Half-Trek Criterion for Identifiability of Latent Variable Models

at 17. Doktorand:innentreffen der Stochastik

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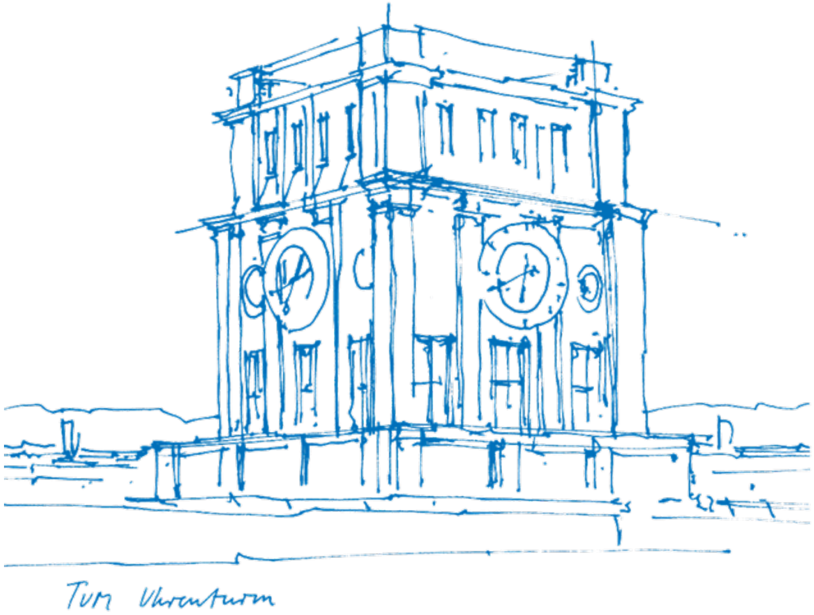
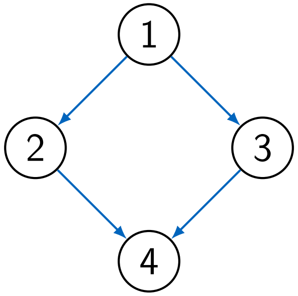
(joint work with Rina Foygel Barber, Mathias Drton, Luca Weihs)



Mathematical Statistics at TUM

About our Research Group

- Chair of Mathias Drton
- Multivariate and high-dimensional Statistics
- Graphical Models and Causality
- Algebraic Statistics



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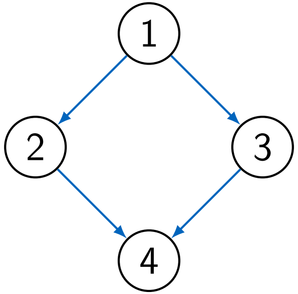


In Klagenfurt...

Philipp Dettling

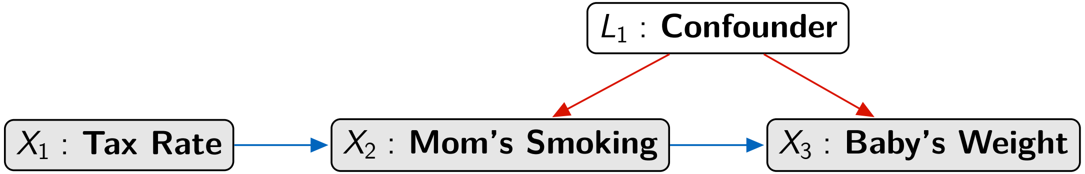
Leopold Mareis

David Strieder

Nils Sturma

Linear Structural Equation/ Causal Models

Each model is induced by a directed graph:



Linear structural equations:

$$
\begin{aligned}
X_1 &= \varepsilon_1, \\
X_2 &= \lambda_{12} X_1 + \gamma_2 L_1 + \varepsilon_2, \\
X_3 &= \lambda_{23} X_2 + \gamma_3 L_1 + \varepsilon_3, \\
L_1 &= \varepsilon_\ell.
\end{aligned}
$$

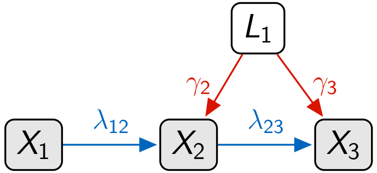
Independent errors:

$$\varepsilon_1 \perp\!\!\!\perp \varepsilon_2 \perp\!\!\!\perp \varepsilon_3 \perp\!\!\!\perp \varepsilon_\ell$$

$$\mathrm{Var}[\varepsilon_v] = \omega_v < \infty$$

Topic of the talk: If L_1 is latent, can we recover the direct effects $(\lambda_{12}, \lambda_{23})$ from $\Sigma = \mathrm{Var}[X]$?

Example: Instrumental Variable Model



$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} 0 & \lambda_{12} & 0 \\ 0 & 0 & \lambda_{23} \\ 0 & 0 & 0 \end{pmatrix}^T \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} + \begin{pmatrix} 0 \\ \gamma_2 \\ \gamma_3 \end{pmatrix} L_1 + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{pmatrix}$$

Observed covariance matrix:

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \cdot & \sigma_{22} & \sigma_{23} \\ \cdot & \cdot & \sigma_{33} \end{pmatrix} = \begin{pmatrix} \omega_1 & \boxed{\omega_1\lambda_{12}} & \boxed{\omega_1\lambda_{12}}\lambda_{23} \\ \cdot & \omega_2 + \gamma_2^2 + \omega_1\lambda_{12}^2 & \gamma_2\gamma_3 + \lambda_{23}\sigma_{22} \\ \cdot & \cdot & \omega_3 + \gamma_3^2 + 2\gamma_2\gamma_3\lambda_{23} + \lambda_{23}^2\sigma_{22} \end{pmatrix}$$

We see that

$$\lambda_{12} = \frac{\sigma_{12}}{\sigma_{11}} \qquad \text{with } \sigma_{11} > 0,$$

$$\lambda_{23} = \frac{\sigma_{13}}{\sigma_{12}} \qquad \text{with } \sigma_{12} = \omega_1\lambda_{12} \neq 0 \text{ ‘almost surely’}.$$

Setup

Variables:

Observed: $X = (X_v)_{v \in V}$ Latent: $L = (L_h)_{h \in \mathcal{L}}$

Graph:

Directed graph $G = (V \dot{\cup} \mathcal{L}, D)$ with directed cycles allowed.

Latent-factor assumption:

All latent variables are latent factors $\equiv$ all nodes in $\mathcal{L}$ are source nodes of G.

Structural equation model:

$$X = \Lambda^\top X + \Gamma^\top L + \varepsilon$$

- all latent factors and error terms in (L, ε) are mutually independent, so $\Omega_{\text{diag}} = \text{Var}[\varepsilon] = \text{diag}(\omega_v : v \in V)$ diagonal, and $\text{Var}[L] = I$ without loss of generality.
- parameter matrices Λ and Γ are sparse and supported over edge set D.

Identifiability

- Every latent-factor graph G yields a parametrization of the observed covariance matrix:

$$\phi_G : (\Lambda, \Gamma, \Omega_{\text{diag}}) \longmapsto \underbrace{(I - \Lambda)^{-\top}(\Omega_{\mathrm{diag}} + \Gamma^\top \Gamma)(I - \Lambda)^{-1}}_{=\Sigma=\text{Var}[X]}.$$

- The model given by G is rationally identifiable if

$$\exists \text{ rational map } \psi_G \ : \quad \psi_G \circ \phi_G(\Lambda, \Gamma, \Omega_{\text{diag}}) = \Lambda \quad \text{for 'almost all'} \ (\Lambda, \Gamma, \Omega_{\text{diag}}).$$

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- The problem may be solved via a Gröbner basis computation. . . on small scale.

- Main Contribution:
  - Sufficient graphical condition for rational identifiability.
  - Recursive polynomial time algorithm.

    (caveat: polynomial time when bounding a matrix rank in a search step)
  - Condition is not necessary but 'effective'; see simulations in paper.

Using Algebraic Relations in Latent Covariance Matrix

- Latent covariance matrix

$$\Omega \;\equiv\; \mathrm{Var}[\Gamma^\top L + \varepsilon] \;=\; \mathrm{Var}[\varepsilon] + \Gamma^\top \mathrm{Var}[L]\Gamma \;=\; \Omega_{\mathrm{diag}} + \Gamma^\top \Gamma.$$

- Observe that

$$\Sigma = (I - \Lambda)^{-\top}\Omega(I - \Lambda)^{-1} \iff \boxed{\Omega \;=\; (I - \Lambda)^T \Sigma (I - \Lambda)}$$

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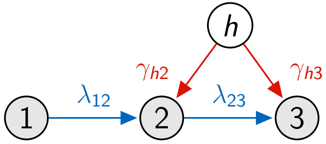
- Algebraic relations between entries of $\Omega = \Omega_{\mathrm{diag}} + \Gamma^\top\Gamma$ yield relations between entries of Λ and Σ:

$$f(\Omega) \;=\; 0 \iff f((I-\Lambda)^T\Sigma(I-\Lambda)) = 0.$$

- Example:

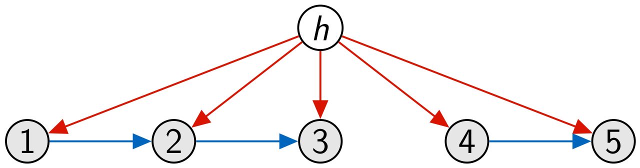


$$\Omega = \begin{pmatrix} \omega_1 & 0 & \mathbf{0} \\ 0 & \omega_2 + \gamma_{h2}^2 & \gamma_{h2}\gamma_{h3} \\ \mathbf{0} & \gamma_{h2}\gamma_{h3} & \omega_3 + \gamma_{h3}^2 \end{pmatrix}$$

$$\left[(I-\Lambda)^T\Sigma(I-\Lambda)\right]_{13} = \sigma_{13} - \lambda_{23}\,\sigma_{12} = 0$$

Latent Low Rank Structure

- Lots of existing work is based on using zero entries in latent covariance matrix.
- However, the resulting methods cannot cover situations such as



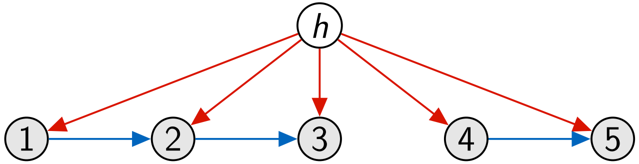
where the latent covariance matrix is dense:

$$\Omega = \Omega_{\text{diag}} + \gamma_h \gamma_h^\top = \text{diagonal} + \text{dense rank 1}.$$

- New paper: Generalize beyond zeros by exploiting

latent low rank structure.

Example: Latent Low Rank Structure



$$\Omega = \begin{pmatrix} \omega_1 & \gamma_{h1}\gamma_{h2} & \gamma_{h1}\gamma_{h3} & \gamma_{h1}\gamma_{h4} & \gamma_{h1}\gamma_{h5} \\ \gamma_{h1}\gamma_{h2} & \omega_2 + \gamma_{h2}^2 & \gamma_{h2}\gamma_{h3} & \gamma_{h2}\gamma_{h4} & \gamma_{h2}\gamma_{h5} \\ \gamma_{h1}\gamma_{h3} & \gamma_{h2}\gamma_{h3} & \omega_3 + \gamma_{h3}^2 & \gamma_{h3}\gamma_{h4} & \gamma_{h3}\gamma_{h5} \\ \gamma_{h1}\gamma_{h4} & \gamma_{h2}\gamma_{h4} & \gamma_{h3}\gamma_{h4} & \omega_4 + \gamma_{h4}^2 & \gamma_{h4}\gamma_{h5} \\ \gamma_{h1}\gamma_{h5} & \gamma_{h2}\gamma_{h5} & \gamma_{h3}\gamma_{h5} & \gamma_{h4}\gamma_{h5} & \omega_5 + \gamma_{h5}^2 \end{pmatrix}$$

Rank-deficient off-diagonal submatrix:

$$\Omega_{\{1,2\},\{3,4\}} = \begin{pmatrix} \gamma_{h1}\gamma_{h3} & \gamma_{h1}\gamma_{h4} \\ \gamma_{h2}\gamma_{h3} & \gamma_{h2}\gamma_{h4} \end{pmatrix} = \begin{pmatrix} \gamma_{h1} \\ \gamma_{h2} \end{pmatrix} \cdot \begin{pmatrix} \gamma_{h3} & \gamma_{h4} \end{pmatrix} \quad \Longrightarrow \quad \det(\Omega_{\{1,2\},\{3,4\}}) = 0.$$

Relations between Λ and Σ:

$$\det\left(\left[(I - \Lambda)^T \Sigma (I - \Lambda)\right]_{\{1,2\},\{3,4\}}\right) = \lambda_{23}\sigma_{12}\sigma_{24} - \lambda_{23}\sigma_{14}\sigma_{22} - \sigma_{13}\sigma_{24} + \sigma_{14}\sigma_{23} = 0.$$

We see that

$$\lambda_{23} = \frac{\sigma_{13}\sigma_{24} - \sigma_{14}\sigma_{23}}{\sigma_{12}\sigma_{24} - \sigma_{14}\sigma_{22}} \qquad \text{with } \sigma_{12}\sigma_{24} - \sigma_{14}\sigma_{22} \neq 0 \text{ 'almost surely'}.$$

New Latent-Factor Half-Trek Criterion: Main Idea

- Digraph $(V \dot\cup \mathcal{L}, D)$ with observed variables in V and latent variables in $\mathcal{L}$.
- Recursive search for linear equation systems that determine columns $\Lambda_{\mathrm{pa}(v),v}$, $v \in V$.

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- To this end, we find a rank-deficient off-diagonal submatrix

$$\Omega_{Y,Z\cup\{v\}} = \left[(I-\Lambda)^T \Sigma (I-\Lambda)\right]_{Y,Z\cup\{v\}} \quad \text{with } |Y| = |Z| + |\text{pa}(v)|.$$

- Our combinatorial conditions ensure a generically unique solution. In particular, we can write $Y = Y_Z \dot{\cup} Y_{\text{pa}(v)}$ such that $\det(\Omega_{Y_Z,Z} \neq 0)$ but

$$\det(\Omega_{Y_Z\cup\{w\},Z\cup\{v\}}) = 0 \quad \text{for all } w \in Y_{\text{pa}(v)}.$$

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- A half-trek from node v to node w is a path of the form:

$$v \to x_1 \to \ldots \to x_\ell \to w \quad \text{or} \quad v \leftarrow \ell \to x_1 \to \ldots \to x_\ell \to w.$$

Relevance: Entries of $(I-\Lambda)^T\Sigma$ are sums over half-treks.

Latent-Factor Half-Trek Criterion (LF-HTC)

Definition

Let $v \in V$ and $Y, Z \subseteq V \setminus \{v\}$ and $H \subseteq \mathcal{L}$. Triple (Y, Z, H) satisfies latent-factor half-trek criterion for v if

(i) $|Y| = |\text{pa}(v)| + |H|$ and $|Z| = |H|$;

(ii) $Y \cap (Z \cup \{v\}) = \emptyset$ and $[\text{pa}_{\mathcal{L}}(Y) \cap \text{pa}_{\mathcal{L}}(Z \cup \{v\})] \subseteq H$;

(iii) There is a system of half-treks from Y to $\text{pa}(v) \cup Z$ without sided intersection and all half-treks ending in Z have form $y \leftarrow \ell \rightarrow z$ for $\ell \in H$.

Theorem

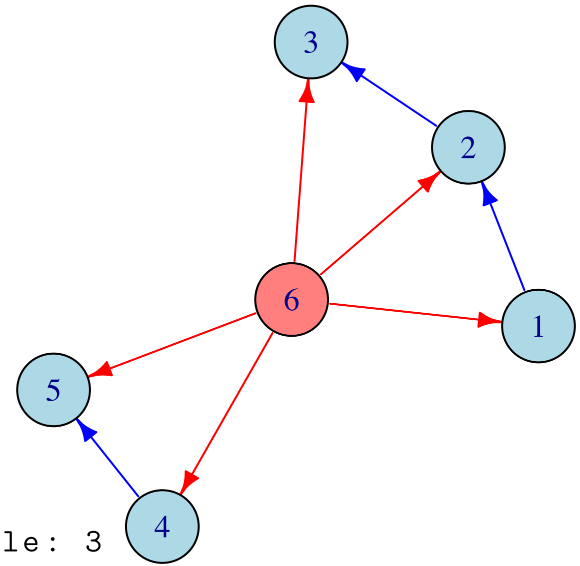
"If the triple (Y, Z, H) satisfies the LF-HTC for $v \in V$ then column $\Lambda_{*,v}$ is a rational function of Σ and certain other columns of Λ."

Our Software: SEMID (R Package)

Algorithm: Recursive Solving.

- Cycle through nodes v and search for LF-HTC triples (Y,Z,H) that allow solving for $\Lambda_{*,v}$.
- Network-flow setup finds LF-HTC triples in polynomial time under a bound on $|Z| = |H|$.

```
> # Define graph
> L = matrix(c(0, 1, 0, 0, 0, 0,
+              0, 0, 1, 0, 0, 0,
+              0, 0, 0, 0, 0, 0,
+              0, 0, 0, 0, 1, 0,
+              0, 0, 0, 0, 0, 0,
+              1, 1, 1, 1, 1, 0), 6, 6, byrow=TRUE)
> observedNodes = seq(1,5)
> latentNodes = c(6)
> g = LatentDigraph(L, observedNodes, latentNodes)
>
> # Check identifiability
> lfhtcID(g)
[1] nr. of edges between observed nodes shown rat. identifiable: 3
[2] rat. identifiable edges: 1->2, 2->3, 4->5
```



Conclusion

- Many applications require modeling effects of latent variables.
- Latent variable models may feature complicated parametrizations and geometry.
- Lots to explore still, in identification and for other problems...

Preprint:

Barber, Drton, Sturma, Weihs (2022).
Half-Trek Criterion for Identifiability of Latent Variable Models. arXiv:2201.04457.