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

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Bernoulli-IMS 10th World Congress in Probability and Statistics

July 19 - 23, 2021

Linear Structural Equation Models

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

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

  Then $X = (I - \Lambda)^{-T}\varepsilon$ has covariance matrix

$$\Sigma = \mathrm{Var}[X] = (I - \Lambda)^{-T}\Omega(I - \Lambda)^{-1}.$$

- We consider homoscedastic errors, $\Omega = \omega \cdot I$, and then focus on the simpler 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

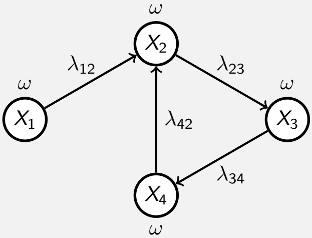
$$M_G = \left\{ s(I - \Lambda)(I - \Lambda)^T : \Lambda \in \mathbb{R}^D_{\mathrm{reg}},\ s > 0 \right\},$$

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

Linear Structural Equation Models: Example

Example 1

$$\begin{aligned} X_1 &= \varepsilon_1 \\ X_2 &= \lambda_{12}X_1 + \lambda_{42}X_4 + \varepsilon_2 \\ X_3 &= \lambda_{23}X_2 + \varepsilon_3 \\ X_4 &= \lambda_{34}X_3 + \varepsilon_4 \end{aligned}$$



$$\Lambda = \begin{pmatrix} 0 & \lambda_{12} & 0 & 0 \\ 0 & 0 & \lambda_{23} & 0 \\ 0 & 0 & 0 & \lambda_{34} \\ 0 & \lambda_{42} & 0 & 0 \end{pmatrix}, \qquad s = \frac{1}{\omega}$$

Here, the graph is simple, but the SEM is non-recursive ($\exists$ cycle)

Identifiability

- Within the class of DAGs (directed acyclic graphs), the graph G is known to be identifiable.
  [Chen, Drton, and Wang 2019; Peters and Bühlmann 2014]
- Is the graph G identifiable more generally? In which sense?

Definition

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

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

- Different dimensions: Automatically generically identifiable
- Same dimension: Intersection of two models is a lower dimensional set

Simple Graphs and Dimension

- We focus on simple directed graphs, allowing cycles

Theorem

Let $G = (V, D)$ be a simple directed graph. Then the model M_G has expected dimension:

$$\dim(M_G) = |D| + 1.$$

Proof.

Fact: $\dim(M_G) =$ maximal rank of the Jacobian of ψ_G.

At $\Lambda = 0$ and $s = 1$, the Jacobian $J(\psi_G)$ contains a diagonal $(|D| + 1) \times (|D| + 1)$ submatrix, with diagonal entries ± 1.

At this point and also generically the Jacobian has full rank $|D| + 1$. □

- Not true for general non-simple graphs

Jacobian: Example

Example 3

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

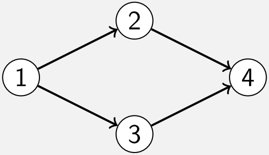


Figure: Example 3

$J(\psi_G)$:

$$\begin{array}{ccccccccccc}
K_{11} & K_{22} & K_{33} & K_{44} & K_{12} & K_{23} & K_{34} & K_{13} & K_{24} & K_{14} & \\
2s\lambda_{12} & 0 & 0 & 0 & -s & 0 & 0 & 0 & 0 & 0 & \lambda_{12} \\
2s\lambda_{13} & 0 & 0 & 0 & 0 & 0 & 0 & -s & 0 & 0 & \lambda_{13} \\
0 & 2s\lambda_{24} & 0 & 0 & 0 & s\lambda_{34} & 0 & 0 & -s & 0 & \lambda_{24} \\
0 & 0 & 2s\lambda_{34} & 0 & 0 & s\lambda_{24} & -s & 0 & 0 & 0 & \lambda_{34} \\
1 + \lambda_{12}^2 + \lambda_{13}^2 & 1 + \lambda_{24}^2 & 1 + \lambda_{34}^2 & 1 & -\lambda_{12} & \lambda_{24}\lambda_{34} & -\lambda_{34} & -\lambda_{13} & -\lambda_{24} & 0 & s
\end{array}$$

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

Jacobian Matroid

Definition

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

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

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

- $E = [r]$ is the ground set, and
- every independent set $S \in \mathcal{I}$ is such that the columns of $J(\phi)$ indexed by S are linearly independent over the fraction field $\mathbb{R}(\theta)$.

- Maximal independent sets determine the Jacobian matriod
- Every maximal independent set is of the size equaling to the rank

Proving Identifiability with Algebraic Matroids

Proposition [Hollering and Sullivant 2021]

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 $\dim(M_1) = \dim(M_2)$

Identifiability Results

Theorem 1

Let $\mathcal{G}$ be a collection of simple directed graphs. If every graph $G \in \mathcal{G}$ has a unique outdegree sequence in the collection, then the models of the graphs in $\mathcal{G}$ are generically identifiable under the homoscedastic errors assumption.

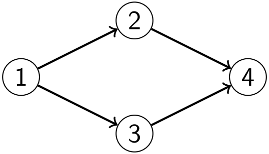


Figure: Example 3

- The outdegree sequence is $\{2, 1, 1, 0\}$.

Identifiability Results

Theorem 2

Let $\mathcal{G}'$ be the collection of transitive triangle-free simple directed graphs with node set V, i.e., $G \in \mathcal{G}'$ has the property $\forall j \in V\ , \forall i \in Ch(j),\ Ch(j) \cap Ch(i) = \emptyset$. Then the models of the graphs in $\mathcal{G}'$ are generically identifiable under the homoscedastic errors assumption.

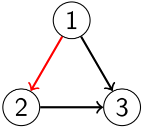


Figure: transitive triangle

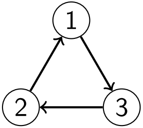


Figure: non-transitive triangle

Identifiability Results

Theorem 3

Let $\mathcal{G}''$ be the collection of simple directed graphs with node set V and the property that $\forall i \in V$, there exists at most one $j \in Ch(i)$ such that $Ch(i) \cap Ch(j) \neq \emptyset$. Then the models of the graphs in collection $\mathcal{G}''$ are generically identifiable under the homoscedastic errors assumption.

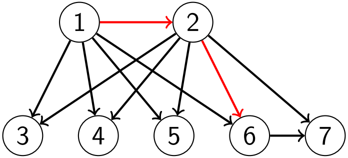


Figure: A graph in $\mathcal{G}''$

Outdegree Proposition

How to certify different matroids?

- If $\exists S$ s.t. $\text{rank}(J^1_S) \neq \text{rank}(J^2_S)$, then J^1 and J^2 have different matroids
- Want to find this kind of set S

Lemma 1

Let $G = (V, D)$ be a directed graph such that $\dim(M_G) = |D| + 1$. If G is not complete, then for every node i and any column set S of size $|D| + 1$ such that $\{K_{i1}, K_{i2}, ..., K_{i(i-1)}, K_{ii}, K_{i(i+1)}, ...\} \cap S = \emptyset$, the submatrix J_S has rank at most $|D| - |Ch(i)| + 1$.

Proof Idea.

Counting zero rows.

Outdegree Proposition

Lemma 2

Let $G = (V, D)$ be a simple directed graph. If G is not complete, then for every node i, there exists a column set S of size $|D| + 1$ such that $\{K_{i1}, K_{i2}, ..., K_{i(i-1), K_{ii}, K_{i(i+1)}, ...}\} \cap S = \emptyset$ and the submatrix J_S has rank at least $|D| - |Ch(i)| + 1$.

Proof Idea.

$$
\begin{array}{cccccccc}
K_{j_0 j_0} & \cdots & K_{j_1 j_1} & \cdots & K_{j_q j_q} & K_{l_1 l_2} & \cdots & K_{l_m l_n} \\
\left(\begin{array}{cccccccc}
0 & \cdots & 0 & \cdots & 0 & -1 & \cdots & O(\varepsilon) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & \cdots & 0 & O(\varepsilon) & \cdots & -1 \\
0 & \cdots & 2\varepsilon & \cdots & 0 & \times & \cdots & \times \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & 0 & \cdots & 2\varepsilon & \times & \cdots & \times \\
0 & \cdots & \times & \cdots & \times & \times & \cdots & \times \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & \times & \cdots & \times & \times & \cdots & \times \\
1 & \cdots & 2 & \cdots & 2 & 0 & \cdots & 0
\end{array}\right)
\end{array}
$$

$\#\{uncertain\ rows\}$

$= |Ch(i)|$

Outdegree Proposition

Proposition 1

Let $G_1 = (V, D_1)$, $G_2 = (V, D_2)$ be two simple directed graphs. If one of the graphs is not complete and there exists a node i such that G_1 and G_2 have outgoing edge set at i of different size, then G_1 and G_2 have different Jacobian matroids. Additionally, if G_1 and G_2 are complete but i is not a sink node in either graph, the difference property still holds.

- A large proportion of the possible pairs of graphs can be certified to give different matroids.
- However there exist still rather simple counterexamples.

Example: Outdegree Proposition Not Applicable

Example 4

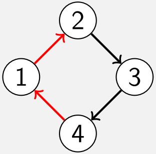


Figure: G_1

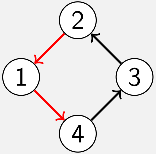


Figure: G_2

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

$$J_S^1 = \begin{array}{c} \begin{array}{ccccc} K_{22} & K_{33} & K_{23} & K_{34} & K_{14} \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 2s\lambda_{23} & 0 & -s & 0 & 0 \\ 0 & 2s\lambda_{34} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -s \\ 1+\lambda_{23}^2 & 1+\lambda_{34}^2 & -\lambda_{23} & -\lambda_{34} & -\lambda_{41} \end{pmatrix} \end{array} \begin{array}{c} \lambda_{12} \\ \lambda_{23} \\ \lambda_{34} \\ \lambda_{41} \\ s \end{array}, \quad \mathrm{rank}(J_S^1) = 4,$$

$$J_S^2 = \begin{array}{c} \begin{array}{ccccc} K_{22} & K_{33} & K_{23} & K_{34} & K_{14} \end{array} \\ \begin{pmatrix} 2s\lambda_{21} & 0 & 0 & 0 & 0 \\ 0 & 2s\lambda_{32} & -s & 0 & 0 \\ 0 & 0 & 0 & -s & 0 \\ 0 & 0 & 0 & 0 & -s \\ 1+\lambda_{21}^2 & 1+\lambda_{32}^2 & -\lambda_{32} & -\lambda_{43} & -\lambda_{14} \end{pmatrix} \end{array} \begin{array}{c} \lambda_{21} \\ \lambda_{32} \\ \lambda_{43} \\ \lambda_{14} \\ s \end{array}, \quad \mathrm{rank}(J_S^2) = 5.$$

Certifying Different Matroids

Proposition 2

Let $\mathcal{G}'$ be the collection of transitive triangle-free simple directed graphs with node set V, i.e., $G \in \mathcal{G}'$ has the property $\forall j \in V \ , \forall i \in Ch(j), \ Ch(j) \cap Ch(i) = \emptyset$. Let $G_1 = (V, D_1)$, $G_2 = (V, D_2)$ be two different graphs in $\mathcal{G}'$. Then G_1 and G_2 have different Jacobian matroids.

Proposition 3

Let $\mathcal{G}''$ be the collection of simple directed graphs with node set V and has the property that $\forall i \in V$, there exists at most one $j \in Ch(i)$ such that $Ch(i) \cap Ch(j) \neq \emptyset$. Let $G_1 = (V, D_1)$, $G_2 = (V, D_2)$ be two different graphs in $\mathcal{G}''$. Then G_1 and G_2 have different Jacobian matroids.

Computational checks for $|V| \leq 6$

Methods

- $|V| = 3$: Manual computations
- $|V| = 4, 5$: Complete symbolic rank checks
- $|V| = 6$: Brute force check is extremely time-consuming!

To resolve the issue:

- Comparisons: within the subclasses indexed by outdegree sequences
- Valid outdegree sequences and simple graphs: depth first search
- 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 node variances

References

- Chen, Wenyu, Mathias Drton, and Y Samuel Wang (2019). "On causal discovery with an equal-variance assumption". In: *Biometrika* 106.4, pp. 973–980.
- 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.

THANK YOU!