CoLiDE: Concomitant Linear DAG Estimation

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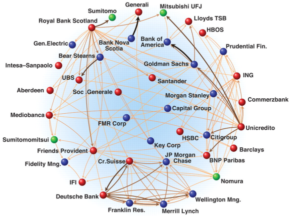
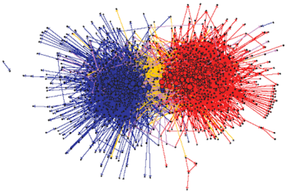
Learning from relational data

- Graphs are natural models for relational data that can help to learn in various timely applications

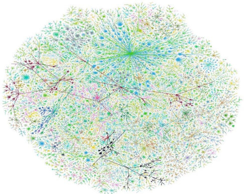
Economic Networks



Social and Information Networks

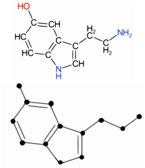


Internet

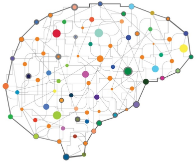


3D Meshes

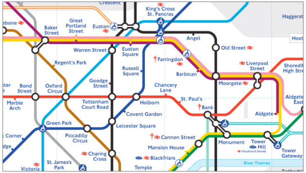
Molecules



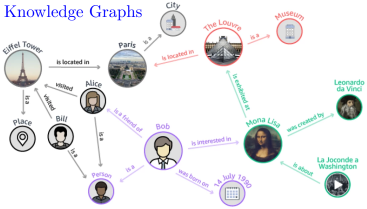
Brain Connectomes



Transportation Networks



Knowledge Graphs

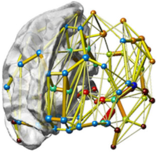


Learning graphs from data: Accounting for directionality and cycles

- Undirected topology inference from nodal observations [Kolaczyk'09]
  - Partial correlations and conditional dependence [Dempster'74]
  - Sparsity [Friedman et al'07] and consistency [Meinshausen-Buhlmann'06]
- Key in neuroscience and bioinformatics

  ⇒ Functional network from fMRI signals [Sporns'10]

  ⇒ Gene-regulatory networks from microarray data [Mazumder-Hastie'12]

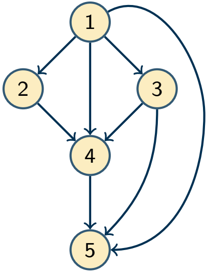


- **This work:** learn the structure of directed acyclic graphs (DAGs)
- DAGs have become prominent models in various ML applications

  ⇒ Conditional independences among variables in Bayesian networks

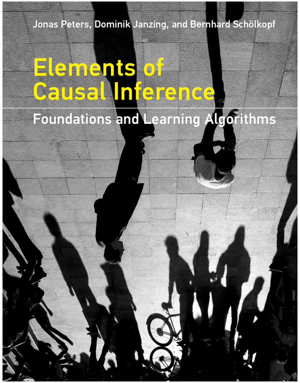
  ⇒ DAG edges may have causal interpretations

  ⇒ Bio [Sachs et al'05], genetics [Zhang et al'13], finance [Sanford-Moosa'12]
- **Challenges:** directionality, acyclicity (combinatorial constraint), identifiability



Causal reasoning and machine learning

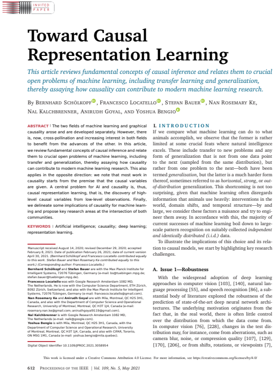
- While our focus is on how optimization and statistical learning can aid inference of causal structures. . .



Jonas Peters, Dominik Janzing, and Bernhard Schölkopf

Elements of Causal Inference

Foundations and Learning Algorithms



INVITED PAPER

Toward Causal Representation Learning

This article reviews fundamental concepts of causal inference and relates them to crucial open problems of machine learning, including transfer learning and generalization, thereby assaying how causality can contribute to modern machine learning research.

By Bernhard Schölkopf, Francesco Locatello, Stefan Bauer, Nan Rosemary Ke,
Nal Kalchbrenner, Anirudh Goyal, and Yoshua Bengio

ABSTRACT | The two fields of machine learning and graphical causality arose and are developed separately. However, there is, now, cross-pollination and increasing interest in both fields to benefit from the advances of the other. In this article, we review fundamental concepts of causal inference and relate them to crucial open problems of machine learning, including transfer and generalization, thereby assaying how causality can contribute to modern machine learning research. This also applies in the opposite direction: we note that most work in causality starts from the premise that the causal variables are given. A central problem for AI and causality is, thus, causal representation learning, that is, the discovery of high-level causal variables from low-level observations. Finally, we delineate some implications of causality for machine learning and propose key research areas at the intersection of both communities.

KEYWORDS | Artificial intelligence; causality; deep learning; representation learning.

I. INTRODUCTION

If we compare what machine learning can do to what animals accomplish, we observe that the former is rather limited at some crucial feats where natural intelligence excels. These include transfer to new problems and any form of generalization that is not from one data point to the next (sampled from the same distribution), but rather from one problem to the next—both have been termed *generalization*, but the latter is a much harder form thereof, sometimes referred to as *horizontal*, *strong*, or *out-of-distribution* generalization. This shortcoming is not too surprising, given that machine learning often disregards information that animals use heavily: interventions in the world, domain shifts, and temporal structure—by and large, we consider these factors a nuisance and try to engineer them away. In accordance with this, the majority of current successes of machine learning boil down to large-scale pattern recognition on suitably collected *independent and identically distributed (i.i.d.)* data.

To illustrate the implications of this choice and its relation to causal models, we start by highlighting key research challenges.

A. Issue 1—Robustness

With the widespread adoption of deep learning approaches in computer vision [103], [140], natural language processing [55], and speech recognition [86], a substantial body of literature explored the robustness of the prediction of state-of-the-art deep neural network architectures. The underlying motivation originates from the fact that, in the real world, there is often little control over the distribution from which the data come from. In computer vision [76], [228], changes in the test distribution may, for instance, come from aberrations, such as camera blur, noise, or compression quality [107], [129], [170], [206], or from shifts, rotations, or viewpoints [7],

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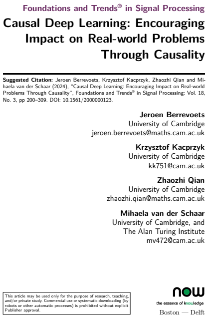

Foundations and Trends® in Signal Processing

Causal Deep Learning: Encouraging Impact on Real-world Problems Through Causality

Suggested Citation: Jeroen Berrevoets, Krzysztof Kacprzyk, Zhaozhi Qian and Mihaela van der Schaar (2024), "Causal Deep Learning: Encouraging Impact on Real-world Problems Through Causality", Foundations and Trends® in Signal Processing: Vol. 18, No. 3, pp 200–309. DOI: 10.1561/2000000123.

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now
the essence of knowledge
Boston — Delft

. . . causal reasoning can inform how we do ML (transferability, generalization, distribution shifts)

Roadmap

Background: Score-based learning of DAG structure

Concomitant linear DAG estimation

Experimental performance evaluation

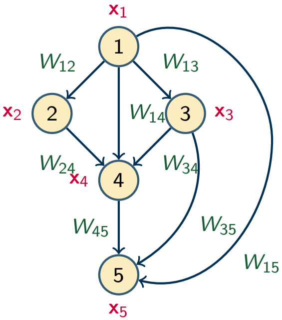
Conclusions

Linear structural equation (causal) models

- DAG $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathbf{W}) \in \mathbb{D}$, vertices $\mathcal{V} = \{1, \ldots, d\}$, edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
  - $\Rightarrow$ Adjacency matrix $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_d] \in \mathbb{R}^{d \times d}$ of edge weights
  - $\Rightarrow$ Entry $W_{ij} \neq 0$ indicates a directed link from node i to j
- Random vector $\mathbf{x} = [x_1, \ldots, x_d] \in \mathbb{R}^d$, joint $p(\mathbf{x})$ Markov w.r.t. $\mathcal{G} \in \mathbb{D}$
  - $\Rightarrow$ DAG $\mathcal{G}$ encodes conditional independencies among variables in $\mathbf{x}$
  - $\Rightarrow$ Each x_i depends only on its parents $\text{PA}_i = \{j \in \mathcal{V} \, : \, W_{ji} \neq 0\}$
- Linear structural equation model (SEM) to generate $p(\mathbf{x})$ consists of

$$x_i = \mathbf{w}_i^\top \mathbf{x} + z_i, \quad \forall i \in \mathcal{V}$$

  - $\Rightarrow$ Mutually independent, exogenous noises $\mathbf{z} = [z_1, \ldots, z_d]^\top \in \mathbb{R}^d$
  - $\Rightarrow$ Ex: $x_4 = \mathbf{w}_4^\top \mathbf{x} + z_4 = W_{14}x_1 + W_{24}x_2 + W_{34}x_3 + z_4$



- **Q:** Estimate $\mathbf{W}$ (learn DAG $\mathcal{G}$) using dataset $\mathbf{X} \in \mathbb{R}^{d \times n}$ with n i.i.d. samples from $p(\mathbf{x})$?

Score-based methods: Problem statement

Given the data matrix $\mathbf{X}$ adhering to a linear SEM, learn the latent DAG $\mathcal{G} \in \mathbb{D}$ by estimating its adjacency matrix $\mathbf{W}$ as the solution to the score-minimization problem

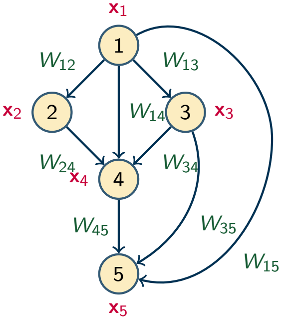
$$\min_{\mathcal{G}(\mathbf{W})} \; \mathcal{S}(\mathcal{G}(\mathbf{W}); \mathbf{X}) \; \text{ subject to } \; \mathcal{G}(\mathbf{W}) \in \mathbb{D}$$

- Learning a DAG solely from observational data $\mathbf{X}$ is NP-hard [Chickering'96]
  - $\Rightarrow$ Combinatorial acyclicity constraint $\mathcal{G} \in \mathbb{D}$ nasty to enforce
  - $\Rightarrow$ Multiple DAGs may generate the same observational distribution $p(\mathbf{x})$
- **Discrete optimization:** combinatorial search methods
  - $\Rightarrow$ Penalized (BIC, MDL) likelihood and Bayesian scoring functions [Peters et al'17]
  - $\Rightarrow$ $|\mathbb{D}|$ grows superexponentially in d, methods face scalability issues
  - $\Rightarrow$ Approximate greedy search [Ramsey et al'17] and order-based methods [Park-Klabjan'17]

Order-based methods: Recent advances

- If DAG's causal (partial) order were known $\Rightarrow$ $\mathbf{W}$ is upper-triangular

$$\mathbf{W} = \begin{bmatrix} 0 & W_{12} & W_{13} & W_{14} & W_{15} \\ 0 & 0 & 0 & W_{24} & 0 \\ 0 & 0 & 0 & W_{34} & W_{35} \\ 0 & 0 & 0 & 0 & W_{45} \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$



- Exploit neat parameterization $\mathcal{G}(\mathbf{W}) \in \mathbb{D} \Leftrightarrow \mathbf{W} = \mathbf{\Pi}^\top \mathbf{U} \mathbf{\Pi}$
  - $\Rightarrow$ $\mathbf{U} \in \mathbb{R}^{d \times d}$ is an upper-triangular weight matrix
  - $\Rightarrow$ Permutation matrix $\mathbf{\Pi} \in \{0,1\}^{d \times d}$ encodes the causal ordering

- Search over exact DAGs in an end-to-end differentiable fashion
  - $\Rightarrow$ Learn permutations with Gumbel-Sinkhorn [Cundy et al'21] or SoftSort [Charpentier et al'22]
  - $\Rightarrow$ Bi-level optimization, topological order swaps at the outer level [Deng et al'23]

- Accurately recovering the causal ordering is challenging, especially when data are limited

Breakthrough: From discrete to continuous optimization

- Acyclicity characterization using nonconvex, smooth functions $\mathcal{H}(\mathbf{W}) : \mathbb{R}^{d\times d} \mapsto \mathbb{R}$

  $\Rightarrow$ Zero level set corresponds to DAGs: $\mathcal{H}(\mathbf{W}) = 0 \iff \mathcal{G}(\mathbf{W}) \in \mathbb{D}$

- **Upshot:** from combinatorial search to nonconvex (smooth) continuous optimization

$$\min_{\mathcal{G}(\mathbf{W})} \; \mathcal{S}(\mathcal{G}(\mathbf{W}); \mathbf{X}) \; \text{ subject to } \; \mathcal{G}(\mathbf{W}) \in \mathbb{D} \quad \iff \quad \min_{\mathbf{W}} \; \mathcal{S}(\mathbf{W}; \mathbf{X}) \; \text{ subject to } \; \mathcal{H}(\mathbf{W}) = 0$$

- **Q:** What are these acyclicity functions $\mathcal{H}$? What about the DAG scoring functions $\mathcal{S}$?

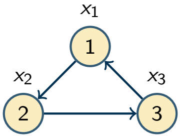
X. Zheng *et al*, "DAGs with NOTEARS: Continuous optimization for structure learning," *NeurIPS*, 2018

Acyclicity functions

- Pioneering NOTEARS formulation proposed $\mathcal{H}_{\text{expm}}(\mathbf{W}) = \operatorname{Tr}\left(e^{\mathbf{W}\circ\mathbf{W}}\right) - d$ [Zheng et al'18]

  $\Rightarrow$ Idea: diagonal entries of powers of $\mathbf{W} \circ \mathbf{W}$ encode information about cycles in $\mathcal{G}$

$$e^{\mathbf{W}} = \sum_{k=0}^{\infty} \frac{(\mathbf{W})^k}{k!} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}}_{\text{self-loops}} + \frac{1}{2} \underbrace{\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}}_{\text{cycles of size 2}} + \frac{1}{6} \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{cycles of size 3}} + \cdots$$



- To speed up computation, [Yu et al'19] advocates $\mathcal{H}_{\text{poly}}(\mathbf{W}) = \operatorname{Tr}\left((\mathbf{I} + \frac{1}{d}\mathbf{W} \circ \mathbf{W})^d\right) - d$

  $\Rightarrow$ Cayley-Hamilton: both $\mathcal{H}_{\text{expm}}$ and $\mathcal{H}_{\text{poly}}$ subsumed by $\operatorname{Tr}\left(\sum_{k=1}^{d} c_k (\mathbf{W} \circ \mathbf{W})^d\right) - d$

- Log-determinant function $\mathcal{H}_{\text{ldet}}(\mathbf{W}; s) = d\log(s) - \log(\det(s\mathbf{I} - \mathbf{W} \circ \mathbf{W})), \quad s > \rho(\mathbf{W} \circ \mathbf{W})$

  $\Rightarrow$ State-of-the-art with several attractive features at the heart of DAGMA

K. Bello *et al*, "DAGMA: Learning DAGs via M-matrices and a log-determinant acyclicity characterization," *NeurIPS*, 2022

Regression-based DAG scoring functions

- Ordinary LS loss augmented with an ℓ_1-norm regularizer

$$\mathcal{S}(\mathbf{W};\mathbf{X}) = \frac{1}{2n}\|\mathbf{X} - \mathbf{W}^\top\mathbf{X}\|_F^2 + \lambda\|\mathbf{W}\|_1$$

$\Rightarrow$ $\lambda \geq 0$ is a tuning parameter that controls edge sparsity

$\Rightarrow$ Computational efficiency, robustness, and even consistency [Loh-Buhlmann'15]

- Multi-task variant of lasso [Tibshirani'96], when response and design matrices coincide

$\Rightarrow$ Optimal rates for $\lambda \asymp \sigma\sqrt{\log d/n}$ [Li et al'20]. But σ^2 is rarely known

- Key limitations we identify:

$\Rightarrow$ Requires carefully retuning λ when unknown σ^2 changes across problems

$\Rightarrow$ Implicitly relies on limiting homoscedasticity assumptions

Contributions

- New convex score function for sparsity-aware learning of linear DAGs
  - ⇒ Incorporate concomitant estimation of scale parameters. Learn $\mathbf{W}$ and σ jointly
  - ⇒ CoLiDE (**C**oncomitant **Li**near **D**AG **E**stimation) decouples λ and σ. No recalibration
  - ⇒ Unlike ordinary LS, it accommodates heteroscedastic exogenous noise profiles
- CoLiDE outperforms state-of-the-art methods across graph ensembles and noise distributions
  - ⇒ Especially when DAGs are larger and the noise level profile is heterogeneous
  - ⇒ Enhanced stability via reduced standard errors across domain-specific metrics

Table: DAG recovery results for 200-node ER4 graphs under homoscedastic Gaussian noise

	Noise variance $= 1.0$				Noise variance $= 5.0$			
	GOLEM	DAGMA	CoLiDE-NV	CoLiDE-EV	GOLEM	DAGMA	CoLiDE-NV	CoLiDE-EV
SHD	468.6±144.0	100.1±41.8	111.9±29	**87.3±33.7**	336.6±233.0	194.4±36.2	157±44.2	**105.6±51.5**
SID	22260±3951	4389±1204	5333±872	**4010±1169**	14472±9203	6582±1227	6067±1088	**4444±1586**
SHD-C	473.6±144.8	101.2±41.0	113.6±29.2	**88.1±33.8**	341.0±234.9	199.9±36.1	161.0±43.5	**107.1±51.6**
FDR	0.28±0.10	0.07±0.03	0.08±0.02	**0.06±0.02**	0.21±0.13	0.15±0.02	0.12±0.03	**0.08±0.04**
TPR	0.66±0.09	0.94±0.01	0.93±0.01	**0.95±0.01**	0.76±0.18	0.92±0.01	0.93±0.01	**0.95±0.01**

S. S. Saboksayr *et al*, "CoLiDE: Concomitant linear DAG estimation," *ICLR*, 2024

Concomitant Linear DAG Estimation

- **Homoscedastic setting:** $z_1, \ldots, z_d$ in the linear SEM have identical variance σ^2
- Inspired by the smoothed concomitant lasso [Ndiaye et al'17], we propose CoLiDE-EV

$$\min_{\mathbf{W}, \sigma \geq \sigma_0} \underbrace{\left[\frac{1}{2n\sigma} \|\mathbf{X} - \mathbf{W}^\top \mathbf{X}\|_F^2 + \frac{d\sigma}{2} + \lambda \|\mathbf{W}\|_1 \right]}_{:=\mathcal{S}(\mathbf{W}, \sigma; \mathbf{X})} \quad \text{subject to} \quad \mathcal{H}(\mathbf{W}) = 0$$

$\Rightarrow$ Can be traced back to the robust linear regression work of [Huber'81]

$\Rightarrow$ Constraint $\sigma \geq \sigma_0$ safeguards against ill-posed scenarios. Set $\sigma_0 = \frac{\|\mathbf{X}\|_F}{\sqrt{dn}} \times 10^{-2}$

- Here λ decouples from σ as minimax optimality now requires $\lambda \asymp \sqrt{\log d/n}$

$\Rightarrow$ Score $\mathcal{S}(\mathbf{W}, \sigma; \mathbf{X})$ is jointly convex w.r.t. $\mathbf{W}$ and σ. Overall nonconvex due to $\mathcal{H}(\mathbf{W})$

$\Rightarrow$ Included $(d\sigma)/2$ so that $\hat{\sigma}^2$ is consistent under Gaussianity

Optimization considerations

- Solve a sequence of unconstrained problems where $\mathcal{H}$ is viewed as a regularizer [Bello et al'22]

  $\Rightarrow$ More effective in practice compared to an augmented Lagrangian method

- Given a decreasing sequence of values $\mu_k \to 0$, at step k of CoLiDE-EV solve

$$\text{(P1)} \quad \min_{\mathbf{W}, \sigma \geq \sigma_0} \mu_k \left[\frac{1}{2n\sigma} \|\mathbf{X} - \mathbf{W}^\top \mathbf{X}\|_F^2 + \frac{d\sigma}{2} + \lambda \|\mathbf{W}\|_1 \right] + \mathcal{H}_{\text{ldet}}(\mathbf{W}, s_k)$$

  $\Rightarrow$ Hyperparameters $\mu_k \geq 0$ and $s_k > 0$ must be prescribed prior to implementation

  $\Rightarrow$ Decreasing the value of μ_k enhances the influence of the acyclicity function

  $\Rightarrow$ Like central path approach of barrier methods. Limit $\mu_k \to 0$ is guaranteed to yield a DAG

Inexact block coordinate descent

- CoLiDE-EV jointly estimates noise level σ and adjacency matrix $\mathbf{W}$ for each μ_k

  $\Rightarrow$ Rely on inexact block coordinate descent (BCD) iterations

- **Step 1:** Fix σ to its most up-to-date value and minimize $\mathcal{S}(\mathbf{W}, \sigma; \mathbf{X})$ inexactly w.r.t. $\mathbf{W}$

  $\Rightarrow$ Run one iteration of the ADAM optimizer

- **Step 2:** Update σ in closed form given the latest $\mathbf{W}$

$$\hat{\sigma} = \max\left(\frac{1}{\sqrt{nd}}\|\mathbf{X} - \mathbf{W}^\top\mathbf{X}\|_F, \sigma_0\right) = \max\left(\sqrt{\mathrm{Tr}\left((\mathbf{I} - \mathbf{W})^\top \mathrm{cov}(\mathbf{X})(\mathbf{I} - \mathbf{W})\right)/d}, \sigma_0\right)$$

  $\Rightarrow$ Precomputed sample covariance matrix $\mathrm{cov}(\mathbf{X}) := \frac{1}{n}\mathbf{X}\mathbf{X}^\top$

- Provably convergent block successive convex approximation (BSCA) algorithm also effective

S. S. Saboksayr *et al*, “Block successive convex approximation for concomitant linear DAG estimation,” *SAM Workshop*, 2024

Heteroscedastic linear SEM

- **Heteroscedastic setting:** noise variables have non-equal variances (NV) $\sigma_1^2, \ldots, \sigma_d^2$

- Mimicking the optimization approach for the EV case, we propose CoLiDE-NV

$$(\text{P2}) \qquad \min_{\mathbf{W}, \boldsymbol{\Sigma} \geq \boldsymbol{\Sigma}_0} \mu_k \left[\frac{1}{2n} \operatorname{Tr}\left((\mathbf{X} - \mathbf{W}^\top \mathbf{X})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{X} - \mathbf{W}^\top \mathbf{X}) \right) + \frac{1}{2} \operatorname{Tr}(\boldsymbol{\Sigma}) + \lambda \|\mathbf{W}\|_1 \right] + \mathcal{H}_{\text{ldet}}(\mathbf{W}, s_k)$$

$\Rightarrow$ $\boldsymbol{\Sigma} = \operatorname{diag}(\sigma_1, \ldots, \sigma_d)$ is a diagonal matrix of exogenous noise standard deviations

$\Rightarrow$ Special case $\boldsymbol{\Sigma} = \sigma \mathbf{I}$ yields CoLiDE-EV score function

- Closed-form solution for $\boldsymbol{\Sigma}$ given $\mathbf{W}$

$$\hat{\boldsymbol{\Sigma}} = \max\left(\sqrt{\operatorname{diag}\left((\mathbf{I} - \mathbf{W})^\top \operatorname{cov}(\mathbf{X})(\mathbf{I} - \mathbf{W}) \right)}, \boldsymbol{\Sigma}_0 \right) \quad \text{or} \quad \hat{\sigma}_i = \max\left(\frac{1}{\sqrt{n}} \|\mathbf{x}_i - \mathbf{w}_i{}^\top \mathbf{X}\|_2, \sigma_0 \right)$$

- CoLiDE's per iteration cost is $\mathcal{O}(d^3)$, on par with state-of-the-art DAG learning methods

Summary and discussion points

```
Algorithm 1: CoLiDE optimization
In: data $\mathbf{X}$ and hyperparameters $\lambda$ and $H = \{(\mu_k, s_k, T_k)\}_{k=1}^{K}$.
Out: DAG $\mathbf{W}$ and the noise estimate $\sigma$ (EV) or $\mathbf{\Sigma}$ (NV).
Compute lower-bounds $\sigma_0$ or $\mathbf{\Sigma}_0$.
Initialize $\mathbf{W} = \mathbf{0}$, $\sigma = \sigma_0 \times 10^2$ or $\mathbf{\Sigma} = \mathbf{\Sigma}_0 \times 10^2$.
foreach $(\mu_k, s_k, T_k) \in H$ do
    for $t = 1, \ldots, T_k$ do
        Apply CoLiDE-EV or NV updates using $\mu_k$ and $s_k$.
```

```
Function CoLiDE-EV update:
    Update W with one iteration of
      a first-order method for (P1)
    Compute $\hat{\sigma}$ in closed form
Function CoLiDE-NV update:
    Update W with one iteration of
      a first-order method for (P2)
    Compute $\hat{\mathbf{\Sigma}}$ in closed form
```

- Decomposable: unlike Gaussian profile log-likelihood in GOLEM [Ng et al'20]

$$\mathcal{S}(\mathbf{W}; \mathbf{X}) = -\frac{1}{2}\sum_{i=1}^{d} \log\left(\left\|\mathbf{x}_i - \mathbf{w}_i^\top \mathbf{X}\right\|_2^2\right) + \log\left(|\det(\mathbf{I} - \mathbf{W})|\right) + \lambda\|\mathbf{W}\|_1$$

- Guarantees: consider general (non-identifiable) linear Gaussian SEMs

  $\Rightarrow$ As $n \to \infty$ CoLiDE-NV outputs a DAG quasi-equivalent to the ground-truth graph

- Flexible: other convex losses beyond LS, other $\mathcal{H}$, nonlinear SEMs, impact to order-based methods

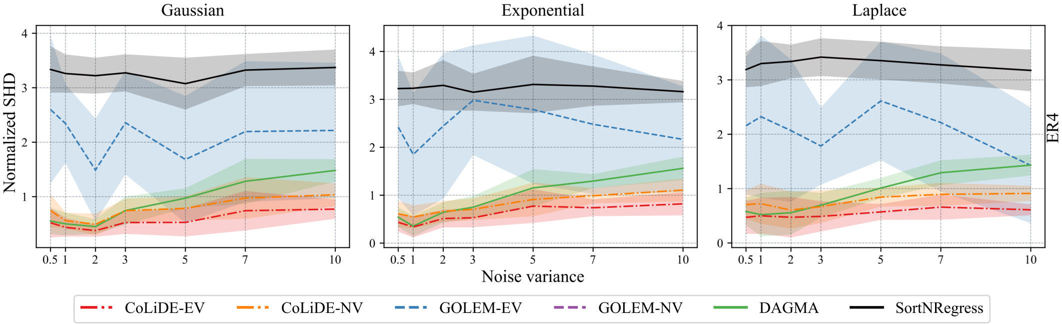
I. Ng *et al*, "On the role of sparsity and DAG constraints for learning linear DAGs," *NeurIPS*, 2020

Experimental performance evaluation

- Comprehensive evaluation to assess the effectiveness of the CoLiDE framework
  - ⇒ Validate DAG recovery performance in synthetic EV and NV settings
  - ⇒ Examine noise estimation performance
  - ⇒ Evaluate DAG recovery performance on real-world datasets
  - ⇒ Compare with other methods such as DAGMA, GOLEM, SortNRegress, GES, . . .
- Tests across graph types (edge weights, average degree), noise distributions, values of d, n, σ
- Reproducibility: code to generate all figures at `https://github.com/SAMiatto/colide`

Experiments: Homoscedastic setting

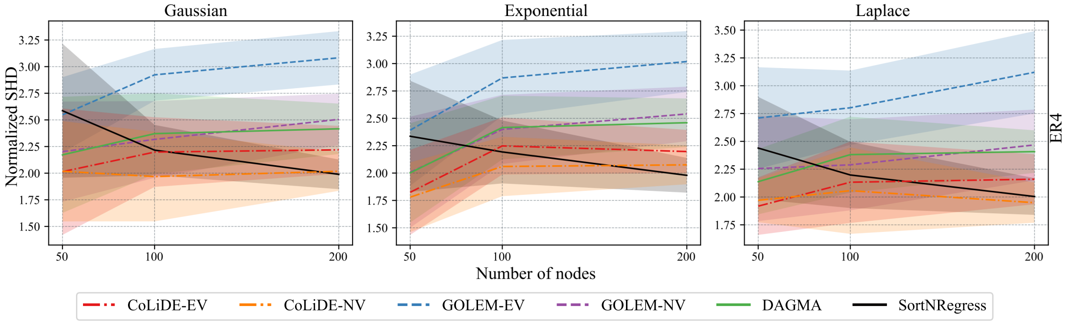
- Investigate the impact of noise level σ^2 on DAG recovery performance
  - Graphs: 200-node ER4 graphs, W_{ij} drawn uniformly from $[-2, -0.5] \cup [0.5, 2]$
  - Data: $n = 1000$ samples via linear SEM, diverse noise distributions
  - Metric: SHD counts number of edge corrections required to recover true graph from estimate



- CoLiDE-EV outperforming DAGMA clearly demonstrates the gains come from $\mathcal{S}(\mathbf{W}, \sigma; \mathbf{X})$

Experiments: Heteroscedastic setting

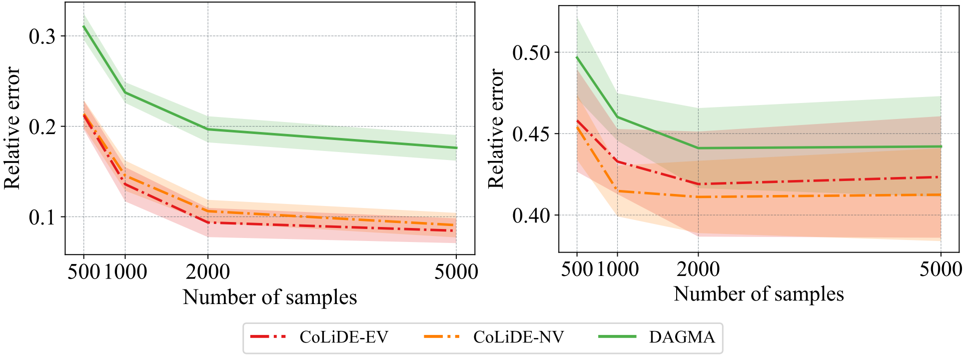
- Heteroscedastic scenario poses further challenges $\Rightarrow$ Non-indentifiable from observational data
  - Noise variance of each node σ_i^2 is uniformly drawn from $[0.5, 10]$
  - Graphs: ER4 graphs varying d; W_{ij} drawn from $[-1, -0.25] \cup [0.25, 1]$ (lower SNR)
  - Data: $n = 1000$ samples via linear SEM, diverse noise distributions



- CoLiDE-NV yields lower deviations than DAGMA and GOLEM, underscoring its robustness

Experiments: Noise estimation

- Method's ability to estimate noise variance $\Rightarrow$ Proficiency in recovering accurate edge weights
  - DAGMA does not explicitly estimate noise level, we use $\hat{\sigma}_i{}^2 = \frac{1}{n}\|\mathbf{x}_i - \hat{\mathbf{w}}_i{}^\top \mathbf{X}\|_2^2$
  - Graphs: 200-node ER4 graphs, W_{ij} drawn uniformly from $[-2, -0.5] \cup [0.5, 2]$
  - Signals: Linear SEM with Gaussian noise; vary n for EV (left) and NV (right) scenarios



- CoLiDE-NV provides lower error even when using half as many samples as DAGMA

Experiments: Cell-signaling data

- Tested CoLiDE on the Sachs dataset [Sachs et al'05]
  - ⇒ Cytometric measurements from human immune system
  - ⇒ Comprises $d = 11$ proteins, 17 edges, and $n = 853$ samples
  - ⇒ Associated DAG is obtained through experimental methods
- CoLiDE-NV attains lowest SHD to date for this problem

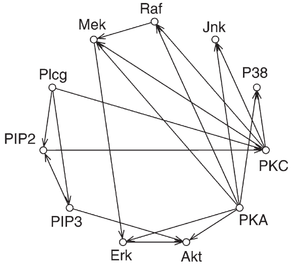


Table: DAG recovery performance on the Sachs dataset

	GOLEM-EV	GOLEM-NV	DAGMA	SortNRegress	DAGuerreotype	GES	CoLiDE-EV	CoLiDE-NV
SHD	22	15	16	13	14	13	13	**12**
SID	49	58	52	47	50	56	47	**46**
SHD-C	19	**11**	15	13	12	**11**	13	14
FDR	0.83	0.66	**0.5**	0.61	0.57	**0.5**	0.54	0.53
TPR	0.11	0.11	0.05	0.29	0.17	0.23	0.29	**0.35**

K. Sachs *et al*, "Causal protein-signaling networks derived from multiparameter single-cell data," *Science*, 2005

Concluding remarks and the road ahead

- DAGs as general descriptors of causal and (in)dependence relationships
  - ⇒ Understanding the enforcement of acyclicty for DAG learning from observational data
  - ⇒ Emphasizing the significance of the score function in continuous-optimization methods
- Proposed framework: CoLiDE (**C**oncomitant **Li**near **D**AG **E**stimation)
  - ⇒ Jointly estimates the DAG structure and noise level
  - ⇒ Adaptivity to changes in noise levels, requires less fine-tuning
  - ⇒ Applicable to challenging heteroscedastic scenarios
  - ⇒ Surpassing state-of-the-art in DAG recovery performance
- Ongoing and future work:
  - ⇒ Non-linear SEMs via neural networks or kernels
  - ⇒ Online DAG learning from streaming signals, time-series data via SVAR models