Identifiability of linear structural equation models with homoscedastic errors using algebraic matroids

Jun Wu 1 , Mathias Drton 1 , Benjamin Hollering 2

¹Technical University of Munich, Germany; TUM School of Computation, Information and Technology, Department of Mathematics and Munich Data Science Institute

²Research Group in Nonlinear Algebra, Max Planck Institute for Mathematics in the Sciences

German Probabiliy and Statistics Day, March 2023

つひつ

- [Structural Identifiability](#page-5-0)
- [Jacobian Matroid](#page-8-0)
- [Outdegree Proposition and etc.](#page-13-0)
- [Identifiability Results](#page-18-0)

- 2 [Structural Identifiability](#page-5-0)
- [Jacobian Matroid](#page-8-0)
- [Outdegree Proposition and etc.](#page-13-0)
- [Identifiability Results](#page-18-0)

Random vector $X=(X_i:i\in V)$ solves

$$
X = \Lambda^T X + \varepsilon, \qquad \text{Var}[\varepsilon] = \Omega.
$$

• We consider homoscedastic errors, $\Omega = \omega \cdot I$, and then focus on the precision matrix:

$$
\psi_G(\Lambda, s) = \Sigma^{-1} = s(I - \Lambda)(I - \Lambda)^T, \quad s = \frac{1}{\omega}.
$$

• The linear homoscedastic Gaussian model given by a directed graph $G = (V, D)$ is

$$
M_G = \left\{ s(I - \Lambda)(I - \Lambda)^T : \Lambda \in \mathbb{R}^D_{\text{reg}}, s > 0 \right\},\,
$$

where $\mathbb{R}^D_{\text{reg}} = \big\{\, \Lambda \in \mathbb{R}^{V\times V} : \Lambda_{ij} = 0 \;\; \text{if} \;\; i \to j \notin D, \; l-\Lambda \; \text{invertible} \big\}.$

Linear Structural Equation Models: Example

Example 1

The graph is simple and the SEM is non-recursive (∃ cycle)

2 [Structural Identifiability](#page-5-0)

- [Jacobian Matroid](#page-8-0)
- [Outdegree Proposition and etc.](#page-13-0)
- [Identifiability Results](#page-18-0)

Question: Can two different graphs have the same model?

- Basic case: Markov equivalent classes of DAGs (directed acyclic graphs)
- \bullet Homoscedastic errors: within the class of DAGs, the graph G is known to be identifiable [Chen, Drton, and Wang [2019;](#page-23-1) Peters and Bühlmann [2014\]](#page-23-2)
- Identifiability results when cycles allowed?

Definition

Let $\{M_i\}_{i=1}^k$ be a finite set of algebraic statistic models given by subsets of \mathbb{R}^m . The indices *i*'s are generically identifiable if for each pair of (i_1,i_2) ,

 $\dim(M_{i_1} \cap M_{i_2}) < \max(\dim(M_{i_1}), \dim(M_{i_2}))$.

How to compare two models?

- Traditional method: Groebner basis (equi.)
- We use: Jacobian matroid (suff., related to graphical criteria)

Our contributions

- Derive graphical criteria certifying two simple directed graphs have distinguishable models
- Give subclasses of graphs that are generically identifiable
- **Computational checks for small-size graphs**

For a simple directed graph $G = (V, D)$,

 $\dim(M_G) := \text{rank}(J(\psi_G)) = |D| + 1.$

- 2 [Structural Identifiability](#page-5-0)
- 3 [Jacobian Matroid](#page-8-0)
- [Outdegree Proposition and etc.](#page-13-0)
- [Identifiability Results](#page-18-0)

 \leftarrow

Jacobian: Example

Example 2

 $G = (V, D)$, with $V = \{1, 2, 3, 4\}$ and $D = \{(1, 2), (2, 4), (1, 3), (3, 4)\}$

Figure: Example 2

 $J(\psi_C)$:

$$
\begin{pmatrix} \begin{array}{cccccccccccc} K_{11} & K_{22} & K_{33} & K_{44} & K_{12} & K_{23} & K_{34} & K_{13} & K_{24} & K_{14} \\ 2s\lambda_{12} & 0 & 0 & 0 & -s & 0 & 0 & 0 & 0 & 0 \\ 2s\lambda_{23} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda_{13} \\ 0 & 0 & 2s\lambda_{24} & 0 & 0 & 0 & s\lambda_{34} & 0 & 0 & -s & 0 \\ 0 & 0 & 2s\lambda_{34} & 0 & 0 & s\lambda_{24} & -s & 0 & 0 & 0 \\ 1+\lambda_{12}^2+\lambda_{13}^2 & 1+\lambda_{24}^2 & 1+\lambda_{34}^2 & 1 & -\lambda_{12} & \lambda_{24}\lambda_{34} & -\lambda_{34} & -\lambda_{13} & -\lambda_{24} & 0 \end{array} & \begin{array}{c} K_{11} \\ K_{22} \\ K_{33} \\ K_{44} \\ K_{55} \\ K_{65} \\ K_{75} \\ K_{86} \\ K_{96} \\ K_{10} \\ K_{11} \\ K_{12} \\ K_{13} \\ K_{14} \\ K_{15} \\ K_{16} \\ K_{17} \\ K_{18} \\ K_{19} \\ K_{10} \\ K_{11} \\ K_{12} \\ K_{13} \\ K_{14} \\ K_{15} \\ K_{16} \\ K_{17} \\ K_{18} \\ K_{19} \\ K_{10} \\ K_{11} \\ K_{12} \\ K_{13} \\ K_{14} \\ K_{15} \\ K_{16} \\ K_{17} \\ K_{18} \\ K_{19} \\ K_{10} \\ K_{11} \\ K_{12} \\ K_{13} \\ K_{24} \\ K_{14} \\ K_{25} \\ K_{26} \\ K_{27} \\ K_{28} \\ K_{29} \\ K_{20} \\ K_{21} \\ K_{22} \\ K_{23} \\ K_{24} \\ K_{23} \\ K_{24} \\ K_{25} \\ K_{26} \\ K_{27} \\ K_{28} \\ K_{29} \\ K_{20} \\ K_{21} \\ K_{22} \\ K_{23} \\ K_{24} \\ K_{25} \\ K_{26} \\ K_{2
$$

 $rank(J_{\{44,12,34,13,24\}})=5$

Definition

Suppose $M = \text{Im}(\phi)$ with parametrization $\phi(\theta) = (\phi_1(\theta), \dots, \phi_r(\theta))$. Let

$$
J(\phi) = \left(\frac{\partial \phi_j}{\partial \theta_i}\right), 1 \le i \le d, 1 \le j \le r
$$

be the Jacobian of ϕ . Then the Jacobian matroid of model M is the matroid $\mathcal{M}(\phi) = (E, \mathcal{I})$, where

- \bullet $E = [r]$, the set of column indices
- A set $S \in \mathcal{I} \subseteq 2^\mathsf{E}$ is called an independent set
- The columns of $J(\phi)$ indexed by S are linearly independent over the fraction field $\mathbb{R}(\theta)$

つひひ

Example 3

$$
\phi(t_1, t_2, t_3) = (t_1, -t_1^2, t_1t_2 + t_3^2),
$$

$$
J = \begin{bmatrix} 1 & -2t_1 & t_2 \\ 0 & 0 & t_1 \\ 0 & 0 & 2t_3 \end{bmatrix}.
$$

• $E = \{1, 2, 3\}$

• The independent sets are

 \emptyset , $\{1\}$, $\{2\}$, $\{3\}$, $\{1,3\}$, $\{2,3\}$

←□

Proposition [Hollering and Sullivant [2021\]](#page-23-3)

Let M_1 and M_2 be two parameterized models in \mathbb{R}^m with parameterization ψ_1 and ψ_2 . Assuming without loss of generality that $\dim(M_1) \geq \dim(M_2)$, if there exists a subset S of the columns such that

 $S \in \mathcal{M}(\psi_2) \setminus \mathcal{M}(\psi_1),$

then $\dim(M_1 \cap M_2) < \min(\dim(M_1), \dim(M_2)).$

• A sufficient condition for generic identifiability

• M_1, M_2 exchangeable when $\dim(M_1) = \dim(M_2)$

- 2 [Structural Identifiability](#page-5-0)
- [Jacobian Matroid](#page-8-0)
- 4 [Outdegree Proposition and etc.](#page-13-0)
	- [Identifiability Results](#page-18-0)

Proposition 1 (Outdegree proposition)

Let G_1, G_2 be non-complete simple directed graphs. If $\exists i$ s.t. $|Ch_1(i)| \neq |Ch_2(i)|$ then $\mathcal{M}(\psi_1) \neq \mathcal{M}(\psi_2)$.

Example 4

€ □ E →同→

Example: Outdegree Proposition Not Applicable

Example 5

Figure:
$$
G_1
$$

Figure: G₂

Let
$$
S = \{22, 33, 23, 34, 14\}
$$
,

$$
J_{\mathcal{S}}^{1} = \begin{pmatrix} \kappa_{22} & \kappa_{33} & \kappa_{23} & \kappa_{34} & \kappa_{14} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -s & 0 & 0 & \lambda_{23} \\ 0 & 0 & 0 & 0 & 0 & \lambda_{34} \\ 0 & 0 & 0 & 0 & -s & \lambda_{41} \\ 1 + \lambda_{23}^{2} & 1 + \lambda_{34}^{2} & -\lambda_{23} & -\lambda_{34} & -\lambda_{41} \end{pmatrix} \xrightarrow[\kappa_{22}]{\lambda_{12}} \kappa_{23} \kappa_{33} \kappa_{34} \kappa_{14}
$$

$$
J_S^2 = \begin{pmatrix} 2s\lambda_{21} & 0 & 0 & 0 & 0 & \lambda_{21} \\ 0 & 2s\lambda_{32} & -s & 0 & 0 & \lambda_{32} \\ 0 & 0 & 0 & -s & 0 & \lambda_{43} \\ 0 & 0 & 0 & 0 & -s & \lambda_{14} \\ 1 + \lambda_{21}^2 & 1 + \lambda_{32}^2 & -\lambda_{32} & -\lambda_{43} & -\lambda_{14} \end{pmatrix} \xrightarrow{\lambda_{21}} \sum_{s=1}^{32} \text{rank}(J_S^2) = 5.
$$

Jun Wu **Internal Internal Internal [Identifiability of linear SEMs using algebraic matroids](#page-0-0)** March 2023 16 / 24

 \sim

Definition

A set $L \in ne(i)$ is called parentally closed w.r.t node *i* if $pa(L) \cap ne(i) \subseteq L$.

Figure: A parentally closed set

 \leftarrow

Proposition 2 (Parentally closed set)

Let $G_1 = (V, D_1)$, $G_2 = (V, D_2)$ be two simple directed graphs, both not complete. For any node i, there are two collections of parentally closed sets $\mathcal{L}^1_i, \mathcal{L}^2_i$, corresponding to G_1 and $G_2.$ If there is a set $L \in \mathcal{L}^k_i$ such that $|Ch_k(i) \cap L| > |Ch_{3-k}(i) \cap L|, k \in \{1,2\}$, then G_1 and G_2 have different matroids.

Corollary 2.1 (Transitive triangle-free)

If two different non-complete simple graphs do not contain transitive triangles $(i \rightarrow i \rightarrow k$ and $i \rightarrow k$), then they have different matroids.

(Every parentally closed set in a transitive triangle-free graph is a singleton!)

 QQ

- 2 [Structural Identifiability](#page-5-0)
- [Jacobian Matroid](#page-8-0)
- [Outdegree Proposition and etc.](#page-13-0)
- 5 [Identifiability Results](#page-18-0)

Identifiability Results

Theorem 1

Let G be the collection of non-complete simple directed graphs. If the collection satisfies one of the following conditions, then the models set of graphs in G is generically identifiable.

I Every graph $G \in \mathcal{G}$ has a unique outdegree sequence

Every graph $G \in \mathcal{G}$ does not contain a transitive triangle $(i \rightarrow j \rightarrow k$ and $i \rightarrow k$

Theorem 2

A DAG and a cyclic graph (generically) generate different distributions under homoscedastic errors condition.

Theorem 3

The collection of all non-complete simple directed graphs with at least 1 source node, and whose strongly connected components contain no transitive triangles are generically identifiable.

- 2 [Structural Identifiability](#page-5-0)
- [Jacobian Matroid](#page-8-0)
- [Outdegree Proposition and etc.](#page-13-0)
- [Identifiability Results](#page-18-0)

Methods

- \bullet $|V|$ < 5: Complete symbolic rank checks
- $|V| = 6$: Brute force check: extremely time-consuming!

To relieve the issue:

- Comparisons: within the subclasses indexed by outdegree sequences
- Parameters: random integers

Results

- Most of the simple directed graphs have unique matroids
- Some graph pairs have the same matroids, but can be distinguished by entries in the precision matrix
- Compatible with parental closed set condition checks

\mathbf{C}

- Natural extension of equal variance (homoscedastic) error assumption from DAGs to directed cyclic graphs
- Partial identifiability results of linear homoscedastic Gaussian models
- Some side-results in algebra

Ω

- Results are not strong enough to cover all cases
- Computation capacity is currently limited to 6-node graphs

つひひ

- Chen, Wenyu, Mathias Drton, and Y Samuel Wang (Sept. 2019). "On causal discovery with an equal-variance assumption". In: Biometrika 106.4, pp. 973–980.
- 昴 Hollering, Benjamin and Seth Sullivant (2021). "Identifiability in phylogenetics using algebraic matroids". In: Journal of Symbolic Computation 104, pp. 142–158.
	- Peters, Jonas and Peter Bühlmann (2014). "Identifiability of Gaussian structural equation models with equal error variances". In: Biometrika 101.1, pp. 219–228.