Hidden Variables in Linear Non-Gaussian Causal Models

Elina Robeva
The University of British Columbia

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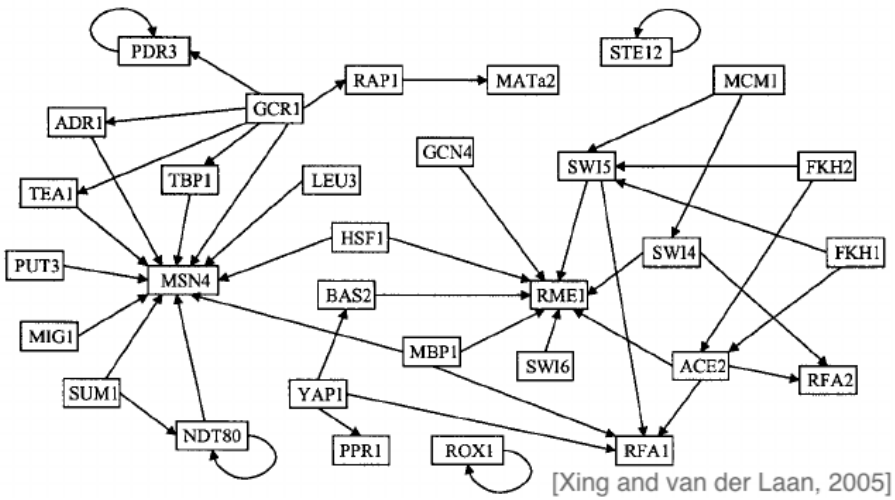
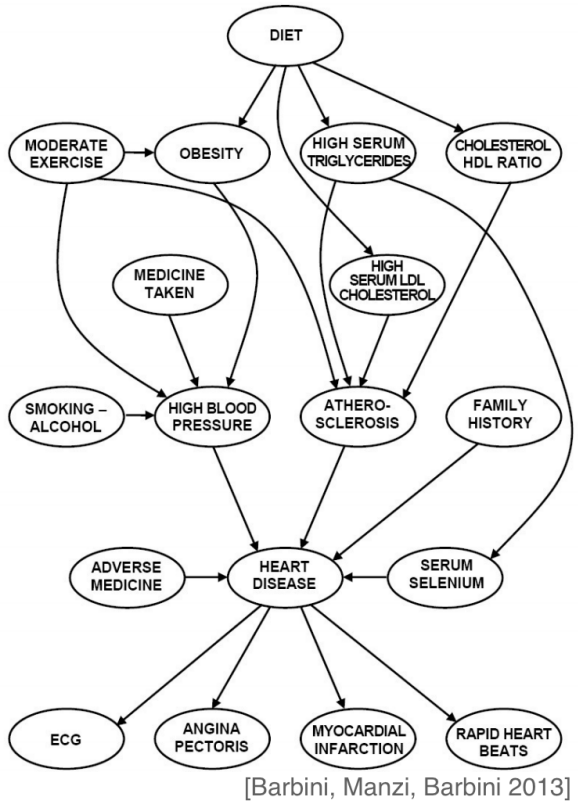
Causal models



Gene regulatory networks



Disease diagnosis graphs

How can we learn the structure of these graphs from observations?

Structural equation models

Definition

A *structural equation model* consists of a directed acyclic graph (DAG) $G = (V, E)$, and a set of equations between random variables $\{X_v : v \in V\}$:

$$X_v = f_v(X_{\mathrm{pa}(v)}, \varepsilon_v), \ v \in V$$

where $X_{\mathrm{pa}(v)} = (X_u : u \to v \in E)$ and ε_v is noise such that $\{\varepsilon_v : v \in V\}$ are independent noise terms.

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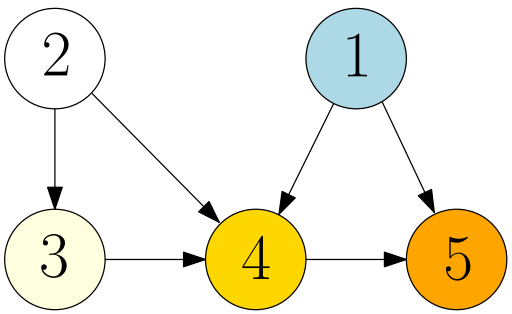

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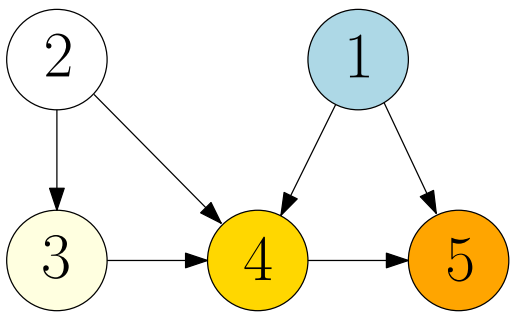

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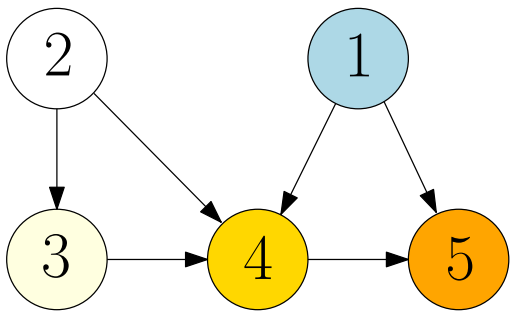

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- Linear structural equation models

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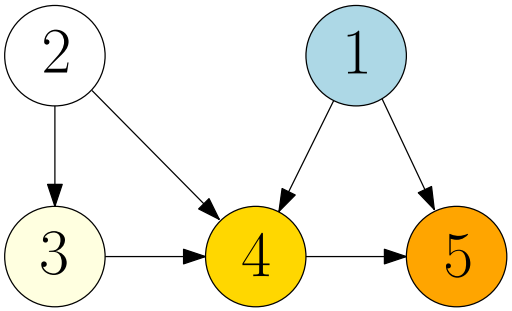

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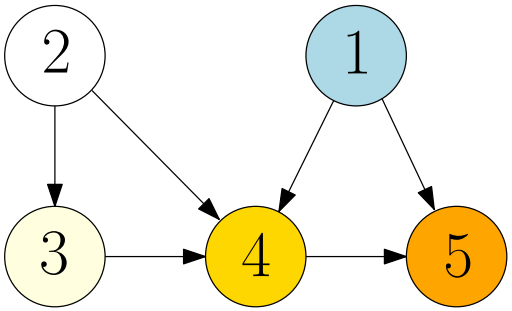

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For a general directed acyclic graph $G = (V, E)$, the *linear structural equation model corresponding to* G consists of the the graph G and the linear equations

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X_i = \sum_{j \in \mathrm{pa}(i)} \lambda_{ji} X_j + \varepsilon_i, \qquad \text{where the variables } \{\varepsilon_i\}_{i \in V} \text{ are independent.}
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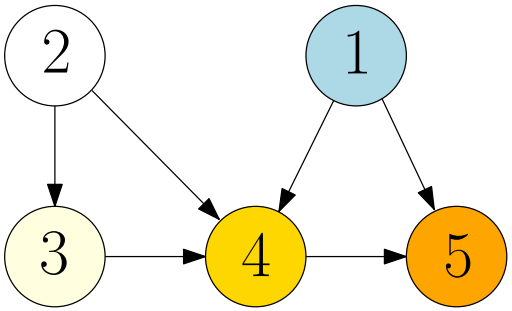

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In matrix-vector form

$$
X = \Lambda^T X + \varepsilon.
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Equivalently,

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X = (I - \Lambda)^{-T} \varepsilon.
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Linear Gaussian models

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

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Thus, $X \sim \mathcal{N}(\mu, \Sigma)$, where

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

The set of distributions $\mathcal{M}_G$ arising from a Gaussian linear causal model with DAG $G = (V, E)$ is called the **directed Gaussian graphical model corresponding to G**, and

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

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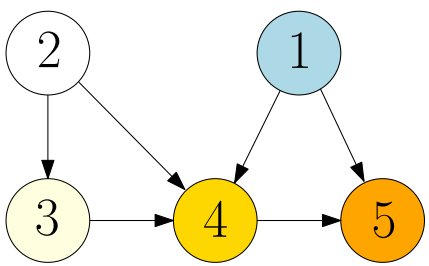

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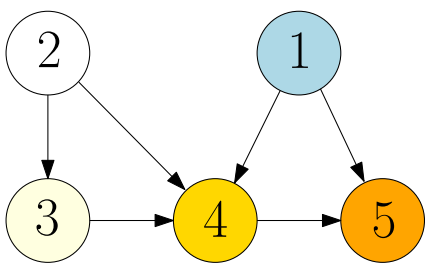

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- Markov equivalence: $\mathcal{M}_G = \mathcal{M}_H \implies$ cannot identify the graph G uniquely.

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Theorem (Comon and Jutten, *Handbook of Blind Source Separation*, 2010)

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- ICA Methods: maximum likelihood estimation, 4th order cumulant tensor decomposition, maximizing |kurtosis| of $A^{-1}X$ (a measure of non-Gaussianity)

Linear Non-Gaussian Acyclic Models (LiNGAM)

$$X = (I - \Lambda)^{-T} \varepsilon.$$

- Shimizu et al., 2006: LiNGAM; use ICA methods; estimate of $(I - \Lambda)$ has all entries non-zero
- Shimizu et al., 2011: Direct-LiNGAM; a source node is independent from regression residuals; does not work if #observations $<$ #variables (high-dimensions)
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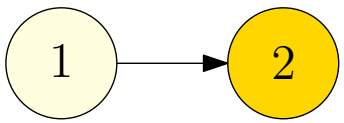

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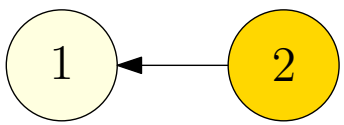


$$\mathbb{E}[X_1X_2]\mathbb{E}[X_1^3] - \mathbb{E}[X_1^2]\mathbb{E}[X_1^2X_2] \neq 0$$

generically, in particular, third order moments need to be non-Gaussian.

Looking at higher moments

$$X = (I - \Lambda)^{-T}\varepsilon.$$

Definition

The *linear structural equation model* $\mathcal{M}^{(2,3)}(G)$ of second and third order moments corresponding to a DAG $G = (V, E)$ with $|V| = n$ is defined as

$$\begin{aligned}\mathcal{M}^{(2,3)}(G) = \{(S = (I - \Lambda)^{-T}\Omega^{(2)}(I - \Lambda)^{-1}, \\ T = \Omega^{(3)} \bullet (I - \Lambda)^{-1} \bullet (I - \Lambda)^{-1} \bullet (I - \Lambda)^{-1}) : \\ \Omega^{(2)} \text{ is } n \times n \text{ positive definite diagonal matrix}, \\ \Omega^{(3)} \text{ is } n \times n \times n \text{ diagonal 3-way tensor, and } \Lambda \in \mathbb{R}^E\}.\end{aligned}$$

Here, $\bullet$ denotes the *Tucker product*.

Theorem (Améndola, Drton, Grosdos, Homs-Pons, and R., 2021+)

The set of second and third order moments (T, S) of a linear non-Gaussian causal model corresponding to a tree DAG are precisely the ones that satisfy certain quadratic binomials which arise as the 2×2 minors of certain matrices constructed from the DAG.

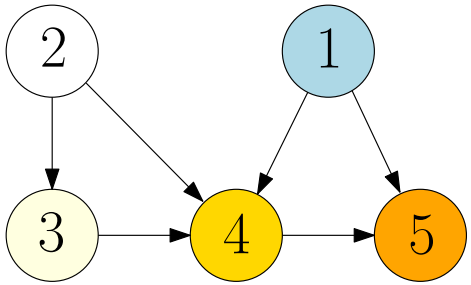
- $s_{ij} = 0$ for all $i, j \in V$ for which there is no 2-trek between i and j;
- $t_{ijk} = 0$ for all $i, j, k \in V$ for which there is no 2-trek between i, j, k;
- the 2×2 minors of the matrix A_{ij} are 0 whenever there is a path from i to j, where

$$A_{ij} = \begin{bmatrix} s_{ik_1} & \cdots & s_{ik_r} & t_{i\ell_1 m_1} & \cdots & t_{i\ell_q m_q} \\ s_{jk_1} & \cdots & s_{jk_r} & t_{j\ell_1 m_1} & \cdots & t_{j\ell_q m_q} \end{bmatrix},$$

where

  - $k_1, \ldots, k_r$ are all vertices such that $\text{top}(i, k_a) = \text{top}(j, k_a)$ and
  - $(l_1, m_1), \ldots, (l_q, m_q)$ are all pairs of vertices such that $\text{top}(i, l_b, m_b) = \text{top}(j, l_b, m_b)$.

Introducing hidden variables



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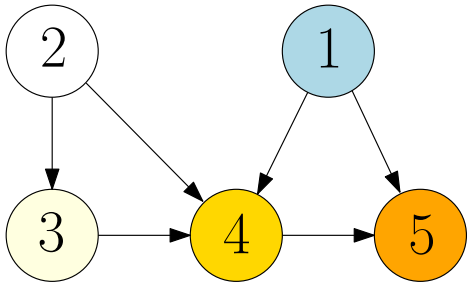

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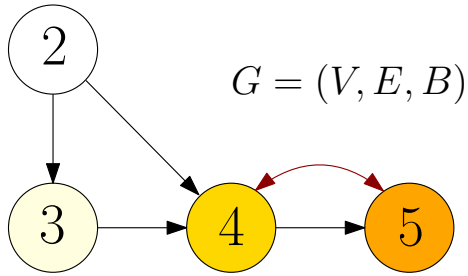

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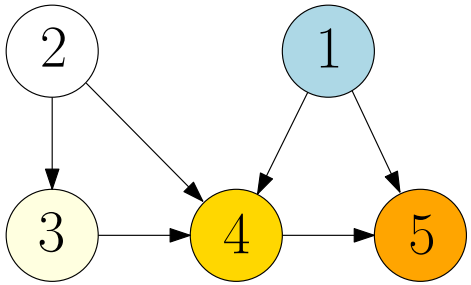

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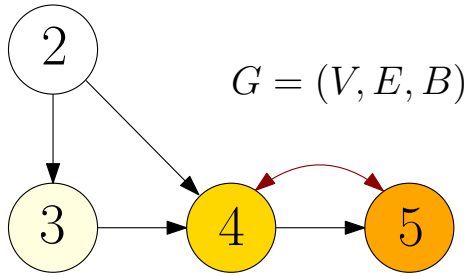

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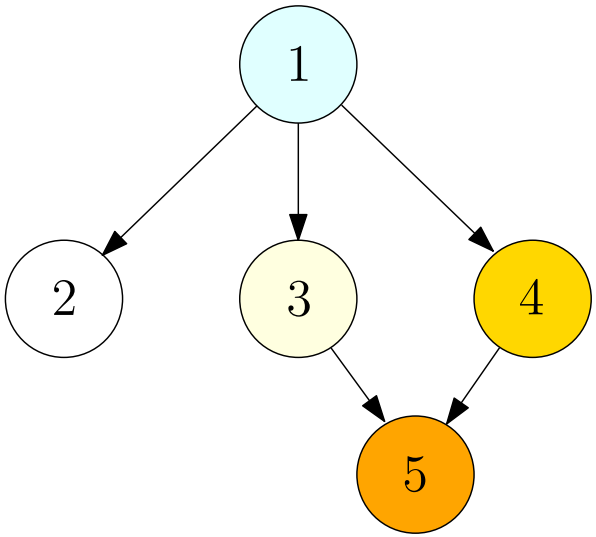

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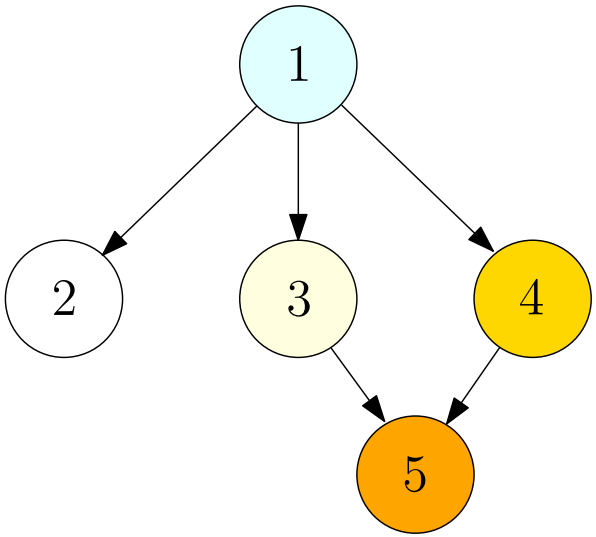

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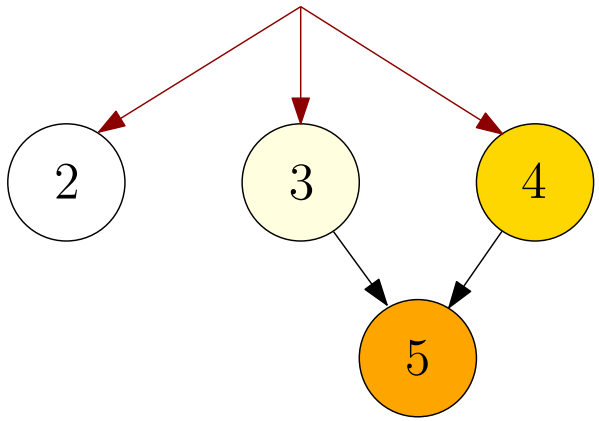

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where $\varepsilon_5 \perp\!\!\!\perp \tilde{\varepsilon}_2, \tilde{\varepsilon}_3, \tilde{\varepsilon}_4$.

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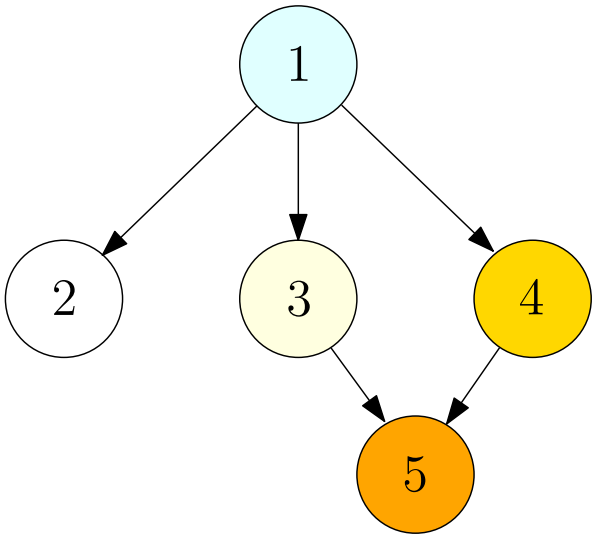

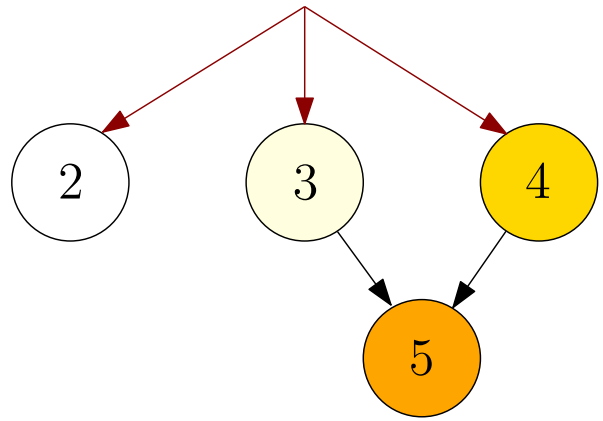

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The new graph $G = (V, E, H)$ has directed edges E and *multi-directed edges* H.

Learning LiNGAMs with hidden variables from observational data

Existing methods for learning $G = (V, E, H)$ either

- Use ICA methods (Hoyer et al., 2008), which don't guarantee convergence to a global optimum, OR
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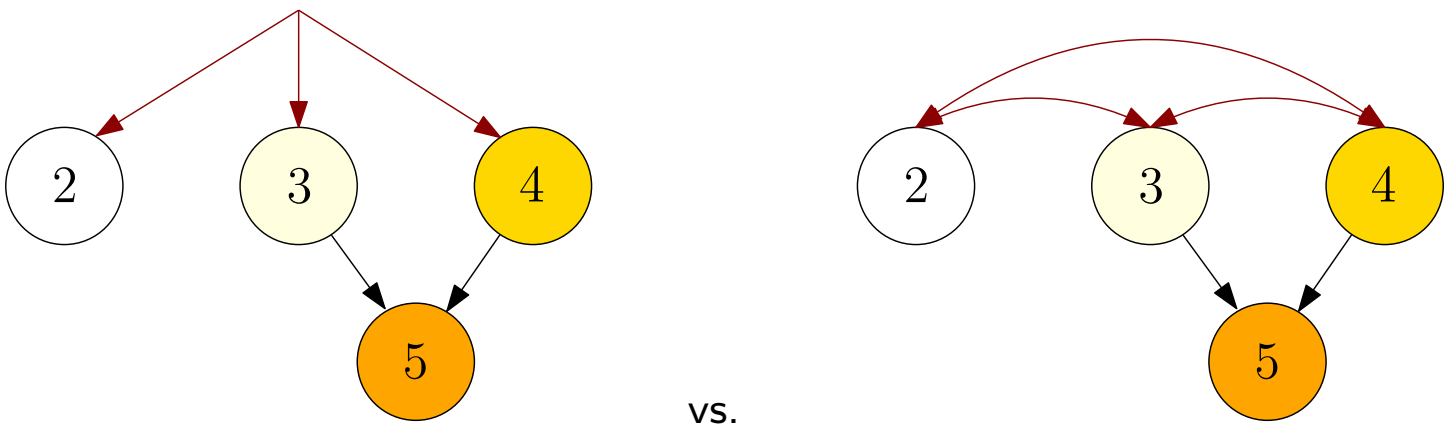

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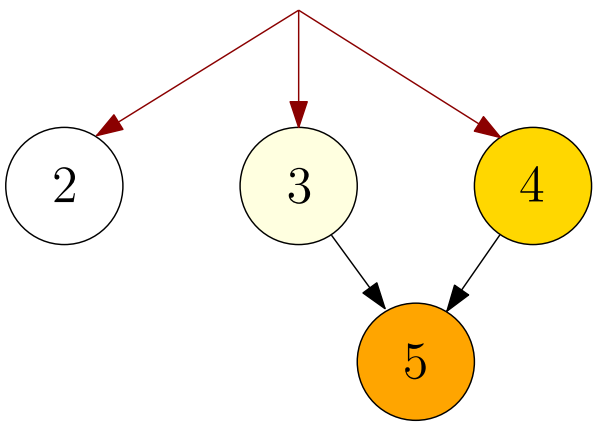

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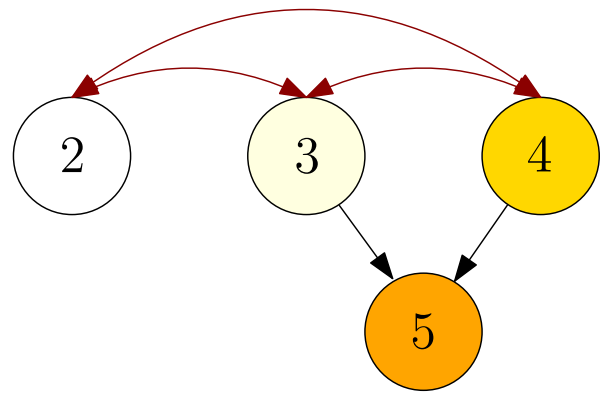

- (Liu, Robeva, Wang, 2020): Learn $G = (V, E, H)$, where H has multidirected edges; G is a bow-free acyclic graph; use high-order cumulant information (Robeva, Seby, 2020)

Vanishing of cumulants

- For a zero-mean random vector $X = (X_1, \ldots, X_d)$, its *k-th order cumulant* is an $d \times \cdots \times d$ (k times) tensor $C^{(k)}$ whose entries can be obtained from the moments of X, e.g. for $k = 4$:

$$C^{(4)}_{i_1,i_2,i_3,i_4} = \mathbb{E}[X_{i_1}X_{i_2}X_{i_3}X_{i_4}] - \mathbb{E}[X_{i_1}X_{i_2}]\mathbb{E}[X_{i_3}X_{i_4}] - \mathbb{E}[X_{i_1}X_{i_3}]\mathbb{E}[X_{i_2}X_{i_4}] - \mathbb{E}[X_{i_1}X_{i_4}]\mathbb{E}[X_{i_2}X_{i_3}].$$

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Theorem (Robeva and Seby, 2020)

If X comes from a linear non-Gaussian acyclic model with graph $G = (V, E, H)$ and X has cumulants $C^{(k)}$, then

$$C^{(k)}_{i_1,\ldots,i_k} = 0$$

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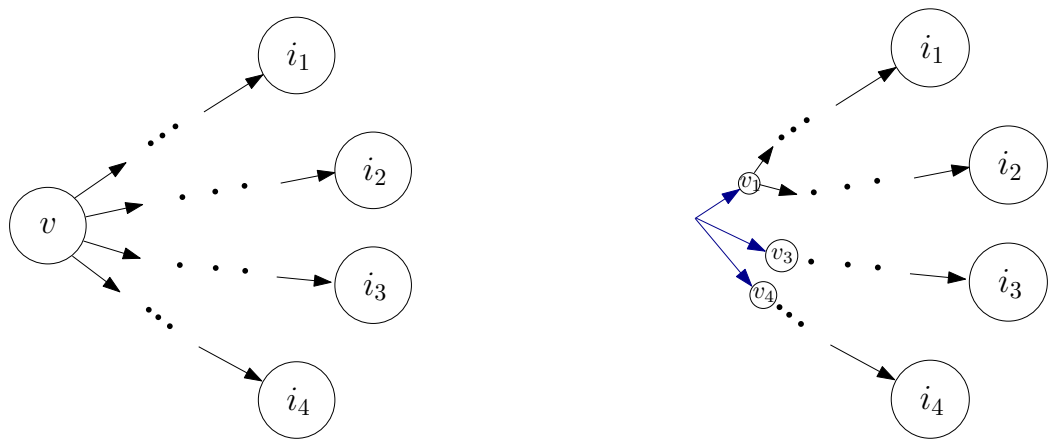

k-treks

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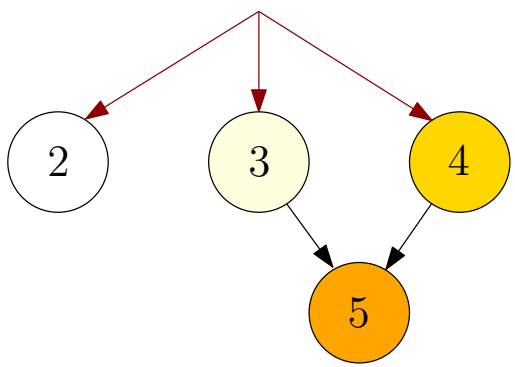
- Thus, we can distinguish:



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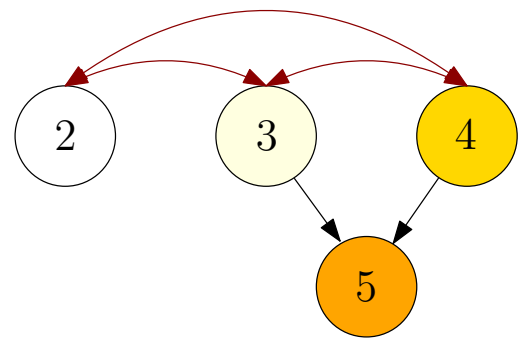
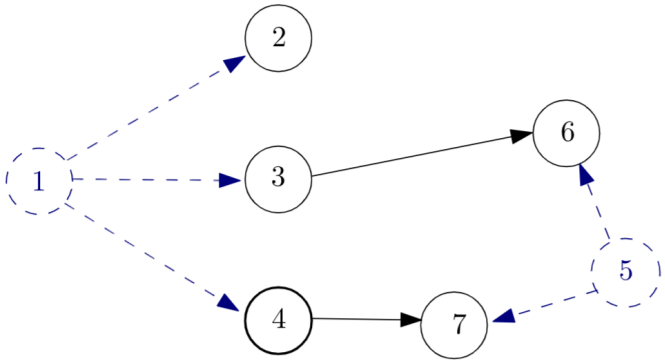


$C^{(3)}_{2,3,4} \neq 0$ $\qquad$ $C^{(3)}_{2,3,4} = 0.$

- Get and algorithm to learn $G = (V, E, H)$ based on high-order cumulants.

Learning $G = (V, E, H)$ [Liu, Robeva, Wang, 2020]



1. Obtain samples $Y = (Y^{(1)}, \ldots, Y^{(N)})$ from LiNGAM with unknown $G = (V, E, H)$

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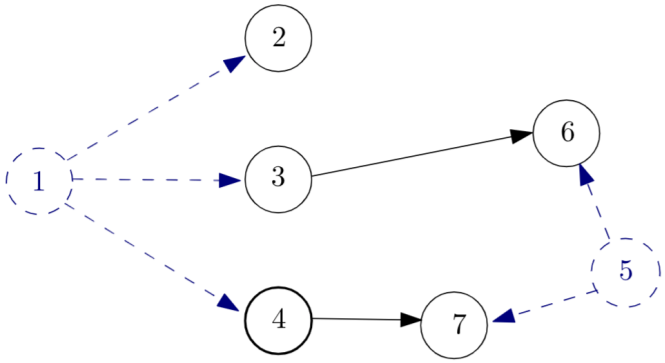

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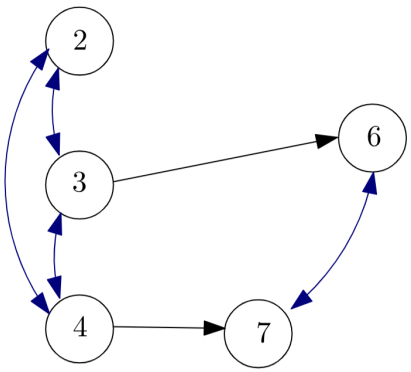

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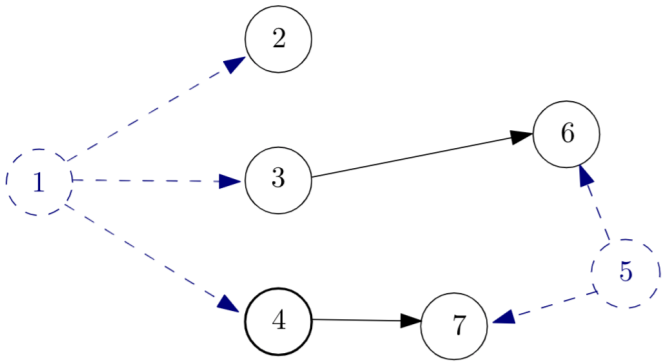

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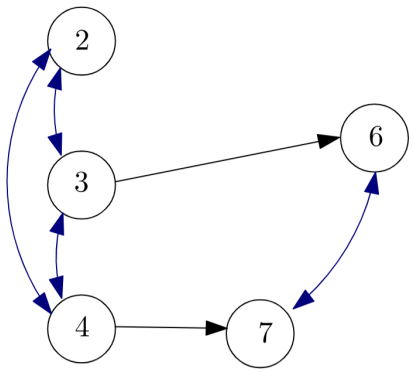

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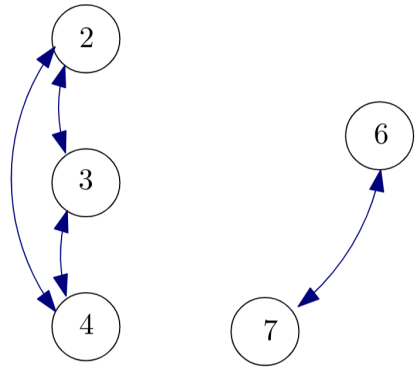

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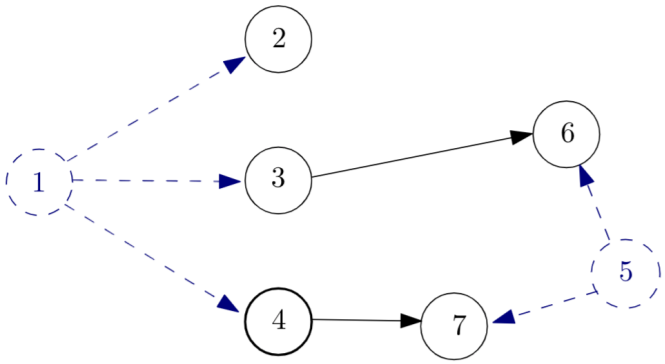

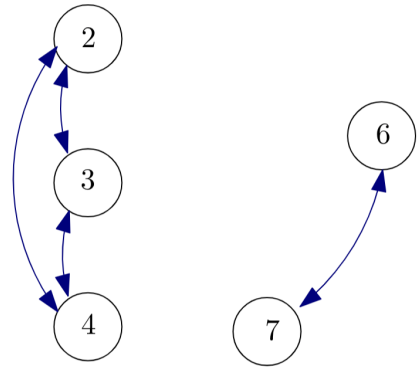

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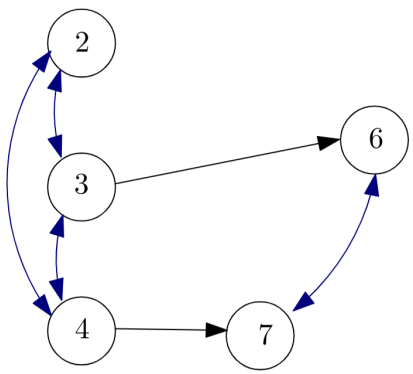

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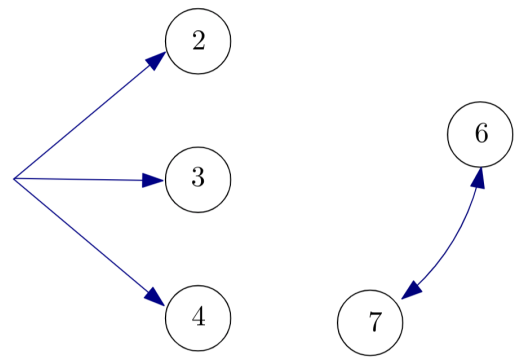

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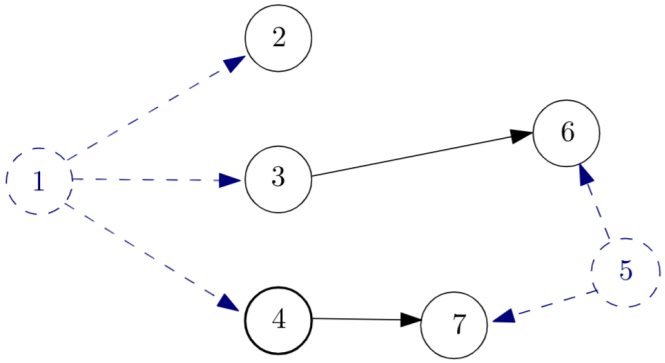

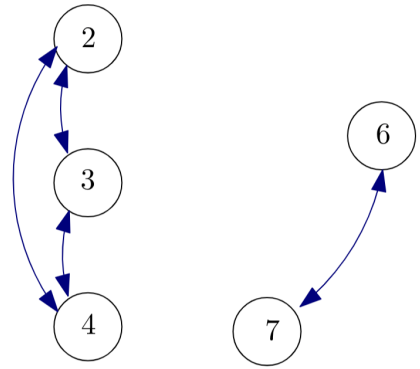

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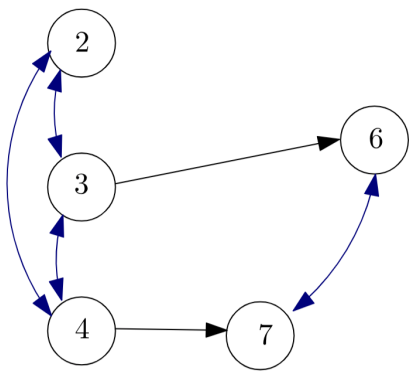

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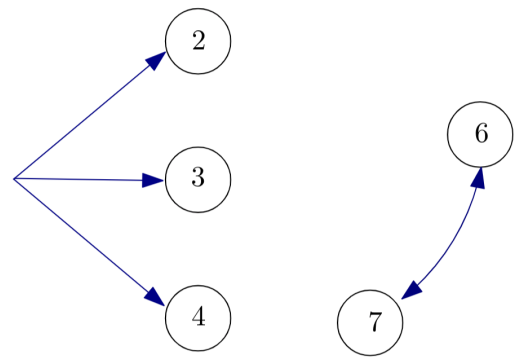

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More algebraic constraints

- (Robeva, Seby, 2020): Characterize vanishing of *determinants of subtensors* of k-th cumulant tensor $C^{(k)}$ in a LiNGAM with graph $G = (V, E, H)$;

$$\det(C^{(k)}_{A_1,\ldots,A_k}) = 0$$

if and only if every system of k-treks between $A_1, \ldots, A_k$ has a sided intersection.

Here:

$$\det(T) = \sum_{\sigma_2,\ldots,\sigma_k \in \mathfrak{S}(d)} \operatorname{sign}(\sigma_2) \cdots \operatorname{sign}(\sigma_k) \prod_{i=1}^{d} T_{i,\sigma_2(i),\ldots,\sigma_k(i)}$$

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- Can we learn such relationships in the case of both cycles and hidden variables?

Thank you!


C. Améndola, M. Drton, A. Grosdos, R. Homs-Pons, and E. Robeva. *Third-order moment varieties of non-Gaussian graphical models*. In preparation.


Y. Liu, E. Robeva, and H. Wang. *Learning Linear Non-Gaussian Graphical Models with Multidirected Edges*. Submitted (2020)


E. Robeva and J.B. Seby. *Multi-trek Separation in Linear Structural Equation Models*. SIAM Journal on Applied Algebra and Geometry (SIAGA) (2021)