Nested Covariance Determinants in Gaussian Graphical Models

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joint work with Mathias Drton and Luca Weihs
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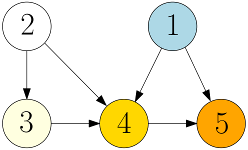
Directed graphical models

Let $G = (V, E)$ be a directed acyclic graph.



The distribution of a random vector $X = (X_1, X_2, X_3, X_4, X_5) \in \prod_{i=1}^{5} \mathcal{X}_i$ with density p lies in the graphical model corresponding to G if

- **Factorization**

$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_2)p(x_3|x_2)p(x_4|x_1, x_2, x_3)p(x_5|x_1, x_4).$$

- **Markov properties**

$$X_1 \perp\!\!\!\perp X_2; \;\; X_2 \perp\!\!\!\perp X_5 | X_1, X_4; \;\; X_3 \perp\!\!\!\perp X_5 | X_1, X_4,$$

  which come from the d-separation statements $1 \perp_d 2; \;\; 2 \perp_d 5|1, 4; \;\; 3 \perp_d 5|1, 4.$

Directed Gaussian graphical models

Let $X \sim \mathcal{N}(\mu, \Sigma)$. When does the distribution of X lie in the model $\mathcal{M}_G$ of Gaussian distributions corresponding to a DAG $G = (V, E)$?

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- d-separation yields: $a \perp_d b | C \implies X_a \perp\!\!\!\perp X_b | X_C \iff |\Sigma_{aC,bC}| = 0$, and

$$\mathcal{M}_G = \{\Sigma \succ 0 \ : \ |\Sigma_{aC,bC}| = 0 \text{ for all } a \perp_d b|C\}.$$

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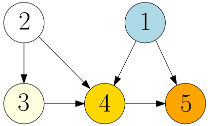

$$1 \perp_d 2; \ \ 2 \perp_d 5 | 1, 4; \ \ 3 \perp_d 5 | 1, 4$$
$$\mathcal{M}_G = \{\Sigma \succ 0 : \Sigma_{12} = 0, \ |\Sigma_{214,514}| = 0, \ |\Sigma_{314,514}| = 0\}.$$

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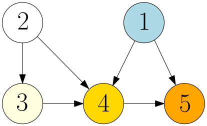

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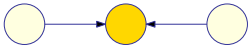
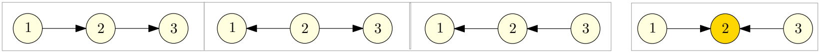
- $\mathcal{M}_G = \mathcal{M}_H$ if and only if G and H have the same skeleton and the same unshielded colliders. 



Directed Gaussian graphical models

$X \sim \mathcal{N}(\mu, \Sigma)$ lies in the model with DAG $G = (V, E)$ if and only if

$$X_i = \sum_{j \in \mathrm{pa}(i)} \lambda_{ji} X_j + \epsilon_i, \quad \text{where } \epsilon \sim \mathcal{N}(\nu, \Omega), \text{ and } \Omega = \mathrm{diag}(\omega_1, \ldots, \omega_n).$$

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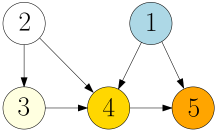

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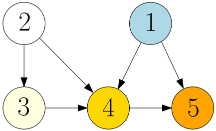

$$\begin{aligned} X_1 &= \epsilon_1 \\ X_2 &= \epsilon_2 \\ X_3 &= \lambda_{23} X_2 + \epsilon_3 \\ X_4 &= \lambda_{14} X_1 + \lambda_{24} X_2 + \lambda_{34} X_3 + \epsilon_4 \\ X_5 &= \lambda_{15} X_1 + \lambda_{45} X_4 + \epsilon_5 \end{aligned}$$

Let

$$\Lambda = \begin{pmatrix} 0 & 0 & 0 & \lambda_{14} & \lambda_{15} \\ 0 & 0 & \lambda_{23} & \lambda_{24} & 0 \\ 0 & 0 & 0 & \lambda_{34} & 0 \\ 0 & 0 & 0 & 0 & \lambda_{45} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^E, \quad \Omega = \begin{pmatrix} \omega_1 & 0 & 0 & 0 & 0 \\ 0 & \omega_2 & 0 & 0 & 0 \\ 0 & 0 & \omega_3 & 0 & 0 \\ 0 & 0 & 0 & \omega_4 & 0 \\ 0 & 0 & 0 & 0 & \omega_5 \end{pmatrix} \succ 0.$$

Then,

$$X = \Lambda^T X + \epsilon \iff X = (I - \Lambda)^{-T} \epsilon,$$

and,

$$\Sigma = (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1}.$$

Directed Gaussian graphical models

The **directed Gaussian graphical model corresponding to a DAG** $G = (V, E)$ is

$$\mathcal{M}_G = \{\Sigma \ : \ \Sigma = (I - \Lambda)^{-T}\Omega(I - \Lambda)^{-1}, \ \Lambda \in \mathbb{R}^E, \Omega \succ 0 \text{ diagonal}\}.$$

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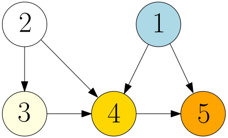
- What happens if we introduce hidden variables?

Introducing hidden variables



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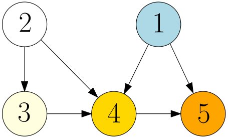

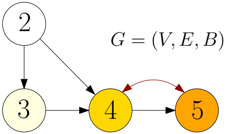

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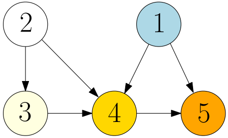

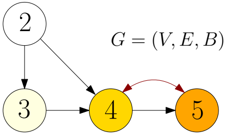

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$$\Sigma = (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1},$$

$$\text{where } \Lambda = \begin{pmatrix} 0 & 0 & 0 & \lambda_{14} & \lambda_{15} \\ 0 & 0 & \lambda_{23} & \lambda_{24} & 0 \\ 0 & 0 & 0 & \lambda_{34} & 0 \\ 0 & 0 & 0 & 0 & \lambda_{45} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^E,$$

$$\Omega = \begin{pmatrix} \omega_{11} & 0 & 0 & 0 & 0 \\ 0 & \omega_{22} & 0 & 0 & 0 \\ 0 & 0 & \omega_{33} & 0 & 0 \\ 0 & 0 & 0 & \omega_{44} & 0 \\ 0 & 0 & 0 & 0 & \omega_{55} \end{pmatrix} \succ 0.$$

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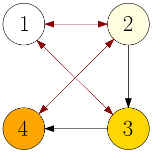
Mixed Gaussian Graphical Models



Given a *mixed graph* $G = (V, E, B)$, take

$$\Lambda = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_{23} & 0 \\ 0 & 0 & 0 & \lambda_{34} \\ 0 & 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^E, \ \Omega = \begin{pmatrix} \omega_{11} & \omega_{12} & \omega_{13} & 0 \\ \omega_{12} & \omega_{22} & 0 & \omega_{24} \\ \omega_{13} & 0 & \omega_{33} & 0 \\ 0 & \omega_{24} & 0 & \omega_{44} \end{pmatrix} \in PD_B.$$

The **mixed Gaussian graphical model corresponding to $G = (V, E, B)$ is**

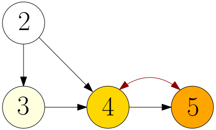
$$\mathcal{M}_G = \{\Sigma \succ 0 \ : \ \Sigma = (I - \Lambda)^{-T}\Omega(I - \Lambda)^{-1}, \ \Lambda \in \mathbb{R}^E, \Omega \in \mathrm{PD}_B\}.$$

Questions:

- How can we describe $\mathcal{M}_G$? Are CI relations/d-separation enough?
- When is $\mathcal{M}_G = \mathcal{M}_H$?

Trek separation

- Conditional independence is not enough:



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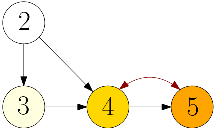

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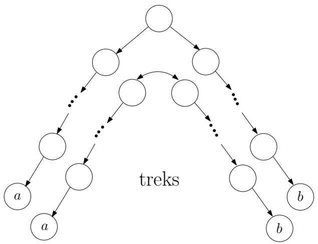
- **Trek separation** is a combinatorial criterion for when we have determinantal constraints.

[Sullivant, Talaska, Draisma 2010]

Trek separation



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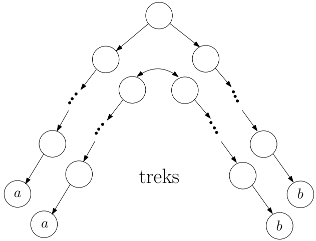
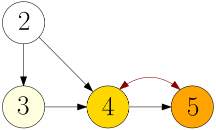


Definition (Sullivant, Talaska, Draisma, 2010)

The sets A and B are trek separated by (E, F) if every trek between $a \in A$ and $b \in B$ intersects either E on the left or F on the right.

Example



$\{2, 3\}$ and $\{4, 5\}$ are trek separated by $(\emptyset, \{4\})$.

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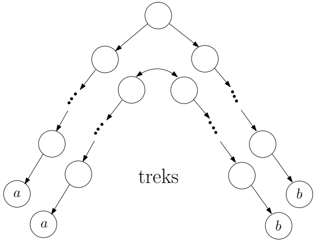

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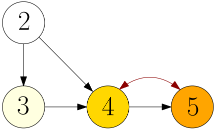

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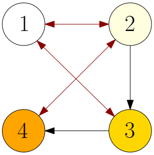
Thus, $|\Sigma_{23,45}| = 0$.

Theorem (Sullivant, Talaska, Draisma, 2010)

For every $A, B \subseteq V$, the submatrix $\Sigma_{A,B}$ has rank at most r if and only if there exist sets $E, F \subseteq V$ such that $|E| + |F| \leq r$ and (E, F) trek-separates *A and B.*

Trek separation might not be enough to describe $\mathcal{M}_G$

- No CI relations and no trek separation:



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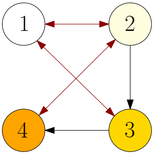

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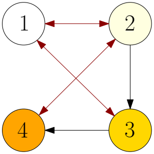

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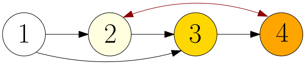

Verma graph

$$\mathcal{M}_G = \{\Sigma \succ 0 \ : \ f_{\text{Verma}}(\Sigma) = 0\},$$

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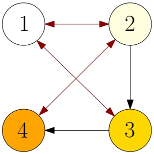

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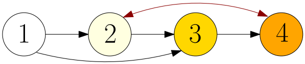

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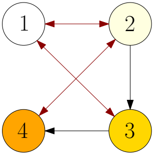
$$f_{Verma}(\Sigma) = \sigma_{11}\sigma_{13}\sigma_{22}\sigma_{34} - \sigma_{11}\sigma_{13}\sigma_{23}\sigma_{24} - \sigma_{11}\sigma_{14}\sigma_{22}\sigma_{33}$$
$$+\sigma_{11}\sigma_{14}\sigma_{23}^2 - \sigma_{12}^2\sigma_{13}\sigma_{34} + \sigma_{12}^2\sigma_{14}\sigma_{33} + \sigma_{12}\sigma_{13}^2\sigma_{24} - \sigma_{12}\sigma_{13}\sigma_{14}\sigma_{23}.$$

Nested determinants

- Constraints are determinants of compound matrices.



$$f(\Sigma) = \begin{vmatrix} |\Sigma_{23,23}| & |\Sigma_{23,24}| \\ \Sigma_{1,3} & \Sigma_{1,4} \end{vmatrix}.$$

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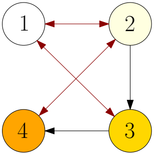

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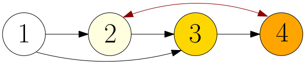

Verma graph

$$f_{\mathsf{Verma}}(\Sigma) = \begin{vmatrix} |\Sigma_{123,123}| & |\Sigma_{123,124}| \\ \Sigma_{1,3} & \Sigma_{1,4} \end{vmatrix}$$

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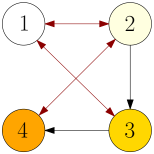

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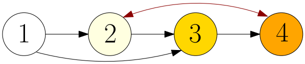

Verma graph

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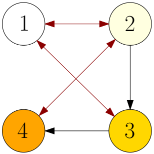
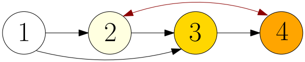
$$= \begin{vmatrix} |\Sigma_{123,134}| & |\Sigma_{123,234}| \\ \Sigma_{1,1} & \Sigma_{1,2} \end{vmatrix} = \begin{vmatrix} |\Sigma_{12,12}| & |\Sigma_{12,13}| \\ |\Sigma_{34,12}| & |\Sigma_{34,13}| \end{vmatrix}$$

Nested determinants

- Constraints are determinants of compound matrices.



$$f(\Sigma) = \begin{vmatrix} |\Sigma_{23,23}| & |\Sigma_{23,24}| \\ \Sigma_{1,3} & \Sigma_{1,4} \end{vmatrix}.$$



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- Can we give a combinatorial criterion for when this happens?
- Are these equations enough to describe the model $\mathcal{M}_G$?

Parentally nested determinants

For $i, j \in V$, $i \neq j$, define the **parentally nested determinant**

$$f_{ij} := \left| \left(|\Sigma_{\mathrm{pa}(r)\cup\{r\},\mathrm{pa}(r)\cup\{c\}}| \right)_{r\in\mathrm{pa}(i)\cup\{j\},c\in\mathrm{pa}(i)\cup\{i\}} \right|.$$

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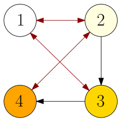
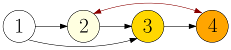


$$f(\Sigma) = \begin{vmatrix} \frac{|\Sigma_{23,23}|}{\Sigma_{1,3}} & \frac{|\Sigma_{23,24}|}{\Sigma_{1,4}} \end{vmatrix} = f_{41}.$$



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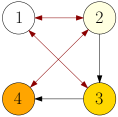

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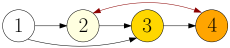

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Proposition (Drton, Robeva, Weihs 2018)

Let i and j be vertices of the mixed graph $G = (V, E, B)$ such that

1. $pa(i) \cap sib(i) = \emptyset$,
2. *all vertices in $pa(i)$ are* **ancestral**, *and*
3. $j \in V \setminus (pa(i) \cup sib(i) \cup \{i\})$.

Then the parentally nested determinant f_{ij} vanishes on $\mathcal{M}(G)$.

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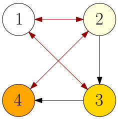

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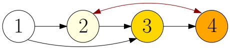

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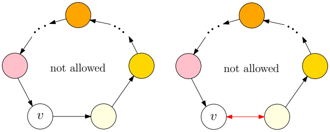
A vertex v is **ancestral** if it does not lie on a cycle, and no sibling of v has a directed path to v.



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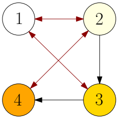

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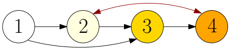

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Parentally nested determinants

Theorem (Drton, Robeva, Weihs 2018)

If $G = (V, E, B)$ *is* **globally identifiable** *and* **almost ancestral**, *then*

$$\mathcal{M}_G = \{\Sigma \succ 0 \ : \ f_{ij}(\Sigma) = 0, \ \forall j \text{ ancestral and } i \neq j\}.$$

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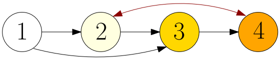
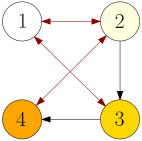




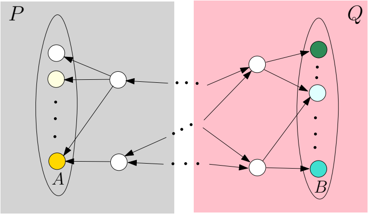
A mixed graph $G = (V, E, B)$ is **almost ancestral** if all of its vertices except for potentially the last one in topological order are ancestral.

A mixed graph $G = (V, E, B)$ is **globally identifiable** if the map

$$(\Lambda, \Omega) \mapsto \Sigma = (I - \Lambda)^{-T}\Omega(I - \Lambda)^{-1}$$

is injective.

Restricted trek separation



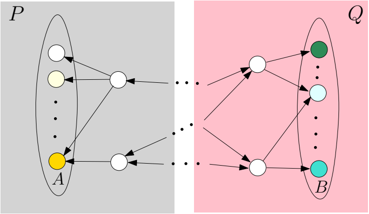
(P, Q)-Restricted Trek Separation

Definition

Let $G = (V, E, B)$ be an acyclic mixed graph. Let $A, B, P, Q, E, F \subseteq V$.

- A trek between $a \in A$ and $b \in B$ is a (P, Q)-*restricted trek* if all vertices on its left lie in P and all vertices on its right lie in Q.
- A and B are *(P, Q)-restricted trek separated by* (E, F) if every (P, Q)-restricted trek between A and B intersects E on left or F on right.

Restricted trek separation



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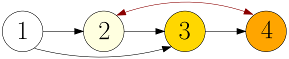

Let $A = \{2, 3\}$, $B = \{2, 4\}$, $P = \{2, 3, 4\}$, $Q = \{2, 4\}$. Then, A and B are (P, Q)-restricted trek separated by $(\{2\}, \emptyset)$.

Restricted trek separation

Proposition (Drton, Robeva, Weihs 2018)

Let $G = (V, E, B)$ *be an acyclic mixed graph. Let* $\Lambda \in \mathbb{R}^E$, $\Omega \in PD_B$*. For* $P, Q \subseteq V$*, consider the matrix*

$$\Sigma^{(P,Q)} = [(I - \Lambda)_{P,P}]^{-T} \Omega_{P,Q} [(I - \Lambda)_{Q,Q}]^{-1}.$$

Then, for $A, B \subseteq V$*, the submatrix* $\Sigma^{(P,Q)}_{A,B}$ *has rank at most*

$$\min\{|E| + |F| : A \text{ and } B \text{ are } (P, Q)\text{-restricted trek separated by } (E, F)\},$$

and is equal to this minimum generically.

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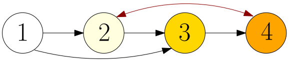

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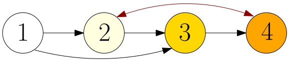
$$\Sigma^{(234,24)}_{23,24} \text{ has rank at most } 1.$$

Restricted trek separation

Theorem (Drton, Robeva, Weihs 2018)

If $A = \{a_1, \ldots, a_n\}$ and $B = \{b_1, \ldots, b_n\}$ are (P, Q)-restricted trek separated, then, under some conditions* *there are sets $C_{ij}, D_{ij} \subseteq V$, such that the matrix with entries $|\Sigma_{C_{ij} \cup \{a_i\}, D_{ij} \cup \{b_j\}}|$ has zero determinant.*



Let $A = \{2, 3\}$, $B = \{2, 4\}$, $P = \{2, 3, 4\}$, $Q = \{2, 4\}$. Then, A and B are (P, Q)-restricted trek separated by $(\{2\}, \emptyset)$, yielding

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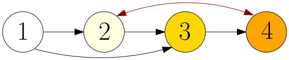

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Corollary

If $G = (V, E, B)$ is globally identifiable and almost ancestral, then the vanishing of the parentally nested determinants $f_{ij}(\Sigma) = \left|(|\Sigma_{pa(r)\cup\{r\}, pa(r)\cup\{c\}}|)_{r \in pa(i)\cup\{j\}, c \in pa(i)\cup\{i\}}\right|$ follows from restricted trek separation.

Remaining questions

- Is restricted trek separation enough to describe $\mathcal{M}_G$ in general?

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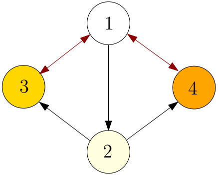
- Recursive nesting:



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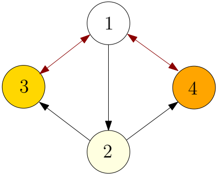

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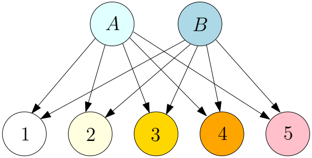
- Other hidden variable models?



$$f = \begin{vmatrix} |\Sigma_{23,45}| & |\Sigma_{25,34}| \\ |\Sigma_{123,145}| & |\Sigma_{125,134}| \end{vmatrix}.$$

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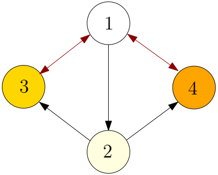

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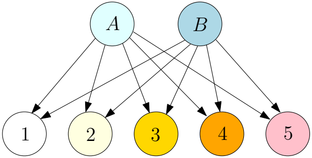

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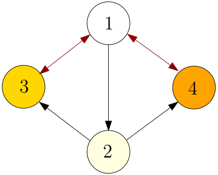

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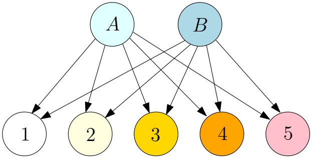

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Thank you!