteq \mathbb{R}^{\binom{|V|+1}{2}}.$$

- Weight matrix:

$$\mathbb{R}^E = \{\Lambda \in \mathbb{R}^{|V|\times|V|} : \lambda_{vu} = 0 \text{ if } u \to v \notin E\}.$$

- Graphical model $\mathcal{M}^{(2)}(G) \subseteq PD(|V|)$ is given by

$$\mathcal{M}^{(2)}(G) = \{\Sigma \in PD(|V|) : \Sigma = (I-\Lambda)^{-1}\Omega(I-\Lambda)^{-\top}\},$$

where $\Lambda \in \mathbb{R}^E, \Omega \in \mathrm{diag}_+$.

Multiple graphical models have a polynomial parameterization.

Example: Gaussian Directed Graphical Models

$$\Lambda = \begin{pmatrix} 0 & 0 & 0 \\ \lambda_{21} & 0 & 0 \\ 0 & \lambda_{32} & 0 \end{pmatrix} \qquad \Omega = \begin{pmatrix} \omega_{11} & 0 & 0 \\ 0 & \omega_{22} & 0 \\ 0 & 0 & \omega_{33} \end{pmatrix}$$

Covariance matrix:

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \cdot & \sigma_{22} & \sigma_{23} \\ \cdot & \cdot & \sigma_{33} \end{pmatrix} = \begin{pmatrix} \omega_{11} & \omega_{11}\lambda_{21} & \omega_{11}\lambda_{21}\lambda_{32} \\ \cdot & \omega_{22} + \omega_{11}\lambda_{21}^2 & \omega_{22}\lambda_{32} + \omega_{11}\lambda_{21}^2\lambda_{32} \\ \cdot & \cdot & \omega_{33} + \omega_{22}\lambda_{32}^2 + \omega_{11}\lambda_{21}^2\lambda_{32}^2 \end{pmatrix}.$$

Graphical model:

$$\mathcal{M}^{(2)}(G) = PD(|V|) \cap \mathbb{V}(\sigma_{12}\sigma_{23} - \sigma_{22}\sigma_{13})$$

Questions of Interest in Graphical Modeling

Statistics

- Model selection.
- Parameter identifiability.
- Parameter estimation.
  (Maximum-Likelihood-Estimation.)
- ...

Algebraic Geometry

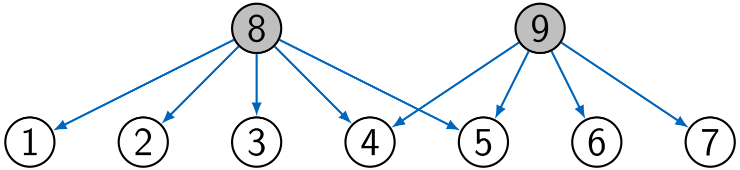
- Vanishing ideal of $\mathcal{M}(G)$.
- Is the parameterization map injective?
- Boundaries and singular locus of $\mathcal{M}(G)$.
  ML degree.
- ...

Interesting:

Hidden variables, i.e., $V = \mathcal{O} \cup \mathcal{H}$. Only observe marginal distribution $X_{\mathcal{O}}$.

Factor Analysis Models

Graph $G = (\mathcal{O} \cup \mathcal{H}, E)$, only edges from latent to observed variables. Usually, $\mathcal{O} = [p]$.



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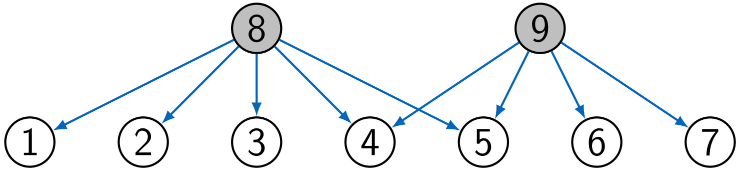

$$\Lambda = \begin{pmatrix} 0 & \Lambda_{\mathcal{O}\mathcal{H}} \\ 0 & 0 \end{pmatrix} \qquad \Omega = \begin{pmatrix} \Omega_{\mathcal{O}\mathcal{O}} & 0 \\ 0 & \Omega_{\mathcal{H}\mathcal{H}} \end{pmatrix}$$

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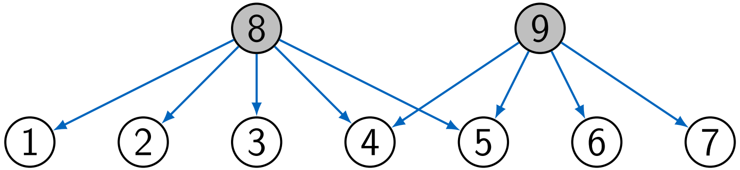


$$\Lambda = \begin{pmatrix} 0 & \Lambda_{\mathcal{O}\mathcal{H}} \\ 0 & 0 \end{pmatrix} \qquad \Omega = \begin{pmatrix} \Omega_{\mathcal{O}\mathcal{O}} & 0 \\ 0 & \Omega_{\mathcal{H}\mathcal{H}} \end{pmatrix}$$

- Covariance matrix:

$$\mathrm{Cov}\left[\begin{pmatrix} X_{\mathcal{O}} \\ X_{\mathcal{H}} \end{pmatrix}\right] = (I - \Lambda)^{-1}\Omega(I - \Lambda)^{-\top} = \begin{pmatrix} \Omega_{\mathcal{O}\mathcal{O}} + \Lambda_{\mathcal{O}\mathcal{H}}\Omega_{\mathcal{H}\mathcal{H}}\Lambda_{\mathcal{O}\mathcal{H}}^\top & \Lambda_{\mathcal{O}\mathcal{H}}\Omega_{\mathcal{H}\mathcal{H}} \\ \Omega_{\mathcal{H}\mathcal{H}}\Lambda_{\mathcal{O}\mathcal{H}}^\top & \Omega_{\mathcal{H}\mathcal{H}} \end{pmatrix}$$

- *Observed* covariance matrix (projection):

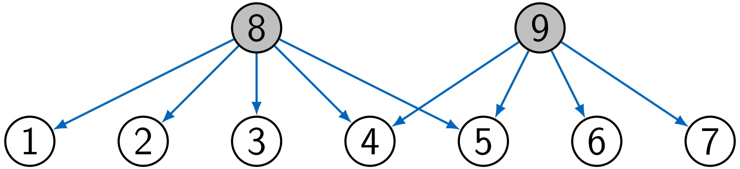
$$\mathrm{Cov}[X_{\mathcal{O}}] = \Omega_{\mathcal{O}\mathcal{O}} + \Lambda_{\mathcal{O}\mathcal{H}}\Omega_{\mathcal{H}\mathcal{H}}\Lambda_{\mathcal{O}\mathcal{H}}^\top$$

- *Observed* covariance model:

$$F_G = \{\widetilde{\Omega} + \widetilde{\Lambda}\widetilde{\Lambda}^\top \in \mathbb{R}^{|\mathcal{O}|\times|\mathcal{O}|} : \widetilde{\Omega} > 0 \text{ diagonal}, \ \widetilde{\Lambda} \in \mathbb{R}^{E_{\mathcal{O}\mathcal{H}}}\}$$

Goals: $\dim(F_G)$? $\quad I(F_G) \subseteq \mathbb{R}[\sigma_{ij}, i < j]$?

Example: Factor Analysis Models



Parameter matrix:

$$\tilde{\Lambda} = \begin{pmatrix} \lambda_{18} & \lambda_{28} & \lambda_{38} & \lambda_{48} & \lambda_{58} & 0 & 0 \\ 0 & 0 & 0 & \lambda_{49} & \lambda_{59} & \lambda_{69} & \lambda_{79} \end{pmatrix}^{\top}, \qquad \widetilde{\Omega} = \mathrm{diag}(\omega_{11}, \omega_{22}, \omega_{33}, \omega_{44}, \omega_{55}, \omega_{66}, \omega_{77}).$$

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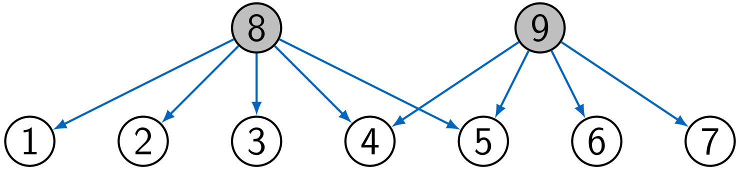

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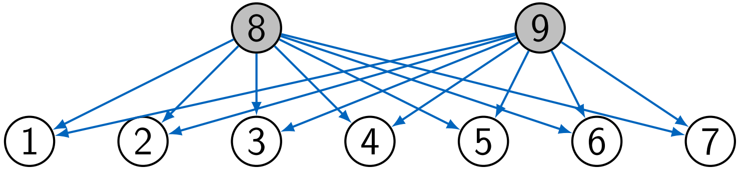
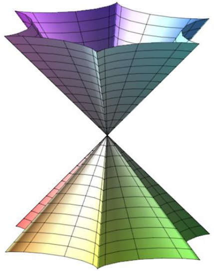
Observed covariance matrix:

$$\Sigma = \begin{pmatrix} \omega_{11} + \lambda_{18}^2 & \lambda_{18}\lambda_{28} & \lambda_{18}\lambda_{38} & \lambda_{18}\lambda_{48} & \lambda_{18}\lambda_{58} & 0 & 0 \\ \lambda_{18}\lambda_{28} & \omega_{22} + \lambda_{28}^2 & \lambda_{28}\lambda_{38} & \lambda_{28}\lambda_{48} & \lambda_{28}\lambda_{58} & 0 & 0 \\ \lambda_{18}\lambda_{38} & \lambda_{28}\lambda_{38} & \omega_{33} + \lambda_{38}^2 & \lambda_{38}\lambda_{48} & \lambda_{38}\lambda_{58} & 0 & 0 \\ \lambda_{18}\lambda_{48} & \lambda_{28}\lambda_{48} & \lambda_{38}\lambda_{48} & \omega_{44} + \lambda_{48}^2 + \lambda_{49}^2 & \lambda_{48}\lambda_{58} + \lambda_{49}\lambda_{59} & \lambda_{49}\lambda_{69} & \lambda_{49}\lambda_{79} \\ \lambda_{18}\lambda_{58} & \lambda_{28}\lambda_{58} & \lambda_{38}\lambda_{58} & \lambda_{48}\lambda_{58} + \lambda_{49}\lambda_{59} & \omega_{55} + \lambda_{58}^2 + \lambda_{59}^2 & \lambda_{59}\lambda_{69} & \lambda_{59}\lambda_{79} \\ 0 & 0 & 0 & \lambda_{49}\lambda_{69} & \lambda_{59}\lambda_{69} & \omega_{66} + \lambda_{69}^2 & \lambda_{69}\lambda_{79} \\ 0 & 0 & 0 & \lambda_{49}\lambda_{79} & \lambda_{59}\lambda_{79} & \lambda_{69}\lambda_{79} & \omega_{77} + \lambda_{79}^2 \end{pmatrix}.$$

Previous work: *Full* Factor Analysis Models





Dimension: [Drton et al., 2007]

$$\dim(F_G) = \min\{p(|\mathcal{H}|+1) - \binom{|\mathcal{H}|}{2}, \binom{p+1}{2}\},$$

where $|\mathcal{O}| = p$.

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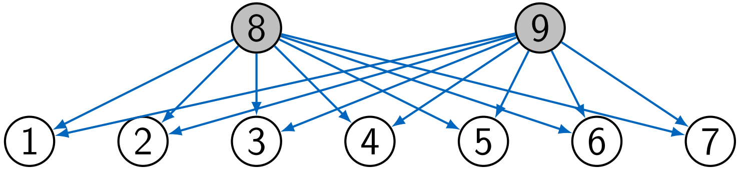

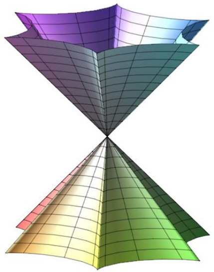

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$$I(F_G) = M_{p,|\mathcal{H}|} \cap \mathbb{R}[\sigma_{ij}, i < j],$$

where $M_{p,|\mathcal{H}|} \subseteq \mathbb{R}[\sigma_{ij}, i \leq j]$ is the ideal generated by all $(|\mathcal{H}| + 1) \times (|\mathcal{H}| + 1)$ minors of a symmetric $p \times p$ matrix.

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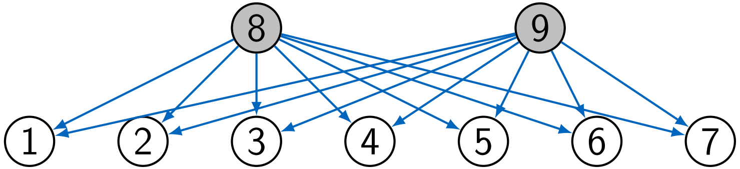

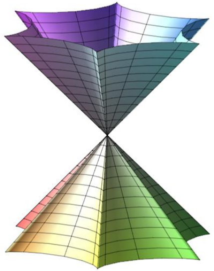

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Gröbner basis:

$|\mathcal{H}| = 1$:

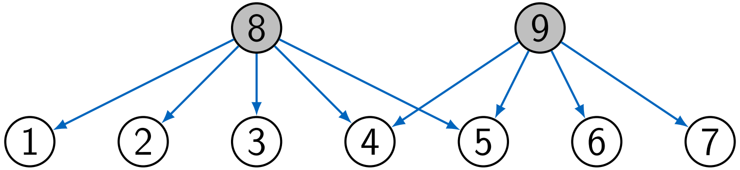
$$G_{p,1} = \{\sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}, \sigma_{il}\sigma_{jk} - \sigma_{ik}\sigma_{jl}$$
$$1 \leq i < j < k < l \leq p\}.$$

$|\mathcal{H}| = 2$:

- $\overline{F_G}$ secant variety of the 1-factor model.
- Delightful strategy. [Sullivant, 2009]

New Project: *Sparse* Factor Analysis Models

At least one edge is missing, only $|\mathcal{H}| = 2$ latent variables.



Dimension:

If $p \geq 5$ and any latent node has at least 3 children, then $\dim(F_G) = p + |E|$.

What about $I(F_G)$?

- If $\text{pa}(u) \cap \text{pa}(v) = \emptyset$, then $\sigma_{uv} = 0$ (singletons).
- Let $A, B \subseteq \mathcal{O}$ be disjoint sets s.t. $|A| = |B| = 2$. If $|\text{pa}(A) \cap \text{pa}(B)| \leq 1$, then $\det(\Sigma_{A,B}) = 0$ (tetrads).

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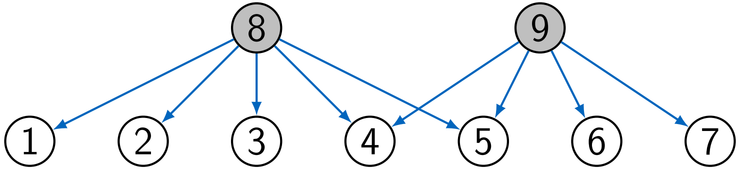

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Theorem:

$$\mathbb{V}(I(F_G)) = \mathbb{V}(\{M_{p,2} + S^{\leq 1}(G)\} \cap \mathbb{R}[\sigma_{ij}, i < j]),$$

where $S^{\leq 1}(G)$ is the ideal generated by all singletons and tetrads corresponding to G.

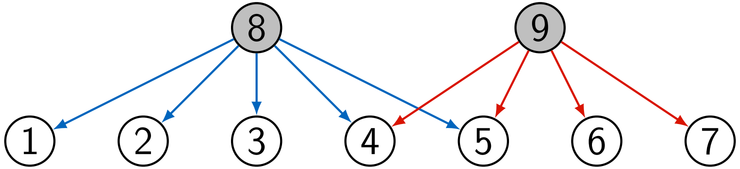
Joins

Join of Varieties:

$$W_1 * W_2 = \overline{\{\lambda w_1 + (1-\lambda) w_2 : w_1 \in W_1, w_2 \in W_2, \lambda \in \mathbb{R}\}}$$

(Sparse) Factor Models = Joins of (Sparse) One-Factor Models:

$$\sigma_{uv} = \begin{cases} \omega_{vv} + \sum_{h \in \mathrm{pa}(v)} \lambda_{vh}^2 & \text{if } u = v, \\ \sum_{h \in \mathrm{pa}(u) \cap \mathrm{pa}(v)} \lambda_{uh}\lambda_{vh} & \text{if } u \neq v. \end{cases}$$



<u>In accordance:</u> For two ideals I_1, I_2, one defines the join ideal $I_1 * I_2$ such that $I_1 * I_2 = I(\mathbb{V}(I_1) * \mathbb{V}(I_2))$.

$$\Longrightarrow \quad I(F_G) = I_1 * I_2$$

Delightful Strategy for Gröbner Basis

Observation:

$\text{in}_\prec(I_1 * I_2) \subseteq \text{in}_\prec(I_1) * \text{in}_\prec(I_2)$ for any term order $\prec$. If equality holds, then $\prec$ is *delightful* for I_1, I_2.

"Delightful" strategy: [Sturmfels, Sullivant, 2006]

Find $G \subseteq I_1 * I_2$ such that $\langle \text{in}_\prec(g) | g \in G \rangle = \text{in}_\prec(I_1) * \text{in}_\prec(I_2)$. Then G is a Gröbner basis.

1. Find delightful term order $\prec$.
2. Understand $\text{in}_\prec(I_1) * \text{in}_\prec(I_2)$.
3. Define polynomials $g \in G$ with correct initial terms.

Circular Term Order

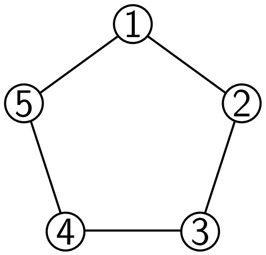
Circular distance on $\mathcal{O} = [p]$:

Length of the shortest path on regular p-gon.

Circular order:

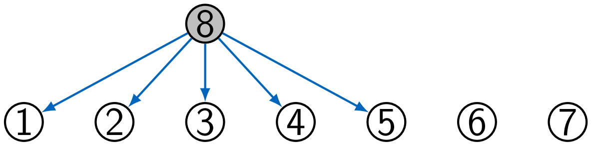
Any block-term order $\prec$ such that $\sigma_{uv} \succ \sigma_{wz}$ whenever the circular distance between u and v is smaller than the circular distance of w and z.

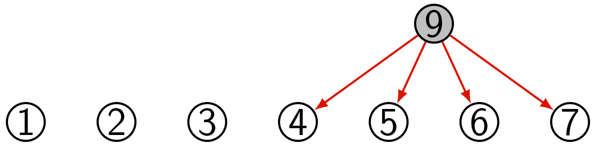
Example:



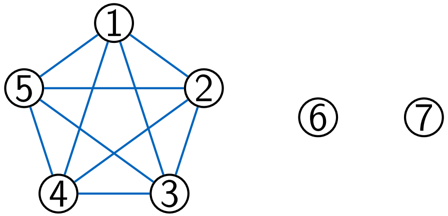
- $\sigma_{15} \succ \sigma_{24}$,
- $\sigma_{34} \succ \sigma_{25}$.

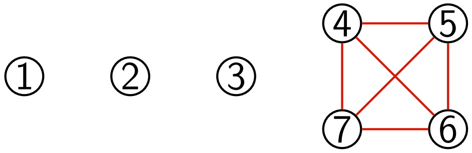
Non-Crossing Edge Graphs



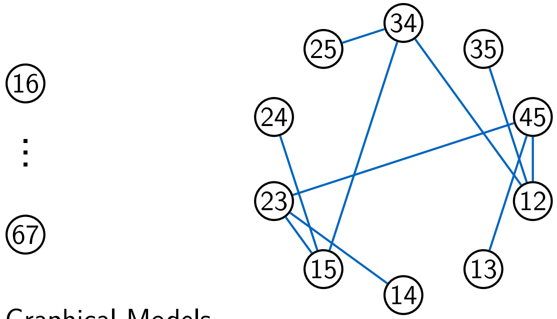


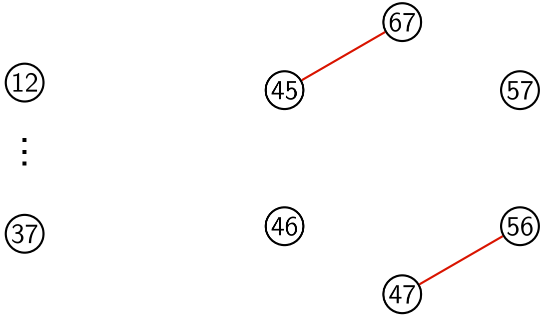
Complete graph on $v \in V$ s.t. $\mathrm{pa}(v) \neq \emptyset$:





Non-crossing edge graph:

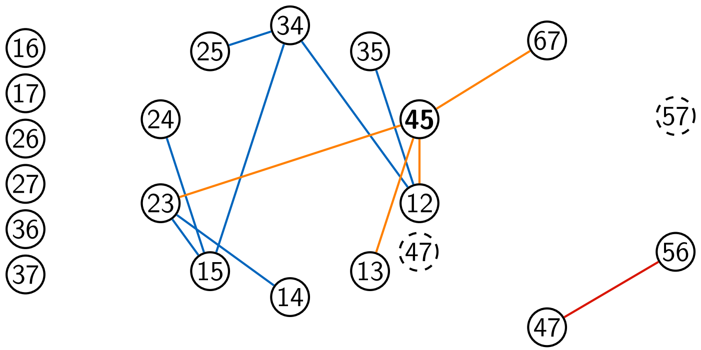




Gröbner Basis for "Overlap = 2"

$in_{\prec}(I_1) * in_{\prec}(I_2)$ is given by the edge ideal of the hypergraph obtained by gluing the non-crossing edge graphs.

Glued Hypergraph



Gröbner basis of $I_1 * I_2 = I(F_G)$

- $\sigma_{16}, \sigma_{17}, \sigma_{26}, \sigma_{27}, \sigma_{36}, \sigma_{37}$.
- $\sigma_{47}\sigma_{56} - \sigma_{57}\sigma_{46}$,
  $\sigma_{12}\sigma_{34} - \sigma_{13}\sigma_{24}$,
  $\sigma_{14}\sigma_{23} - \sigma_{13}\sigma_{24}$,
  $\sigma_{12}\sigma_{35} - \sigma_{13}\sigma_{25}$,
  $\sigma_{15}\sigma_{23} - \sigma_{13}\sigma_{25}$,
  $\sigma_{15}\sigma_{24} - \sigma_{14}\sigma_{25}$,
  $\sigma_{15}\sigma_{34} - \sigma_{14}\sigma_{35}$,
  $\sigma_{25}\sigma_{34} - \sigma_{24}\sigma_{35}$.
- $\sigma_{67}\sigma_{12}\sigma_{45} - \sigma_{67}\sigma_{24}\sigma_{15} - \sigma_{12}\sigma_{47}\sigma_{56}$,
  $\sigma_{67}\sigma_{13}\sigma_{45} - \sigma_{67}\sigma_{34}\sigma_{15} - \sigma_{13}\sigma_{47}\sigma_{56}$,
  $\sigma_{67}\sigma_{23}\sigma_{45} - \sigma_{67}\sigma_{34}\sigma_{25} - \sigma_{23}\sigma_{47}\sigma_{56}$.

Conclusion

- Latent variable models generally feature complicated geometry.
- Even in "simple" factor analysis models there is still lots to explore ...
- Circular term order is not delightful for "overlap $= 3$" ...
- What about $|\mathcal{H}| \geq 3$?

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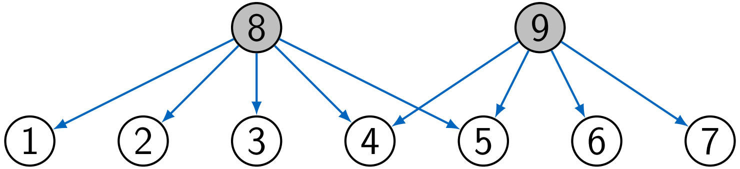
Appendix: Example



Singletons:

$\sigma_{16}, \quad \sigma_{26}, \quad \sigma_{36}, \quad \sigma_{17}, \quad \sigma_{27}, \quad \sigma_{37}.$

Tetrads:

- $A = \{1, 2\}$ and $B = \{4, 5\}$. Then $\text{pa}(A) \cap \text{pa}(B) = \{8\}$ and $\sigma_{14}\sigma_{25} - \sigma_{24}\sigma_{15} \in S^{\leq 1}(G)$.
- $A = \{1, 4\}$ and $B = \{2, 5\}$. Then $\text{pa}(A) \cap \text{pa}(B) = \{8, 9\}$ and $\sigma_{12}\sigma_{45} - \sigma_{24}\sigma_{15} \notin S^{\leq 1}(G)$.