

Identifiability of Gaussian Structural Equation Models with Equal Error Variances

(J.Peters and P.Buhlmann, Biometrika, 2014)

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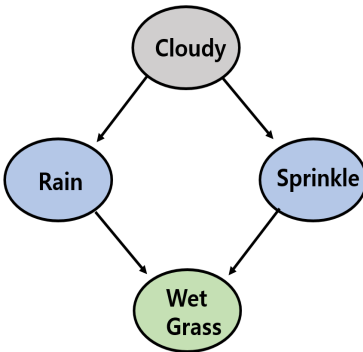
Outline

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1. Introduction

1. Introduction



1.1. Directed Acyclic Graphical(DAG) model

- Directed acyclic graph \mathcal{G} :



- $\mathcal{G} = (V, E)$.
- V : a set of nodes, e.g. $V = \{1, 2, 3\}$.
- E : a set of directed edges, $E = \{(1, 2), (2, 3)\}$.

1.1. Directed Acyclic Graphical(DAG) model

- DAG model:



- $X := (X_j)_{j \in V}$: a set of random variables, e.g.
 $X = \{X_1, X_2, X_3\}$.
- DAG model has the factorization,

$$P(\mathcal{G}) = P(X_1, X_2, \dots, X_p) = \prod_{j=1}^p P(X_j \mid X_{Pa(j)}).$$

- In this graph,

$$P(\mathcal{G}) = P(X_1)P(X_2 \mid X_1)P(X_3 \mid X_2).$$

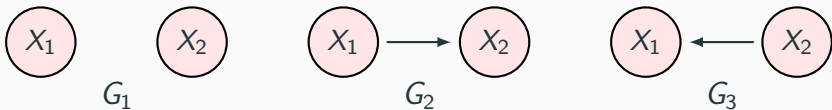
1.2. Identifiability from the distribution

- Problem:

Given the joint distribution $P(\mathcal{G})$, can we recover the graph \mathcal{G}_0 ?

"Negative!!"

- Reason:



- We can distinguish G_2 and G_3 from G_1 .
- We cannot identify a direction of an edge. Hence, we cannot distinguish G_2 and G_3 .

1.2. Identifiability from the distribution

- Exception case:
 1. Linear non-Gaussian SEMs (Shimizu et al., 2006).
 2. Non-parametric SEMs with additive independent noise (Peters et al., 2012).
 3. **Gaussian SEMs with the equal error variances (Peters and Bühlmann, 2013).**

2. Identifiability for Gaussian SEM with equal error variances

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- Gaussian SEM:

$$X_j = \sum_{k \in PA_j^{\mathcal{G}_0}} \beta_{jk} X_k + N_j \quad (j = 1, \dots, p).$$

- V : a set of nodes in a graph, $V = \{1, \dots, p\}$.
- X_j : random variable, $j \in V$.
- N_j : noise term, $N_j \sim^{IID} N(0, \sigma^2)$ with $\sigma^2 > 0$.
- $\beta_{jk} \neq 0$ for all $k \in PA_j^{\mathcal{G}_0}$, otherwise $\beta_{jk} = 0$.

2. Identifiability for Gaussian models with equal error variances

- Theorem 1.

Let $P(\mathcal{G})$ be generated from model Gaussian SEM,

Then \mathcal{G}_0 is identifiable from $P(\mathcal{G})$ and the coefficients β_{jk} can be reconstructed for all j and $k \in PA_j^{\mathcal{G}_0}$.

- Assumptions: **Non-zero coefficient, Causal sufficiency.**
 - Non-zero coefficient: $\beta_{jk} \neq 0$, $k \in PA_j^{\mathcal{G}_0}$.
 - Causal sufficiency: all variables are observed.

3. Penalized maximum likelihood estimator

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- Penalized maximum likelihood estimator:

$$\{\hat{\beta}(\lambda), \hat{\sigma}^2(\lambda)\} = \arg \min_{\beta \in \mathcal{B}, \sigma^2 \in \mathbb{R}^+} -\ell(\beta, \sigma^2; X^{(1)}, \dots, X^{(n)}) + \lambda \|\beta\|_0, \quad (1)$$

where

$$-\ell(\beta, \sigma^2; X^{(1)}, \dots, X^{(n)}) = \frac{np}{2} \log(2\pi\sigma^2) + \frac{n}{2\sigma^2} \text{tr}\{(I - B)^T(I - B)\hat{\Sigma}\}.$$

- B : $p \times p$ matrix with $B_{jk} = \beta_{jk}$.
- $\hat{\Sigma}$: sample covariance matrix.
- σ^2 : error variance.
- $\lambda = \log(n)/2$: the objective function in equation (1) is the BIC score.

3. Penalized maximum likelihood estimator

- Convergence rate:

For $\lambda_n = \log(n)/2$, $n \rightarrow \infty$,

$$\sum_{j,k=1}^p \{\hat{\beta}_{jk}(\lambda_n) - \beta_{jk}^0\}^2 = O_p\{\log(n)n^{-1}\}.$$

- Consistency:

For $\lambda_n = \log(n)/2$, $n \rightarrow \infty$,

$$\text{pr}(\hat{\mathcal{G}}_n = \mathcal{G}_0) \rightarrow 1.$$

3. Penalized maximum likelihood estimator

- Computational complexity:

$$p = 20 \rightarrow 2 \cdot 3 \times 10^{72} \text{ DAG } \mathcal{G}.$$

\Rightarrow Greedy search algorithm

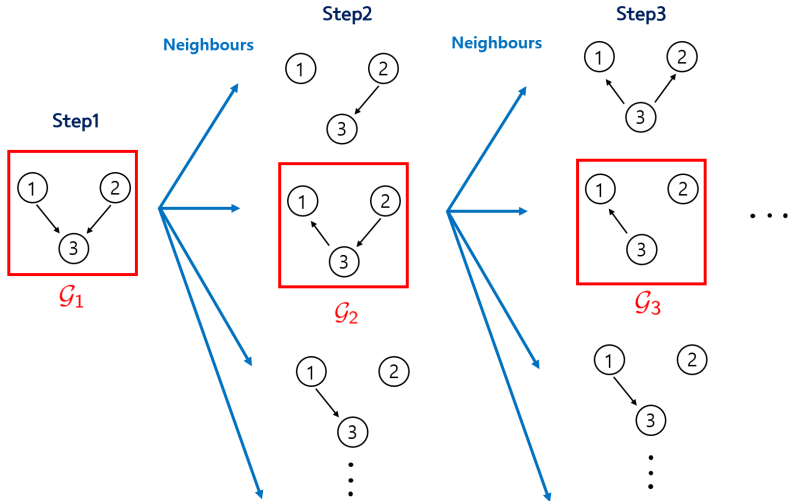
4. Greedy search algorithm

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- We consider at least k neighbours.
 - If the neighbouring \mathcal{G}_t have a lower BIC score than \mathcal{G}_{t-1} , \mathcal{G}_{t-1} move to \mathcal{G}_t .
 - If all neighbours have a higher BIC score than \mathcal{G}_t , the algorithm terminates.
 - $k = p$, $k = 2p$, $k = 3p$, $k = 5p$ and $k = 300$.
- * Neighbour: if they can be transformed into each other by one edge addition, removal or reversal.

4. Greedy search algorithm



5. Experiments

5.1. Existing methods

- Compare three methods:
PC-algorithm, GES, GDS.

- Evaluation:

The structural Hamming distance between the true and estimated DAG.

- * Hamming distance: this assigns a distance of 2 for each pair of reversed edges. all other edge mistakes count as 1.

5.2. Random graphs

- $p=5, 20, 40$.
- $n=100, 500, 1000$.
- β_{jk}^0 : uniformly $[-1, -0.1] \cup [0.1, 1]$.
- Sparse setting: $p_{edge} = 3/(2p - 2)$.
- Dense setting: $p_{edge} = 0.3$.

5.2. Random graphs

- Sparse setting

| | | $n = 100$ | | | $n = 500$ | | | $n = 1000$ | | |
|-----|-------|--------------------|------|------|--------------------|------|------|--------------------|------|------|
| p | | GDS _{EEV} | PC | GES | GDS _{EEV} | PC | GES | GDS _{EEV} | PC | GES |
| 5 | DAG | 1.5 | 3.9 | 3.6 | 0.5 | 2.9 | 2.8 | 0.4 | 3.0 | 2.5 |
| | CPDAG | 1.5 | 2.9 | 2.3 | 0.5 | 1.4 | 1.2 | 0.3 | 1.0 | 0.7 |
| 20 | DAG | 12.2 | 14.1 | 18.0 | 4.5 | 11.1 | 10.3 | 2.7 | 10.1 | 8.7 |
| | CPDAG | 13.9 | 10.9 | 17.0 | 5.2 | 7.7 | 7.6 | 3.0 | 6.9 | 5.6 |
| 40 | DAG | 44.7 | 29.6 | 53.0 | 15.7 | 22.6 | 26.1 | 10.7 | 20.1 | 21.9 |
| | CPDAG | 50.0 | 24.4 | 53.1 | 18.9 | 15.9 | 23.4 | 13.4 | 13.3 | 17.5 |

Average structural Hamming distance

- Except for $p = 40$ and $n = 100$,
GDS method are closer to the true DAG.

5.2. Random graphs

- Dense setting

| | | $n = 100$ | | | $n = 500$ | | | $n = 1000$ | | |
|-----|-------|--------------------|-------|-------|--------------------|-------|-------|--------------------|-------|-------|
| p | | GDS _{EEV} | PC | GES | GDS _{EEV} | PC | GES | GDS _{EEV} | PC | GES |
| 5 | DAG | 1.2 | 2.9 | 3.0 | 0.6 | 2.4 | 2.2 | 0.3 | 2.1 | 2.1 |
| | CPDAG | 1.3 | 2.1 | 1.9 | 0.5 | 1.2 | 0.7 | 0.2 | 0.8 | 0.5 |
| 20 | DAG | 30.0 | 56.6 | 63.9 | 12.5 | 55.7 | 66.3 | 8.2 | 57.6 | 69.1 |
| | CPDAG | 31.0 | 56.1 | 63.2 | 13.1 | 55.5 | 66.2 | 8.8 | 57.5 | 68.5 |
| 40 | DAG | 216.1 | 242.8 | 323.1 | 185.2 | 247.2 | 430.4 | 172.0 | 248.9 | 470.6 |
| | CPDAG | 217.1 | 242.4 | 323.0 | 185.7 | 247.0 | 430.1 | 172.2 | 248.5 | 470.4 |

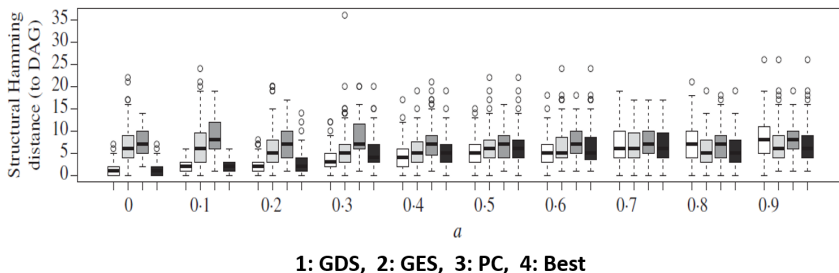
Average structural Hamming distance

- GDS method are closer to the true DAG.

5.3. Deviation from equal error variances

- $p = 10, n = 500$.
- σ_j^2 : uniformly $[1 - a, 1 + a]$, $a = (0.1, 0.2, \dots, 0.9)$.
- p_{edge} : $2/(p - 1)$ on average resulting in p edges.
- β_{jk}^0 : uniformly $[-1, -0.1] \cup [0.1, 1]$.

5.3. Deviation from equal error variances



- For large values of a , the method does not perform worse than the PC-algorithm.
- GDS is relatively robust as the parameter a changes.

* Bestscore method: the result of GDS or GES depending on which 25 / 29

5.4. Real data

Table 3. BIC scores of greedy equivalence search and greedy directed acyclic graph search with equal error variances obtained for different types of microarray data; smaller is better

| | Prostate | Lymphoma | Riboflavin | Leukaemia | Brain | Cancer | Colon |
|--------------------|----------|----------|------------|-----------|-------|--------|-------|
| GES | 4095 | 4560 | 2711 | 5456 | 1411 | 5891 | 3224 |
| GDS _{EEV} | 6057 | 5404 | 3236 | 5481 | 1343 | 6288 | 3201 |

GES, greedy equivalence search; GDS_{EEV}, greedy directed acyclic graph search with equal error variances.

- 7 datasets: Prostate, Lymphoma, Riboflavin, Leukaemia, Brain, Cancer, Colon.
- Brain, Colon datasets: GDS produced a better score than GES.

Summary

Summary

- Identifiability
 - Gaussian SEMs with the equal error variances.
 - Assumptions: Non-zero coefficient, Causal sufficiency.
- Learning
 - Penalized MLE.
 - Greedy search algorithm.

Reference

Reference

- J.Peters and P.Buhlmann, Identifiability of Gaussian Structural Equation Models with Equal Error Variances 2014.
- Park, Gunwoong, High Dimensional Gaussian DAG Model Learning via ℓ_1 - regularized Regression.



THANK YOU

A Newton's cradle with five blue blocks spelling 'THANK' and three blue blocks spelling 'YOU'. The blocks are suspended by thin silver wires. The background is white.