Optimal structure learning and conditional independence testing

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Main Takeaway

Can we understand the statistical optimality of structure learning via CI testing ?

We establish a fundamental connection between the statistical complexity of CI testing and structure learning (SL):

- optimal testing radius (of CI) $\implies$ optimal sample complexity (of SL)
- achieved by an efficient variant of PC algo w/ the optimal test plugged in
- applied to several examples (Bernoulli, Gaussian, nonparam. cts.)

Motivation

Structure learning / causal discovery / DAG learning enjoys extensive algorithmic developments. However, the statistical optimality is less understood.

One special case: Equal-variance model [3, 5, 2]

What about faithfulness? nonparametric models? A general recipe?

Let's leverage CI testing!

- Closely related: e.g. workhorse to (constraint-based) structure learning.
- Extensively studied: e.g. discrete [1]; continuous [4].

Problem Setup

Given a distribution family $\mathcal{P}$ and a dependence measure m:

CI Testing aims to distinguish two hypotheses of distributions:

$$\begin{aligned} \mathcal{H}_0: &\quad p(X,Y,Z) \quad \text{s.t. } m(X;Y \mid Z) = 0 \Leftrightarrow X \perp\!\!\!\perp Y \mid Z \\ \mathcal{H}_1: &\quad p(X,Y,Z) \quad \text{s.t. } m(X;Y \mid Z) \geq r \end{aligned}$$

where $p \in \mathcal{P}$, and r is the signal strength. A CI test ψ is a function of data that outputs a binary decision.

The *optimal testing radius* is the infimum of $r = r_n$ in terms of n s.t. there exists a ψ whose Type-I and Type-II errors are controlled.

Structure Learning (for poly-forest) is to learn the Markov equivalence class of G (a poly-forest) given i.i.d. samples from p where

- p is Markov to G
- p is c-strong tree-faithful to G wrt. m
- $p_{X_j,X_k,X_\ell} \in \mathcal{P}, \forall j,k,\ell \in [d]$

The *optimal sample complexity* is the infimum of sample size n in terms of the number of nodes d and the strong tree-faithfulness parameter c s.t. G can be confidently learned.

A poly-forest is a DAG whose skeleton has any two nodes connected by at most one path.

Markov property: $p(X) = p(X_1,\ldots,X_d) = \prod_{k=1}^{d} p(X_k \mid \mathrm{pa}_G(k))$.

c-strong Tree-faithfulness:

- For any two nodes connected $j-k$, we have $m(X_k;X_j \mid X_\ell) \geq c$ for $\ell \in V \cup \{\emptyset\} \setminus \{k,j\}$;
- For any v-structure $k \to \ell \leftarrow j$, we have $m(X_k;X_j \mid X_\ell) \geq c$.

Main Result

CI testing ⟹ Structure learning for poly-forest

optimal testing radius $\implies$ *optimal sample complexity*

$r_n \asymp n^{-1/\alpha}$ $\qquad$ $n^* \asymp \frac{\log d}{c^\alpha}$

- $\alpha > 0$ depends on the modeling setup
- c is the strong faithfulness parameter
- Applied to Bernoulli and Gaussian ($\alpha = 2$), and nonparametric continuous distributions ($\alpha = \frac{5s+2}{2s} > 2$)
- Optimality achieved by PC-tree with the optimal test plugged in

Applications

Distribution Family $\mathcal{P}$	Parameter α	Testing Radius	Sample Complexity
Bernoulli	$\alpha = 2$	$r_n \asymp n^{-1/2}$	$n^* \asymp \log d / c^2$
Gaussian	$\alpha = 2$	$r_n \asymp n^{-1/2}$	$n^* \asymp \log d / c^2$
Nonparam. Cts. [4]	$\alpha = \frac{5s+2}{2s}$	$r_n \asymp n^{-2s/(5s+2)}$	$n^* \asymp \log d / c^{\frac{5s+2}{2s}}$

- s is a smoothness parameter in the nonparametric function class
- $\alpha = \frac{5s+2}{2s} > 2$ in the nonparametric continuous case is strictly larger than the two parametric cases $\implies$ intrinsic difficulty
- Optimality results for Bernoulli an Gaussian can be extended for poly-tree learning

PC-tree Algorithm

Algorithm 1 PC-Tree

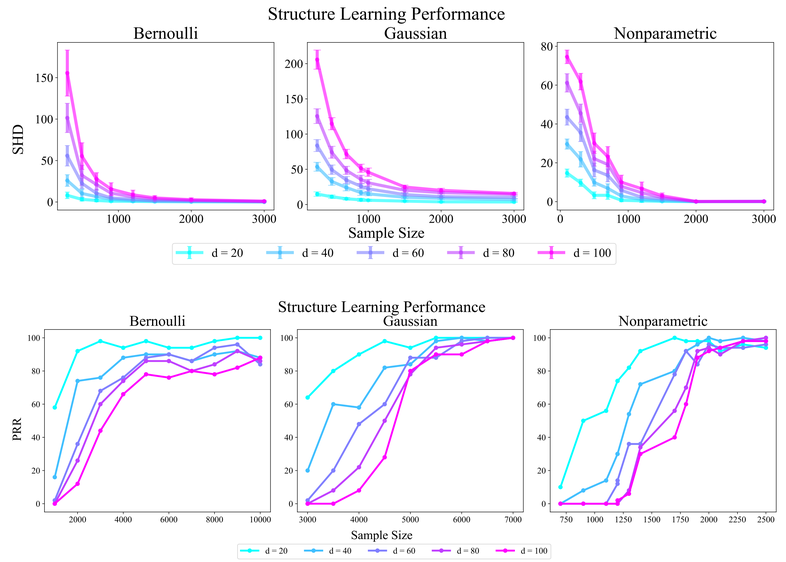
Input: n i.i.d. samples $\{X_1^{(i)},\ldots,X_d^{(i)}\}_{i=1}^n$, CI test ψ as function of data;

1. Let $\widehat{E} = \emptyset$.
2. For each pair (j,k), $0 \leq j < k \leq d$:
   1. For all $\ell \in [d] \cup \{\emptyset\} \setminus \{j,k\}$:
      1. Test $H_0 : X_j \perp\!\!\!\perp X_k \mid X_\ell$ vs. $H_1 : X_j \not\perp\!\!\!\perp X_k \mid X_\ell$ using ψ, store the results.
   2. If all tests reject, then $\widehat{E} \leftarrow \widehat{E} \cup \{j-k\}$.
   3. Else (if some test accepts), let $S(j,k) = \{\ell \in [d] \cup \{\emptyset\} \setminus \{j,k\} : X_j \perp\!\!\!\perp X_k \mid X_\ell\}$.

Output: $\widehat{G} = ([d], \widehat{E})$, separation set S.

The output is refined using orientation rules.

Experiments



More in paper!

References

[1] Clément L Canonne, Ilias Diakonikolas, Daniel M Kane, and Alistair Stewart.
Testing conditional independence of discrete distributions.
In *Proceedings of the 50th Annual ACM SIGACT Symposium on Theory of Computing*, pages 735--748, 2018.

[2] Constantinos Daskalakis, Vardis Kandiros, and Rui Yao.
Learning gaussian dag models without condition number bounds.
In *Forty-second International Conference on Machine Learning*, 2025.

[3] Ming Gao, Wai Ming Tai, and Bryon Aragam.
Optimal estimation of gaussian dag models.
In *International Conference on Artificial Intelligence and Statistics*, pages 8738--8757. PMLR, 2022.

[4] Matey Neykov, Sivaraman Balakrishnan, and Larry Wasserman.
Minimax optimal conditional independence testing.
The Annals of Statistics, 49(4):2151--2177, 2021.

[5] Mishfad Shaikh Veedu, Deepjyoti Deka, and Murti Salapaka.
Information theoretically optimal sample complexity of learning dynamical directed acyclic graphs.
In *International Conference on Artificial Intelligence and Statistics*, pages 4636--4644. PMLR, 2024.