

CoLiDE: Concomitant Linear DAG Estimation

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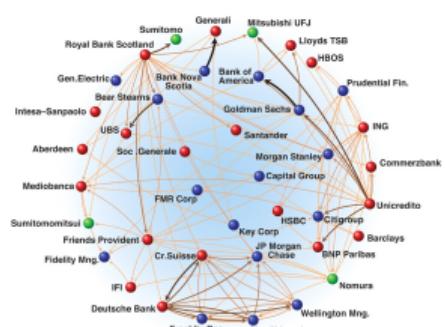
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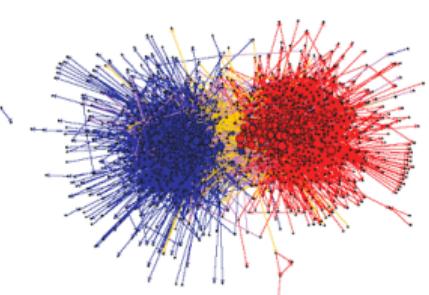
Learning from relational data

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

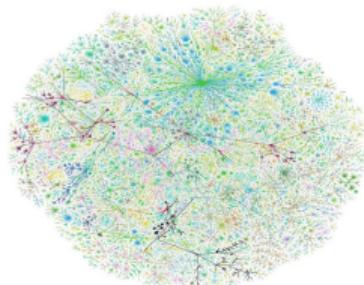
Economic Networks



Social and Information Networks



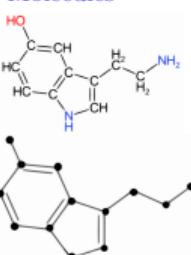
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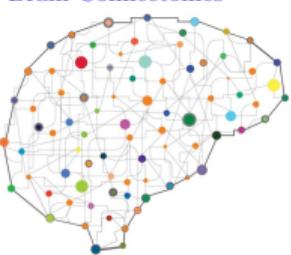
3D Meshes



Molecules



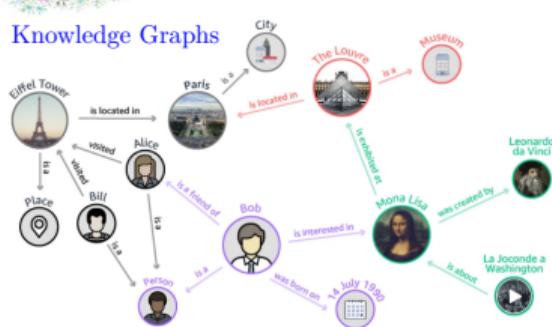
Brain Connectomes



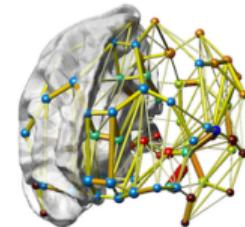
Transportation Networks



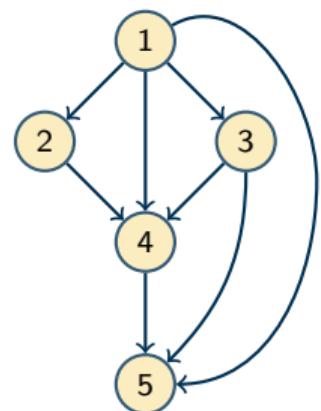
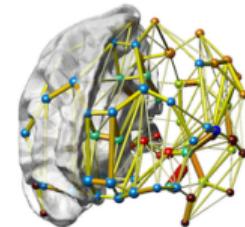
Knowledge Graphs



- ▶ 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]

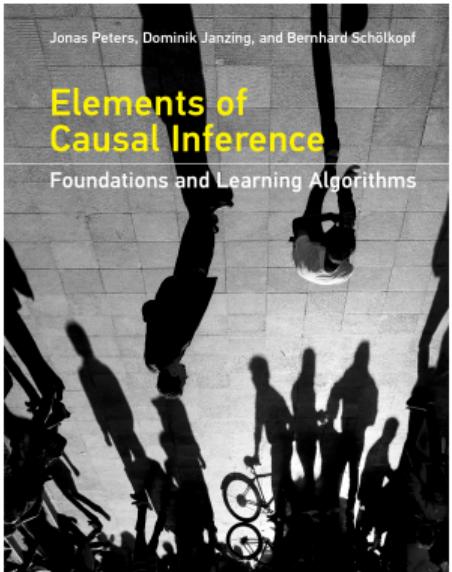


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- ▶ This work: learn the structure of directed acyclic graphs (DAGs)
- ▶ DAGs have become prominent models in various ML applications
 - ⇒ Conditional independences among variables in Bayesian networks
 - ⇒ DAG edges may have causal interpretations
 - ⇒ 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...



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 Schölkopf¹, Francesco Locatello², Stefan Bauer¹, Nan Rosemary Ke,
Nal Kalchbrenner, Anirudh Goyal, and Yairi Feinberg³

ABSTRACT : The two fields of machine learning and graphical causality share some deep theoretical connections. In this article, we review these connections, increasing awareness in machine learning of the advances of the other. In this article, we review fundamental concepts of causal inference and relate them to open problems of machine learning, including transfer learning and generalization. thereby assaying how causality can contribute to modern machine learning research. This also applies to the field of representation learning, where causal inference starts from the premise that the causal variables are generated. A central problem for it is how causality can be used to learn causal variables from low-level observations. Finally, we delineate some implications of causality for machine learning and point to many research areas at the intersection of both communities.

KEYWORDS : Artificial intelligence; causality; deep learning; representation learning

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Foundations and Trends® in Signal Processing Causal Deep Learning: Encouraging Impact on Real-world Problems Through Causality

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now
the essence of knowledge
Boston — Delhi

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

Roadmap

Background: Score-based learning of DAG structure

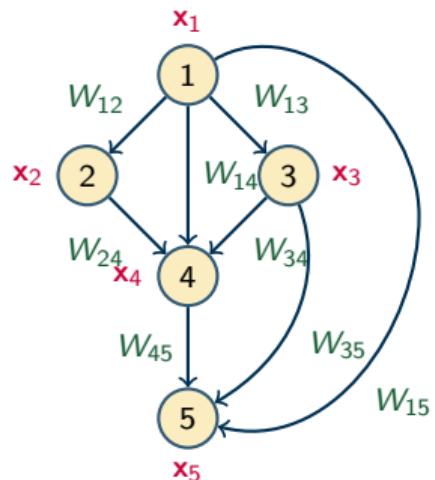
Concomitant linear DAG estimation

Experimental performance evaluation

Conclusions

Linear structural equation (causal) models

- ▶ DAG $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathbf{W}) \in \mathbb{D}$, vertices $\mathcal{V} = \{1, \dots, d\}$, edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
 - \Rightarrow Adjacency matrix $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_d] \in \mathbb{R}^{d \times d}$ of edge weights
 - \Rightarrow Entry $W_{ij} \neq 0$ indicates a directed link from node i to j
- ▶ Random vector $\mathbf{x} = [x_1, \dots, x_d] \in \mathbb{R}^d$, 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 $\text{PA}_i = \{j \in \mathcal{V} : W_{ji} \neq 0\}$

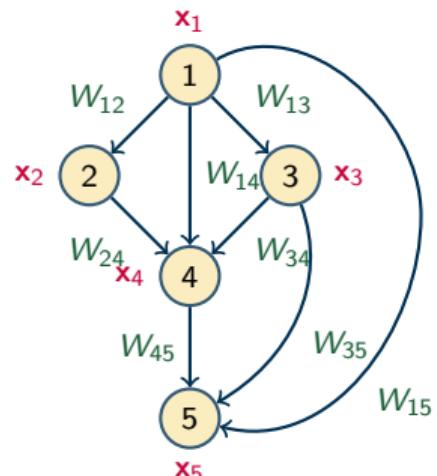


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- ▶ Linear structural equation model (SEM) to generate $p(\mathbf{x})$ consists of

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

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



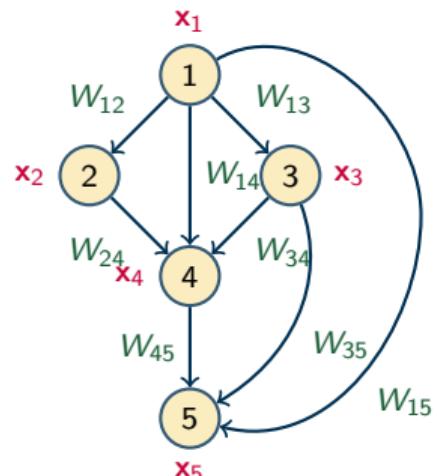
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- ▶ **Q:** Estimate \mathbf{W} (learn DAG \mathcal{G}) using dataset $\mathbf{X} \in \mathbb{R}^{d \times n}$ with n i.i.d. samples from $p(\mathbf{x})$?



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]
 - ⇒ Combinatorial acyclicity constraint $\mathcal{G} \in \mathbb{D}$ nasty to enforce
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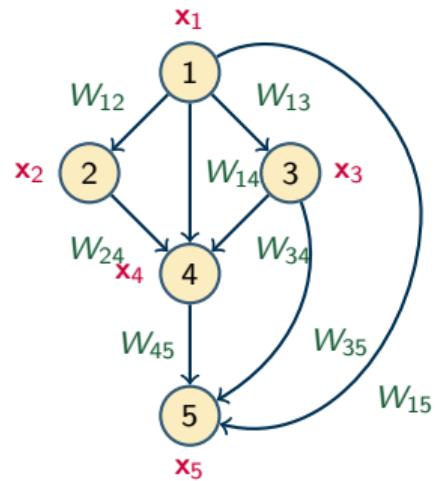
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- ▶ Discrete optimization: combinatorial search methods
 - ⇒ Penalized (BIC, MDL) likelihood and Bayesian scoring functions [Peters et al'17]
 - ⇒ $|\mathbb{D}|$ grows superexponentially in d , methods face scalability issues
 - ⇒ Approximate greedy 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

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

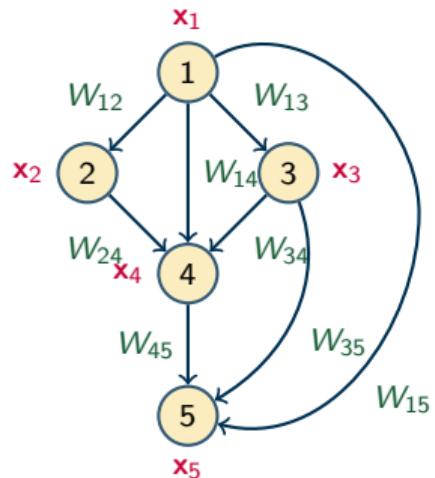


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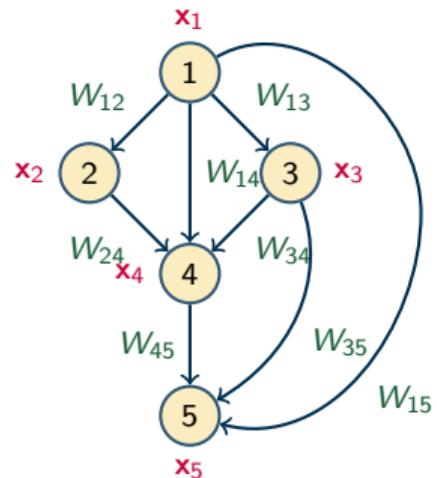
- Exploit neat parameterization $\mathcal{G}(\mathbf{W}) \in \mathbb{D} \Leftrightarrow \mathbf{W} = \boldsymbol{\Pi}^T \mathbf{U} \boldsymbol{\Pi}$
 - $\Rightarrow \mathbf{U} \in \mathbb{R}^{d \times d}$ is an upper-triangular weight matrix
 - \Rightarrow Permutation matrix $\boldsymbol{\Pi} \in \{0,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



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- 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



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

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

- ▶ **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

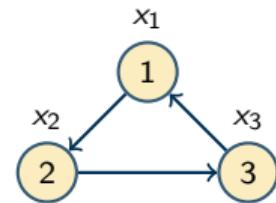
Acyclicity functions

- ▶ Pioneering **NOTEARS** formulation proposed $\mathcal{H}_{\text{expm}}(\mathbf{W}) = \text{Tr}(e^{\mathbf{W} \circ \mathbf{W}}) - d$ [Zheng et al'18]
⇒ Idea: diagonal entries of powers of $\mathbf{W} \circ \mathbf{W}$ encode information about **cycles** in \mathcal{G}

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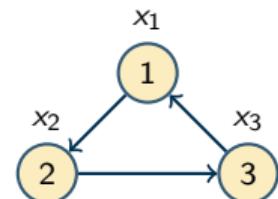
$$e^{\mathbf{W}} = \sum_{k=0}^{\infty} \frac{(\mathbf{W})^k}{k!} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{self-loops}} + \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}}_{\text{cycles of size 2}} + \frac{1}{2} \underbrace{\begin{bmatrix}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



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- To speed up computation, [Yu et al'19] advocates $\mathcal{H}_{\text{poly}}(\mathbf{W}) = \text{Tr}((\mathbf{I} + \frac{1}{d}\mathbf{W} \circ \mathbf{W})^d) - d$
 ⇒ Cayley-Hamilton: both $\mathcal{H}_{\text{expm}}$ and $\mathcal{H}_{\text{poly}}$ subsumed by $\text{Tr} \left(\sum_{k=1}^d c_k (\mathbf{W} \circ \mathbf{W})^k \right) - d$
- Log-determinant function $\mathcal{H}_{\text{ldet}}(\mathbf{W}; s) = d \log(s) - \log(\det(s\mathbf{I} - \mathbf{W} \circ \mathbf{W}))$, $s > \rho(\mathbf{W} \circ \mathbf{W})$
 ⇒ State-of-the-art with several attractive features at the heart of **DAGMA**

- ▶ Ordinary LS loss augmented with an ℓ_1 -norm regularizer

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

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

⇒ Computational efficiency, robustness, and even consistency [Loh-Buhlmann'15]

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⇒ Computational efficiency, robustness, and even consistency [Loh-Buhlmann'15]

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

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

- ▶ Key limitations we identify:

⇒ Requires carefully retuning λ when unknown σ^2 changes across problems

⇒ Implicitly relies on limiting homoscedasticity assumptions

- ▶ New convex score function for sparsity-aware learning of linear DAGs
 - ⇒ Incorporate concomitant estimation of scale parameters. Learn \mathbf{W} and σ jointly
 - ⇒ CoLiDE (Concomitant Linear DAG Estimation) decouples λ and σ . No recalibration
 - ⇒ Unlike ordinary LS, it accommodates heteroscedastic exogenous noise profiles

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 (**Concomitant Linear DAG Estimation**) 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. Saboktasir et al., "CoLiDE: Concomitant linear DAG estimation," ICLR, 2024

- **Homoscedastic setting:** z_1, \dots, 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**

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

- ⇒ Can be traced back to the **robust linear regression** work of [Huber'81]
- ⇒ Constraint $\sigma \geq \sigma_0$ safeguards against **ill-posed** scenarios. Set $\sigma_0 = \frac{\|\mathbf{X}\|_F}{\sqrt{dn}} \times 10^{-2}$

- **Homoscedastic setting:** z_1, \dots, 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**

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

- ⇒ Can be traced back to the **robust linear regression** work of [Huber'81]
- ⇒ 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 $\lambda \asymp \sqrt{\log d/n}$
 - ⇒ Score $\mathcal{S}(\mathbf{W}, \sigma; \mathbf{X})$ is **jointly convex** w.r.t. \mathbf{W} and σ . Overall nonconvex due to $\mathcal{H}(\mathbf{W})$
 - ⇒ Included $(d\sigma)/2$ so that $\hat{\sigma}^2$ is **consistent** under **Gaussianity**

- ▶ Solve a **sequence of unconstrained** problems where \mathcal{H} is viewed as a regularizer [Bello et al'22]
 - ⇒ More **effective** in practice compared to an **augmented Lagrangian** method
- ▶ Given a **decreasing** sequence of values $\mu_k \rightarrow 0$, at step k of **CoLiDE-EV** solve

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

- ⇒ Hyperparameters $\mu_k \geq 0$ and $s_k > 0$ must be **prescribed** prior to implementation
- ⇒ **Decreasing** the value of μ_k **enhances** the influence of the acyclicity function
- ⇒ Like central path approach of barrier methods. **Limit** $\mu_k \rightarrow 0$ 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
 - ⇒ 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}
 - ⇒ Run one iteration of the ADAM optimizer
- ▶ Step 2: Update σ in closed form given the latest \mathbf{W}

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

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

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

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

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

⇒ $\boldsymbol{\Sigma} = \text{diag}(\sigma_1, \dots, \sigma_d)$ is a diagonal matrix of exogenous noise **standard deviations**

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

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

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

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

- ▶ 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 λ and $H = \{(\mu_k, s_k, T_k)\}_{k=1}^K$.
Out: DAG \mathbf{W} and the noise estimate σ (EV) or Σ (NV).
 Compute lower-bounds σ_0 or Σ_0 .
 Initialize $\mathbf{W} = \mathbf{0}$, $\sigma = \sigma_0 \times 10^2$ or $\Sigma = \Sigma_0 \times 10^2$.
foreach $(\mu_k, s_k, T_k) \in H$ **do**
for $t = 1, \dots, T_k$ **do**
 Apply CoLiDE-EV or NV updates using μ_k and s_k .

Function *CoLiDE-EV update*:

Update \mathbf{W} with one iteration of
 a first-order method for (P1)
 Compute $\hat{\sigma}$ in closed form

Function *CoLiDE-NV update*:

Update \mathbf{W} with one iteration of
 a first-order method for (P2)
 Compute $\hat{\Sigma}$ in closed form

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

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

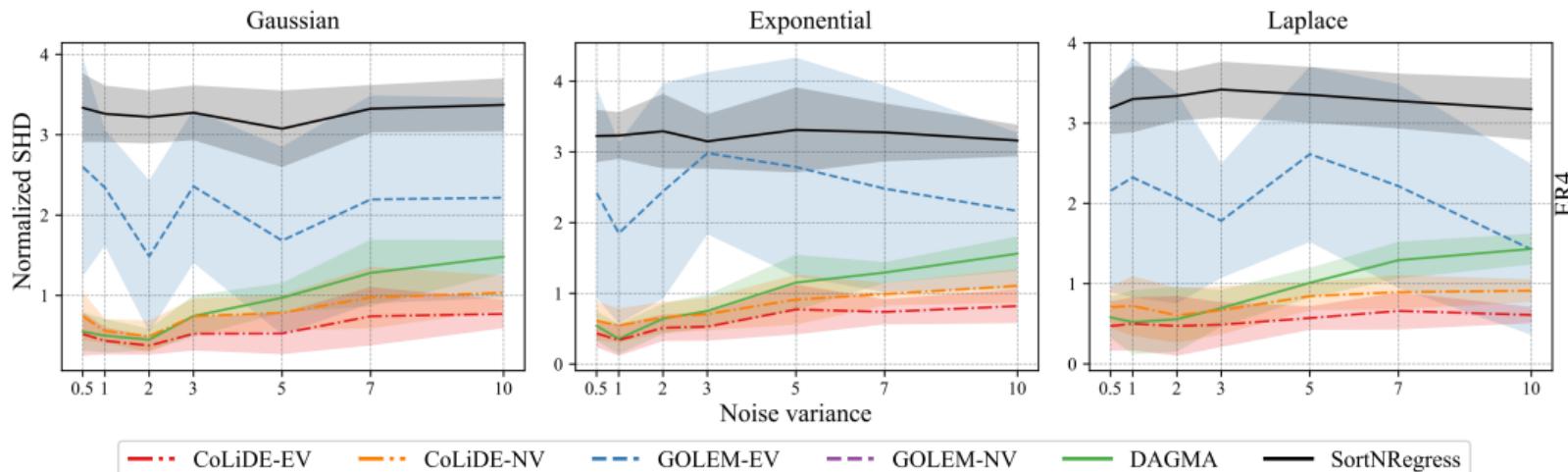
- ▶ **Guarantees:** consider general (non-identifiable) linear **Gaussian SEMs**
 ⇒ As $n \rightarrow \infty$ **CoLiDE-NV** outputs a DAG quasi-equivalent to the ground-truth graph
- ▶ **Flexible:** other convex losses beyond LS, other \mathcal{H} , nonlinear SEMs, impact to order-based methods

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

- ▶ 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

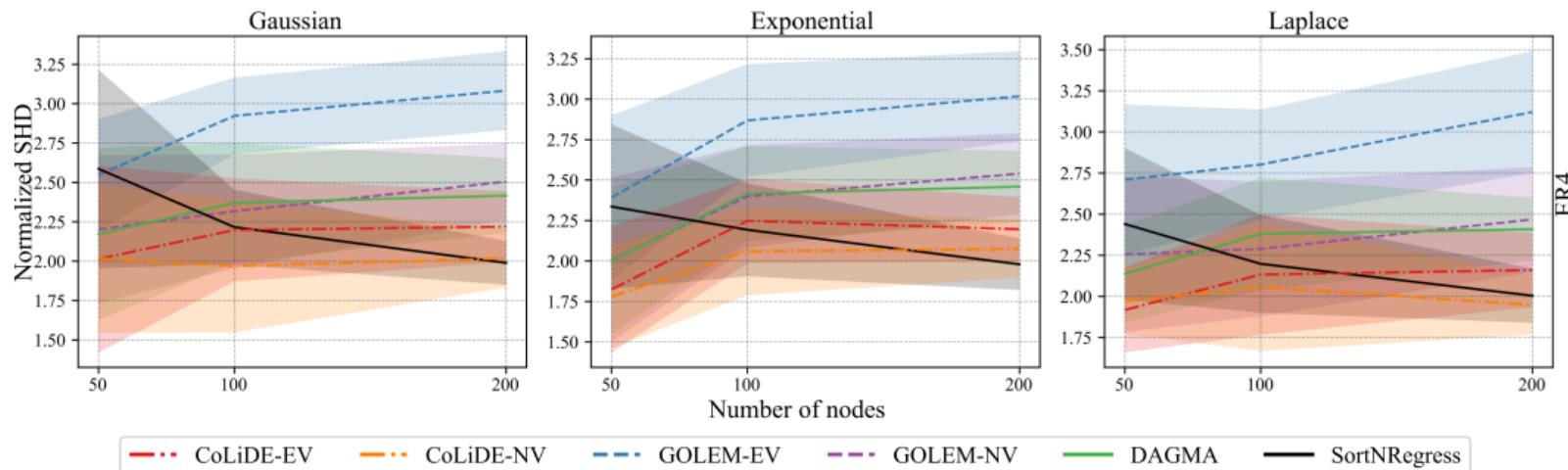
- ▶ Investigate the impact of **noise level** σ^2 on DAG recovery performance
 - ▶ **Graphs:** 200-node ER4 graphs, W_{ij} drawn uniformly from $[-2, -0.5] \cup [0.5, 2]$
 - ▶ **Data:** $n = 1000$ samples via **linear SEM**, diverse noise distributions
 - ▶ **Metric:** SHD counts number of edge corrections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



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

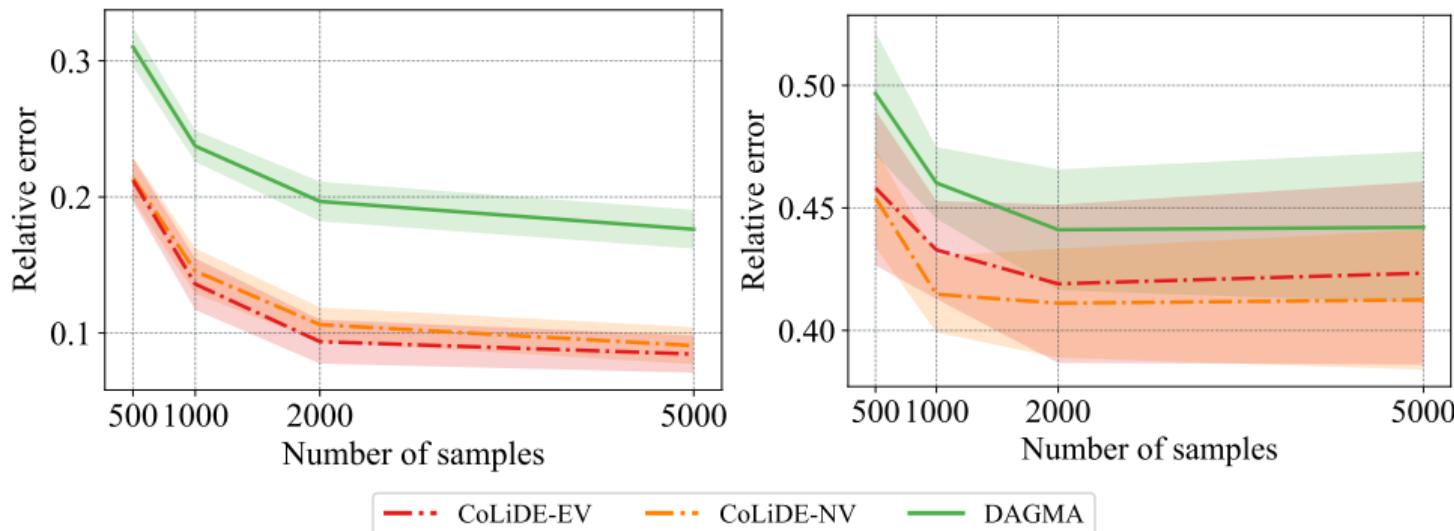
Experiments: Heteroscedastic setting

- 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

- ▶ 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

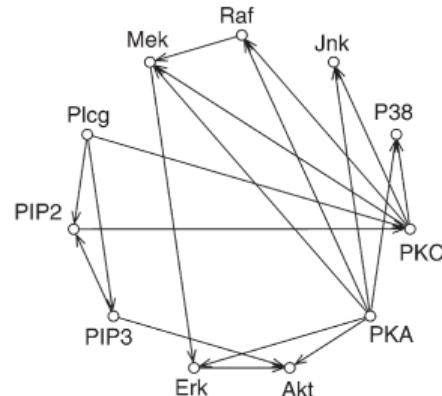


Table: DAG recovery performance on the Sachs dataset

	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 **acyclicity** for DAG learning from **observational data**
 - ⇒ Emphasizing the significance of the **score function** in continuous-optimization methods
- ▶ Proposed framework: **CoLiDE** (**C**oncomitant **L**inear **DAG** **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

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 - ⇒ 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