Learning Causal Structures via Gradient-Based Optimization

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Overview

- Causality Framework
  - Causal Graphical Models
  - Motivating example
  - Markov Equivalence and Structure Identifiability
- Causal Structure Learning
  - Problem formulation
  - Discrete Search Algorithms
  - Gradient-Based Algorithms
- GraN-DAG & extensions
  - The algorithm
  - With interventional data
  - Neural Autoregressive Flows

Causal graphical models (CGM)

- Random vector $X \in \mathbb{R}^d$ (d variables)
- Let $\mathcal{G}$ be a **directed acyclic graph** (DAG)
- Assume $p(x) = \prod_{i=1}^{d} p(x_i | x_{\pi_i^{\mathcal{G}}})$
  $\pi_i^{\mathcal{G}} =$ parents of i in $\mathcal{G}$
- Encodes **(conditional) independence statements** (via *d-separation*, see [Koller & Friedman, 2009])
- Almost identical to Bayesian Networks but allows for **interventional distributions:** $p(x|do(z))$

Simple example

$\mathcal{G} = (V, E)$

$$p(x, y, z) = p(x)p(z \mid x)p(y \mid z)$$

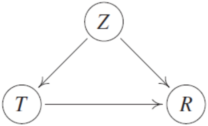
$$\implies p(x, y|z) = p(x|z)p(y|z)$$

i.e. $X \perp\!\!\!\perp Y \mid Z$

The **do operator** will be explained in the following example...

Why should you care: Kidney Stone Treatment

T = Treatment $\in \{A, B\}$
Z = Stone size $\in \{\text{small}, \text{large}\}$
R = Patient recovered $\in \{0, 1\}$



	Overall	Patients with small stones	Patients with large stones
Treatment *a*: Open surgery	78% (273/350)	**93%** (81/87)	**73%** (192/263)
Treatment *b*: Percutaneous nephrolithotomy	**83%** (289/350)	87% (234/270)	69% (55/80)

(Example taken from *Element of Causal Inference* by Peters et al. p111)

Why should you care: Kidney Stone Treatment

Pay attention to these two questions...
Assuming the size of your stone is unknown...

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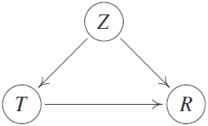

What is your chance of recovery knowing that the doctor gave you treatment A?

- Knowing that your doctor gave you treatment A tells you that you probably have a large kidney stone ... $P(Z = large | T = A) = 0.75$

- ... which reduces your chance of recovery $P(R = 1 | T = A, Z = large) = 0.73 < 0.93 = P(R = 1 | T = A, Z = small)$

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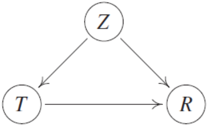

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What is your chance of recovery if you decide to take treatment A?

- Your really don't know anything about your kidney stone
- **You taking treatment A is not a function of any variable**

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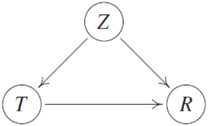

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$P(R = 1|T = A) = 0,78$ $P(R = 1|T = B) = \mathbf{0,83}$

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$$
\begin{tikzcd}
 & Z \arrow[dl] \arrow[dr] & \\
T \arrow[rr] & & R
\end{tikzcd}
$$

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What is your chance of recovery if you decide to take treatment A?

$P(R = 1|do(T = A)) = \mathbf{0{,}832}$ $\quad$ $P(R = 1|do(T = B)) = 0,782$

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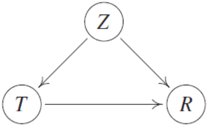

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But how do we compute these **interventional distributions**?!

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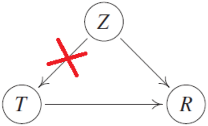


$$P(R, Z|do(T = A)) = P(R|Z, T = A)\underbrace{\cancel{P(T = A|Z)}}_{\text{The decision of taking treatment } A \text{ does not depend on } Z \text{ anymore}} P(Z)$$

Then simply marginalize as usual:

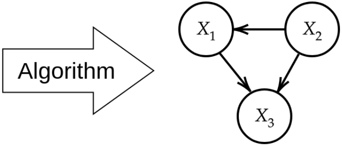
$$P(R = 1|do(T = A)) = \sum_Z P(R = 1, Z|do(T = A))$$
$$= \sum_Z P(R = 1|Z, T = A)P(Z) = 0,832$$

Structure Learning

- In the kidney stone example, **the causal graph was known**
- What if we don't have it? **Learn it!**

Purely observational data

	X_1	X_2	X_3
sample 1	1.76	10.46	0.002
sample2	3.42	78.6	0.011
...		...	
sample n	4.56	9.35	1.96



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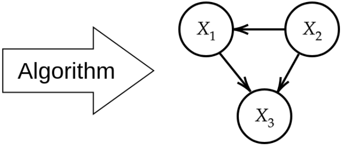

Is it even possible?

Identifiability

- In general, this is impossible without interventional data...

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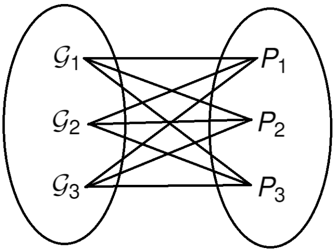
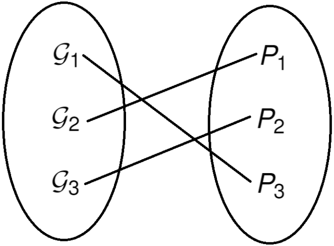
- Multiple DAGs can express the same distribution...



Identifiability

- If we assume causal mechanisms are "simple", then $\mathcal{G}$ can be identified...



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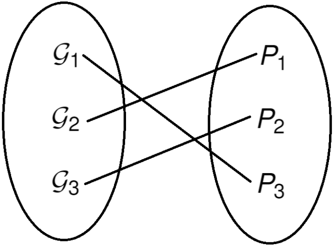

An example (useful later!)

If data follows this model...

$$X_i | X_{\pi_i^{\mathcal{G}}} \sim \mathcal{N}(f_i(X_{\pi_i^{\mathcal{G}}}), \sigma_i^2)$$

...then **correct causal DAG $\mathcal{G}$ can be identified from purely observational data** (see [Peters et al., 2014] for proof and regularity conditions)

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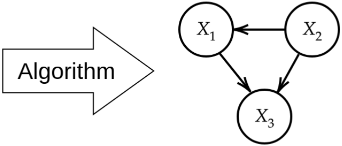


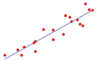
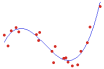
Score-based algorithms

$$\hat{\mathcal{G}} = \arg\max_{\mathcal{G} \in \text{DAG}} \text{Score}(\mathcal{G})$$

Often, $\text{Score}(\mathcal{G}) =$ regularized maximum likelihood under $\mathcal{G}$

Structure Learning

Taxonomy of score-based algorithms (non-exhaustive)

		Discrete optim.	Continuous optim.
	Linear	GES [Chickering, 2003]	NOTEARS [Zheng et al., 2018]
	Nonlinear	CAM [Bühlmann et al., 2014]	GraN-DAG [Lachapelle et al., 2020]

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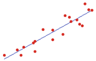
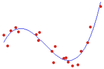
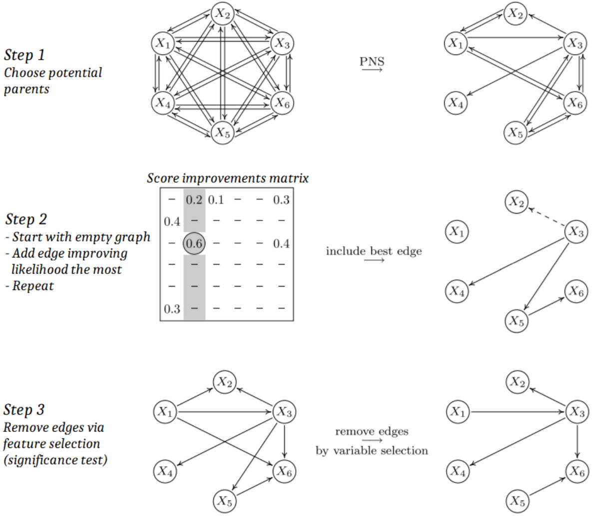
	Linear	GES [Chickering, 2003]	NOTEARS [Zheng et al., 2018]
	Nonlinear	**CAM** **[Bühlmann et al., 2014]**	GraN-DAG [Lachapelle et al., 2020]

A greedy algorithm - CAM [Bühlmann et al., 2014]



Figures from [Bühlmann et al., 2014]

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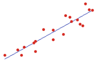
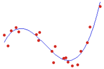
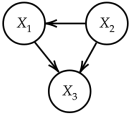
	Linear	GES [Chickering, 2003]	**NOTEARS [Zheng et al., 2018]**
	Nonlinear	CAM [Bühlmann et al., 2014]	GraN-DAG [Lachapelle et al., 2020]

NOTEARS: Continuous optimization for structure learning

- Encode graph as a **weighted adjacency matrix** $U = [u_1 | \dots | u_d] \in \mathbb{R}^{d \times d}$



$$\underbrace{A = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}}_{\text{Adjacency matrix}} \quad \underbrace{U = \begin{pmatrix} 0 & 0 & 4.8 \\ 0.2 & 0 & -1.7 \\ 0 & 0 & 0 \end{pmatrix}}_{\text{Weighted adjacency matrix}}$$

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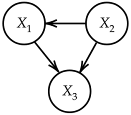

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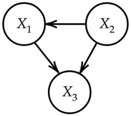

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- For an arbitrary U, associated graph might be cyclic

Acyclicity constraint

NOTEARS [Zheng et al., 2018] uses this **differentiable acyclicity constraint**:

$$\operatorname{Tr} e^{U \odot U} - d = 0 \qquad \left(e^M \triangleq \sum_{k=0}^{\infty} \frac{M^k}{k!} \right)$$

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NOTEARS: Continuous optimization for structure learning

- NOTEARS [Zheng et al., 2018]:
  Solve this **continuous constrained optimization problem**:

$$\max_{U} \underbrace{-\|\mathbf{X} - \mathbf{X}U\|_F^2 - \lambda\|U\|_1}_{\text{Score}} \quad \text{s.t.} \quad \operatorname{Tr} e^{U \odot U} - d = 0$$

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- where $\mathbf{X} \in \mathbb{R}^{n \times d}$ is the design matrix containing all n samples
- Solve approximately using an **Augmented Lagrangian method**
- Amounts to maximizing (with gradient ascent)

$$-\|\mathbf{X} - \mathbf{X}U\|_F^2 - \lambda\|U\|_1 - \alpha_t(\operatorname{Tr} e^{U \odot U} - d) - \frac{\mu_t}{2}(\operatorname{Tr} e^{U \odot U} - d)^2$$

- while gradually increasing α_t and μ_t

NOTEARS: The acyclicity constraint

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Suppose $A \in \{0,1\}^{d \times d}$ is an adjacency matrix for a certain directed graph

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Graph acyclic $\iff$ $(A^k)_{ii} = 0$ for all i and all k

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\end{aligned}$$

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The argument is almost identical when using weighted adjacency U instead of A...

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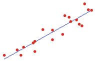
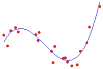
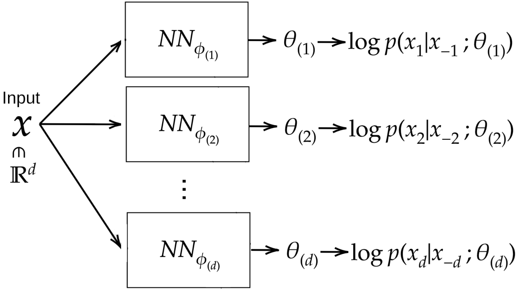
	Linear	GES [Chickering, 2003]	NOTEARS [Zheng et al., 2018]
	Nonlinear	CAM [Bühlmann et al., 2014]	**GraN-DAG** **[Lachapelle et al., 2020]**

Gradient-Based Neural DAG Learning

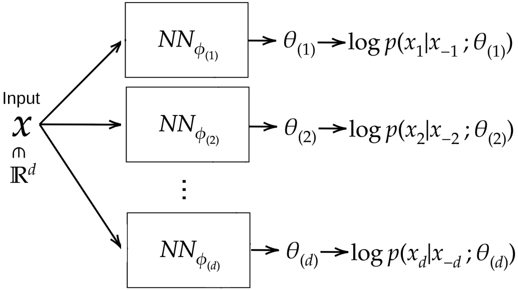


$\phi_{(i)} \triangleq \{W_{(i)}^{(1)}, \dots, W_{(i)}^{(L+1)}\}$

$W_{(i)}^{(\ell)} = \ell$th weight matrix of $NN_{\phi_{(i)}}$

$\phi \triangleq \{\phi_{(i)}\}_{i=1}^{d}$

Gradient-Based Neural DAG Learning



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$W^{(\ell)}_{(i)} =$ ℓth weight matrix of $NN_{\phi_{(i)}}$

$\phi \triangleq \{\phi_{(i)}\}_{i=1}^d$

$\prod_{i=1}^d p(x_i|x_{-i};\theta_{(i)})$ does not decompose according to a DAG!

We need to constrain the networks to be acyclic! How?

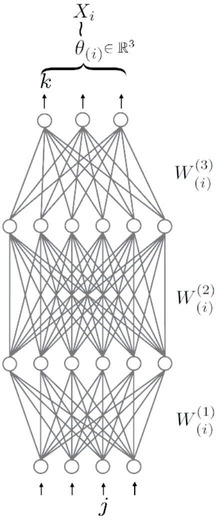
Gradient-Based Neural DAG Learning

Key idea:
Construct a **weighted adjacency matrix** A_ϕ (analogous to U from the linear case) which could be used in the acyclicity constraint

Then maximize likelihood under acyclicity constraint via **augmented Lagrangian**

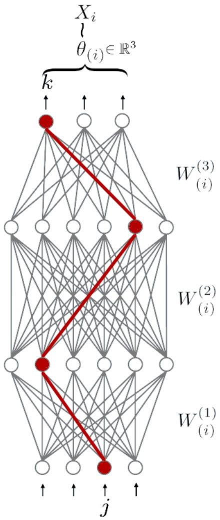
$$\max_{\phi} \underbrace{\mathbb{E}_{X\sim P_X} \sum_{i=0}^{d} \log p_\phi(X_i|X_{-i}) - \alpha_t(\mathrm{Tr}\, e^{A_\phi} - d) - \frac{\mu_t}{2}(\mathrm{Tr}\, e^{A_\phi} - d)^2}_{\text{Augmented Lagrangian}}$$

Constructing weighted adjacency matrix A_ϕ



Let's measure the "strength" of edge $X_j \rightarrow X_i$

Constructing weighted adjacency matrix A_ϕ



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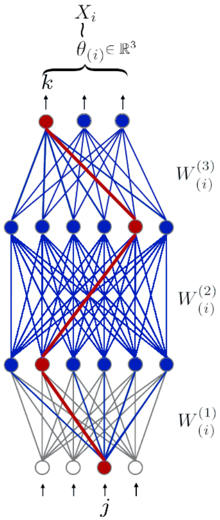
- **Path product:**
  $|W^{(1)}_{h_1 j}||W^{(2)}_{h_2 h_1}||W^{(3)}_{k h_2}| \geq 0$

Constructing weighted adjacency matrix A_ϕ



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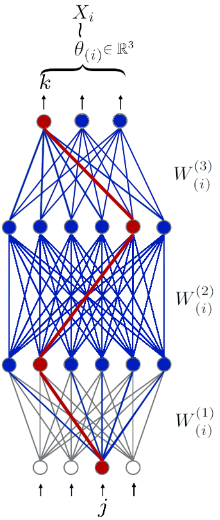
- $C \triangleq |W^{(3)}||W^{(2)}||W^{(1)}|$
  "Connection strength" from X_j to $\theta_{(i)}$:
  $\sum_{k=1}^{m} C_{kj} \geq 0$

Constructing weighted adjacency matrix A_ϕ



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- $\sum_{k=1}^{m} C_{kj} = 0 \Rightarrow$ All paths from X_j to X_i are **inactive!**

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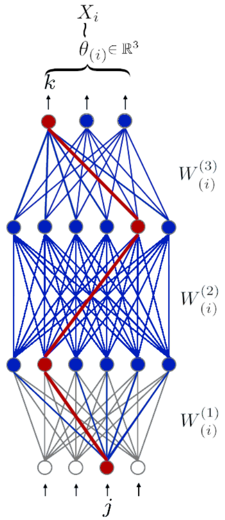
Constructing weighted adjacency matrix A_ϕ



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$$(A_\phi)_{ji} \triangleq \begin{cases} \sum_{k=1}^m \left(C_{(i)}\right)_{kj}, & \text{if } i \neq j \\ 0, & \text{otherwise} \end{cases}$$

Gradient-Based Neural DAG Learning

The algorithm:

1. Preliminary neighborhood selection (analogous to CAM)
   i.e. for each node, select potential parents via any *variable selection* approach
2. Maximize likelihood under acyclicity constraint via **augmented Lagrangian**

$$\max_{\phi} \underbrace{\mathop{\mathbb{E}}_{X\sim P_X} \sum_{i=0}^{d} \log p_\phi(x_i|x_{-i}) - \alpha_t(\operatorname{Tr} e^{A_\phi} - d) - \frac{\mu_t}{2}(\operatorname{Tr} e^{A_\phi} - d)^2}_{\text{Augmented Lagrangian}}$$

3. DAG Pruning (analogous to CAM)
   i.e. for each node, get rid of some parents via any *variable selection* approach

Step 1 and 3 helps reducing overfitting.
Important since **adding edges cannot reduce maximum likelihood**

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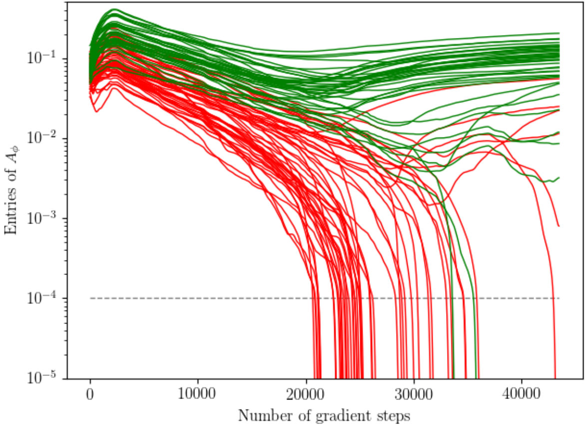
Gradient-Based Neural DAG Learning



Correct edges
Wrong edges

Experiments

Synthetic data: $X_i | X_{\pi_i^{\mathcal{G}}} \sim \mathcal{N}(f_i(X_{\pi^{\mathcal{G}}}), \sigma_i^2)$ $\quad f_i \sim$ Gaussian Process

Models: GraN-DAG, NOTEARS and CAM makes the Gaussian assumption

Real data: Measurements of expression levels of proteins and phospholipids in human immune system cells [Sachs et al., 2005]

		Synthetic (50 nodes)		Protein data set	
		SHD	SID	SHD	SID
Continuous	**GraN-DAG**	**102.6±21.2**	**1060.1±109.4**	**13**	**47**
	DAG-GNN	191.9±15.2	2146.2±64	16	44
	NOTEARS	202.3±14.3	2149.1±76.3	21	44
Discrete	**CAM**	**98.8±20.7**	**1197.2±125.9**	**12**	**55**
	RANDOM	708.4±234.4	1921.3±203.5	21	60

DAG-GNN [Yu et al., 2019]

Experiments

- In previous setup, synthetic data generation and model matched
- Here: **model misspecification**

Synthetic post nonlinear data sets

		PNL-GP		PNL-MULT	
		SHD	SID	SHD	SID
10 nodes ER1	GraN-DAG	**1.6±3.0**	**3.9±8.0**	**13.1±3.8**	35.7±12.3
	DAG-GNN	11.5±6.8	32.4±19.3	17.900±6.2	40.700±14.743
	NOTEARS	10.7±5.5	34.4±19.1	**14.0±4.0**	38.6±11.9
	CAM	**1.5±2.6**	**6.8±12.1**	**12.0±6.4**	36.3±17.7
	GSF	**6.2±3.3**	[7.7±8.7, 18.9±12.4]	**10.7±3.0**	**[9.8±11.9, 25.3±11.5]**
	RANDOM	23.8±2.9	36.8±19.1	23.7±2.9	37.7±20.7

GSF [Huang et al., 2018a]

Experiments: Effect of sample size

- Previous experiment: relatively small dataset: 1000 examples
- GraN-DAG is more expressive than CAM
- Advantage shows up in large sample size regimes

Effect of sample size - Gauss-ANM 50 nodes ER4 (averaged over 10 datasets)

Sample size	Method	SHD	SID
500	CAM	123.5 ± 13.9	1181.2 ± 160.8
	GraN-DAG	130.2 ± 14.4	1246.4 ± 126.1
1000	CAM	103.7 ± 15.2	1074.7 ± 125.8
	GraN-DAG	104.4 ± 15.3	942.1 ± 69.8
5000	CAM	74.1 ± 13.2	845.0 ± 159.8
	GraN-DAG	71.9 ± 15.9	554.1 ± 117.9
10000	CAM	66.3 ± 16.0	808.1 ± 142.9
	GraN-DAG	65.9 ± 19.8	453.4 ± 171.7

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GraN-DAG with interventions [Brouillard et al., 2020]

Can we make use of **interventional data**?

GraN-DAG with interventions [Brouillard et al., 2020]

Some **terminology** and **setting**:

- $I \subset \{1, ..., n\}$ is an *interventional target* (set of nodes on which we intervene)

- **Definition** of *stochastic intervention*:

$$p(x_1, ..., x_d | do(X_I)) \triangleq \prod_{j \notin I} p_j(x_j | x_{\pi_j^{\mathcal{G}}}) \prod_{j \in I} \tilde{p}_j(x_j)$$

  where $\tilde{p}_j(x_j)$ is the *new marginal* replacing $p_j(x_j | x_{\pi_j^{\mathcal{G}}})$ (parents are "cut out")

GraN-DAG with interventions [Brouillard et al., 2020]

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- **Observed:** $\{(X^{(1)}, I^{(1)}), ..., (X^{(n)}, I^{(n)})\}$ where $I^{(i)}$ is the interventional target associated to observation $X^{(i)}$.

$$I^{(i)} \sim P(I) \text{ i.i.d. } \forall i$$
$$X^{(i)} | I^{(i)} \sim P(X | I = I^{(i)}) \triangleq p(x_1, ..., x_d | do(X_{I^{(i)}})) \; \forall i \quad (1)$$

  where $P(I)$ is a distribution over a collection of interventional targets $\mathcal{I}$

GraN-DAG with interventions [Brouillard et al., 2020]

- Think about a CGM as a family of models of the form

$$\left\{ \prod_{j \notin I} p_j(x_j | x_{\pi_j^{\mathcal{G}}}; \phi_j) \prod_{j \in I} \tilde{p}_j(x_j; \omega_j^I) | I \in \mathcal{I} \right\}$$

  where $\omega^I \triangleq \{\omega_j^I\}_{j \in I}$ for each $I \in \mathcal{I}$ are learnable parameters.

- The natural **optimization problem:**

$$\max_{\phi, \{\omega^I\}_{I \in \mathcal{I}}} \mathbb{E}_{(X,I) \sim P(X,I)} \left[\sum_{j \notin I} \log p_j(X_j | X_{-j}; \phi_j) + \sum_{j \in I} \log p_j(X_j; \omega_j^I) \right] \quad \text{s.t.} \quad \mathrm{Tr}\, e^{A_\phi} = d$$

- But we do not really care about learning the $p_j(X_j; \omega_j^I)$ ...

- ... and problem trivially decomposes as a sum of $\max_\phi$ and $\max_{\{\omega^I\}_{I \in \mathcal{I}}}$ so ...

GraN-DAG with interventions [Brouillard et al., 2020]

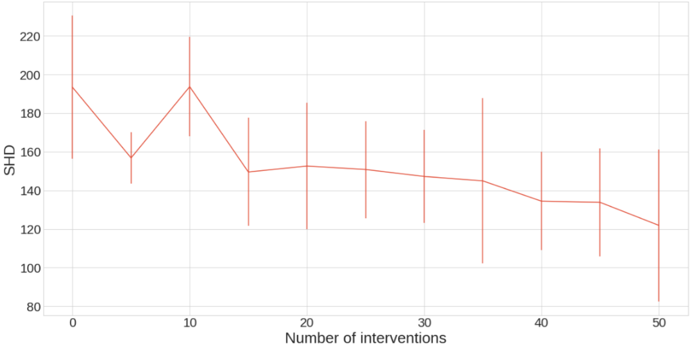
- ... can forget about $p_j(X_j; \omega_j^I)$ altogether and get

The optimization problem:

$$\max_{\phi} \mathbb{E}_{(X,I)\sim P(X,I)} \sum_{j \notin I} \log p(X_j | X_{-j}; \phi_j) \quad \text{s.t.} \quad \mathrm{Tr}\, e^{A_\phi} = d$$

In a nutshell: We throw out the conditionals associated with the intervention variables

GraN-DAG with interventions [Brouillard et al., 2020]



- Linear data (unidentifiable without interventions)
- 50 nodes and $\approx$ 200 edges
- Intervention on one node at a time

GraN-DAG with interventions [Brouillard et al., 2020]

- Nonlinear data

	20 nodes, $e = 1$		20 nodes, $e = 4$		50 nodes, $e = 1$		50 nodes, $e = 4$	
Method	SHD	SID	SHD	SID	SHD	SID	SHD	SID
GraN-DAG	**1.0** ± 1.2	**1.9** ± 3.7	**33.3** ± 10.0	**138.9** ± 21.0	**85.3** ± 20.2	**885.3** ± 151.4	**3.2** ± 2.8	**12.7** ± 13.6
GraN-DAG no interv	**0.7** ± 0.8	**1.1** ± 2.3	**41.5** ± 8.0	164.2 ± 27.9	109.8 ± 17.6	**1021.7** ± 109.0	**4.1** ± 2.3	**18.6** ± 15.1
GIES	14.6 ± 5.8	34.9 ± 23.1	64.3 ± 6.1	282.7 ± 36.7	170.2 ± 21.1	1820.7 ± 183.0	41.6 ± 9.9	107.9 ± 48.9
CAM*	1.9 ± 2.5	4.8 ± 6.3	48.8 ± 23.5	144.3 ± 38.6	**91.9** ± 11.9	**1024.4** ± 118.0	**4.7** ± 3.8	**24.5** ± 18.1

- Linear data

	20 nodes, $e = 1$		20 nodes, $e = 4$		50 nodes, $e = 1$		50 nodes, $e = 4$	
Method	SHD	SID	SHD	SID	SHD	SID	SHD	SID
GraN-DAG	5.7 ± 5.4	31.3 ± 37.5	**24.5** ± 7.4	**159.6** ± 34.9	12.5 ± 7.2	63.4 ± 36.0	**52.7** ± 16.0	**699.9** ± 166.3
GraN-DAG no interv	17.7 ± 8.2	91.8 ± 71.9	88.3 ± 23.2	275.2 ± 17.0	41.2 ± 7.3	163.8 ± 70.4	193.4 ± 39.3	1667.7 ± 169.2
GIES	**2.4** ± 1.1	**0.0** ± 0.0	**29.7** ± 28.2	**122.3** ± 103.7	13.9 ± 3.8	**0.0** ± 0.0	129.7 ± 75.1	**757.8** ± 477.7
CAM*	6.5 ± 8.7	19.0 ± 35.0	59.2 ± 27.2	173.1 ± 69.2	**1.9** ± 2.4	9.8 ± 16.5	135.4 ± 29.8	1484.1 ± 274.8

- More experiments in workshop paper...

GraN-DAG with Neural Autoregressive flows

- In previous experiments, GraN-DAG models was:

$$X_i = NN_{\phi_i}(X_{\pi_i^{\mathcal{G}}}) + \sigma_i Z \quad \text{with} \quad Z \sim \mathcal{N}(0,1) \ \ \forall i$$

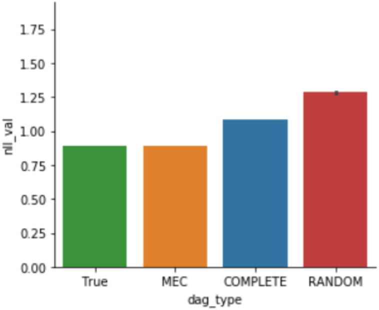
- GraN-DAG's framework allows for usage of "Neural Autoregressive Flows" [Huang et al., 2018b]

$$X_i = NAF(Z; NN_{\phi_i}(X_{\pi_i^{\mathcal{G}}})) \quad \text{with} \quad Z \sim \mathcal{N}(0,1) \ \ \forall i$$

- The function $NAF(\cdot; NN_{\phi_i}(X_{\pi_i^{\mathcal{G}}}))$ is **invertible** and with **tractable Jacobian** so the likelihood of X can be computed exactly and maximized

GraN-DAG with Neural Autoregressive flows

- Without interventions, we run into identifiability problems ...



- **Future work:** make it works with interventional data (since identifiability is less of a problem)

Conclusion and future work

Gradient-based DAG search...

- ... performs similarly to its discrete analogs
- ... scales well with number of samples (since amenable to stochastic optimization)
- ... can be easily adapted to work with interventional data
- ... allows for very expressive density models (Neural Autoregressive flow)

Future work:

- DAGs appear in many places, could we adapt the neural acyclicity constraint to other problems? (Not causality?)
- Drawing links between causality and representation learning

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