DAGs with No Curl:

An Efficient DAG Structure Learning Approach

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DAG Learning: SoTA Methods

- DAG learning plays a vital part in other machine learning sub-areas such as causal inference However, it is proven to be NP-hard.

- **Conventional DAG learning methods:**

  1) Make a parametric (e.g. Gaussian) assumption for continuous variables: may result in model misspecification.

  2) Perform score-and-search for **discrete variables**: with a constraint stating that the graph must be acyclic.

$$A^* = \underset{A}{\operatorname{argmin}} \quad F(A, \mathbf{X}), \qquad \text{subject to} \qquad \mathcal{G}_A \in \mathbb{D}$$

- **DAG learning as a continuous optimization:**

  An equivalent acyclicity constraint by Zheng et al*: $\mathcal{G}_A \in \mathbb{D} \Longleftrightarrow h(A) = \operatorname{tr}(\exp(A \circ A)) - m = 0$

continuous constraint optimization

$$A^* = \underset{A}{\operatorname{argmin}} \quad F(A, \mathbf{X}), \qquad \text{subject to} \qquad h(A) = 0,$$

Zheng, X., Aragam, B., Ravikumar, P. K., Xing, E. P. (2018). DAGs with NO TEARS: Continuous Optimization for Structure Learning. In Advances in Neural Information Processing Systems (pp. 9472-9483).

An Equivalent DAG Space

Idea: Can we remove the constraint, by solving directly in the DAG space?

- Reformulate the DAG space: **acyclic = a (curl-free) gradient flow**

Topological Ordering!!

Theorem 1:
Consider a complete undirected graph G(V,E), given any function $p \in L^2(V) = \mathbb{R}^m$ and any skew-symmetric matrix $W \in \mathbb{R}^{m\times m}$, $W \circ \mathrm{ReLU}(\mathrm{grad}(p))$ is the weighted adjacency matrix of a DAG.

Theorem 2:
Let $A \in \mathbb{R}^{m\times m}$ be the weighted adjacency matrix of a DAG, then there exists a skew-symmetric matrix $W \in \mathbb{R}^{m\times m}$ and a potential function $p \in L^2(V) = \mathbb{R}^m$ such that $A = W \circ \mathrm{ReLU}(\mathrm{grad}(p))$.

⇒ $$\{\mathcal{G}_{W\circ \mathrm{ReLU}(\mathrm{grad}(p))}\} = \{\mathrm{DAGs}\}.$$

An Efficient Projection Algorithm

Idea: Can we remove the constraint, by solving directly in the DAG space?

- Reformulate the DAG space: $W \in \mathbb{R}^{m \times m},\ \ p \in L^2(V) = \mathbb{R}^m$

$$\{\mathcal{G}_{W \circ \mathrm{ReLU}(\mathrm{grad}(p))}\} = \{\mathrm{DAGs}\}.$$

- A new continuous optimization **without constraint**:

$$(W^*, p^*) = \underset{W \in \mathbb{R}^{m \times m}, W = -W^T, p \in \mathbb{R}^m}{\mathrm{argmin}} F(W \circ \mathrm{ReLU}(\mathrm{grad}(p)), \mathbf{X})$$

- Instead of solving for A, we solve for W and p, then obtain an optimal DAG via:

$$A^* = W^* \circ \mathrm{ReLU}(\mathrm{grad}(p^*))$$

However, like NOTEARS, this optimization problem is non-convex, even for linear SEM

An Efficient Projection Algorithm

Idea: Can we provide initial guesses by projecting any cyclic graph to the DAG space?

- How to solve the non-convex optimization problem

$$(W^*, p^*) = \underset{W \in \mathbb{R}^{m\times m}, W=-W^T, p\in\mathbb{R}^m}{\operatorname{argmin}} F(W \circ \mathrm{ReLU}(\mathrm{grad}(p)), \mathbf{X})$$

Theorem 3 (Projection Method):
Let $A \in \mathbb{R}^{m\times m}$ be the weighted adjacency matrix of a DAG, C(A) denotes the connectivity matrix of A, then

$$p = -\Delta_0^{\dagger}\mathrm{div}\left(\frac{1}{2}(C(A) - C(A)^T)\right),$$

preserves the topological order in A. Moreover, taking

$$[W]_{ij} = \begin{cases} 0, & \text{if } p(i) = p(j) \text{ or } A(i,j) = A(j,i) = 0; \\ \frac{A(i,j)}{p(j)-p(i)}, & \text{if } A(i,j) \neq 0 \text{ and } A(j,i) = 0; \\ \frac{A(j,i)}{p(j)-p(i)}, & \text{if } A(i,j) = 0 \text{ and } A(j,i) \neq 0. \end{cases}$$

we have $A = W \circ \mathrm{ReLU}(\mathrm{grad}(p))$

For any (cyclic) A, we can project it to the DAG space.

DAG-NoCurl

Overall recipe for DAG-NoCurl

1. **Prediction phase**: Solve for an initial prediction $A^{pre} \in \mathbb{R}^{m \times m}$ via:

$$A^{pre} = \underset{A}{\operatorname{argmin}} \; F(A, \mathbf{X}) + \lambda h(A)$$

2. **Projection phase**: Based on A^{pre}, obtain an approximate solution of p with the projection method:

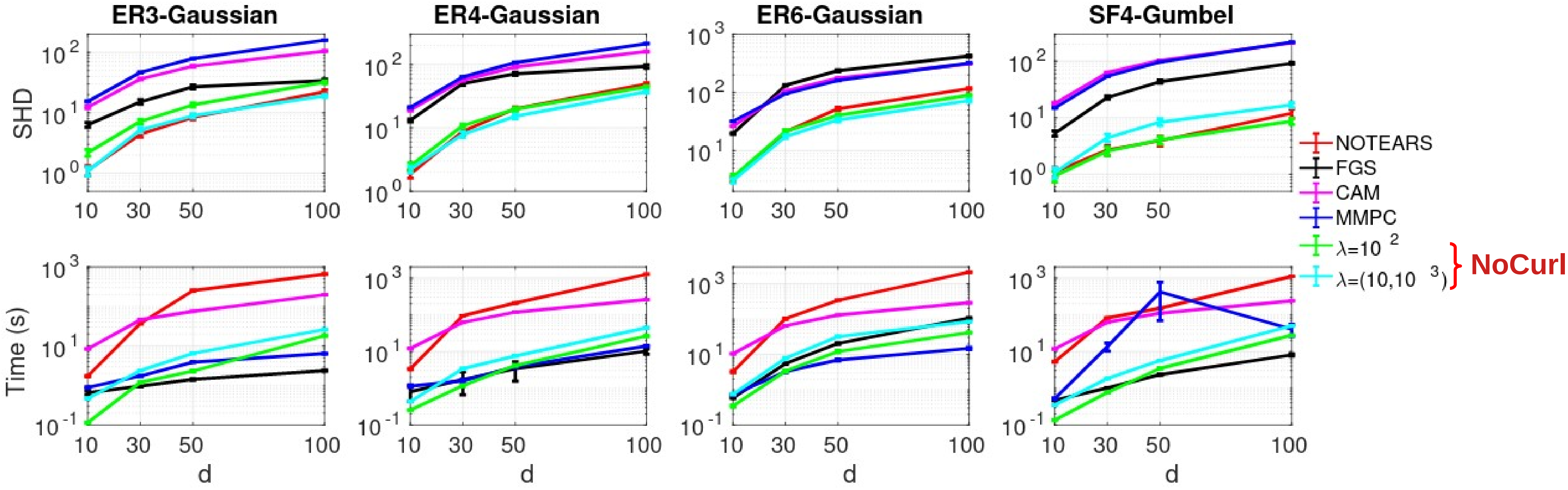
$$\tilde{p} = -\Delta_0^{\dagger} \operatorname{div} \left(\frac{1}{2} (C(A^{pre}) - C(A^{pre})^T) \right),$$

and solve for W via: $$\tilde{W} = \underset{W \in S}{\operatorname{argmin}} \; F(W \circ \operatorname{ReLU}(\operatorname{grad}(\tilde{p})), \mathbf{X}).$$

3. **Final approximation**: $\tilde{A} = \tilde{W} \circ \operatorname{ReLU}(\operatorname{grad}(\tilde{p}))$ and apply thresholding to remove false discoveries.

DAG-NoCurl

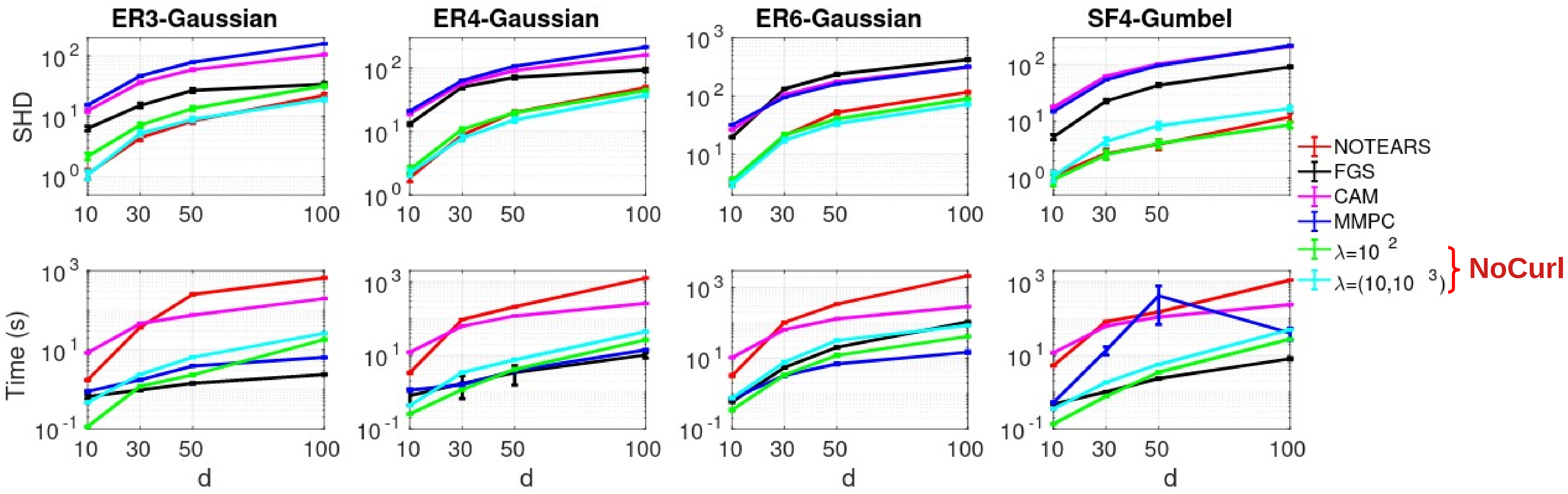
Results: linear SEM



Accuracy: NoCurl achieves a similar accuracy, and sometimes beats NOTEARS, especially on dense and large graphs

DAG-NoCurl

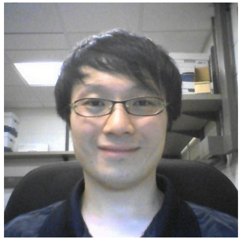
Results: linear SEM



Efficiency: NoCurl requires a similar runtime as FGS and MMPC, which is faster than NOTEARS by one or two orders of magnitude.

Thank You!

- Co-authors:
  Tian Gao (IBM), Naiyu Yin, Qiang Ji (RPI).



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- For further analysis and results on nonlinear and real-world datasets, please stop by our poster.

Poster ID: 937

- Codes and datasets are available at
  https://github.com/fishmoon1234/DAG-NoCurl