



Deutsches Zentrum
für Luft- und Raumfahrt
German Aerospace Center

Necessary and sufficient graphical conditions for optimal adjustment sets in causal graphical models with hidden variables (#3495)

Prof. Dr. Jakob Runge

October 18, 2021

Knowledge for Tomorrow

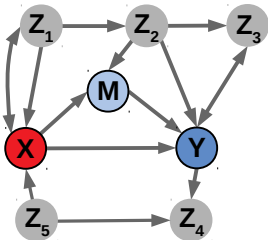
DLR Institute of Data Science and TU Berlin



Causal inference preliminaries

Task Given a qualitative causal graph and data, estimate causal effect of X on Y [Pearl, 2009]:

$$p(Y \mid do(X = x))$$

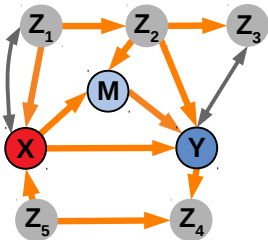


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Graph type Acyclic directed mixed graph (ADMG) $\mathcal{G} = (\mathbf{V}, \mathcal{E})$ with **directed** (\rightarrow) and **bi-directed** (\leftrightarrow) edges representing arbitrary latent confounders

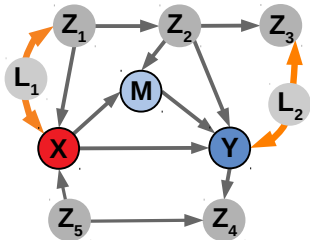


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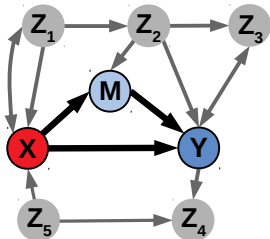


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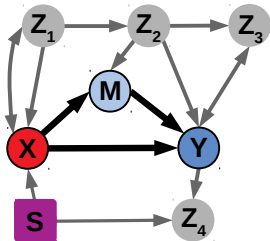
Different types of effects Here total causal effect through direct and indirect path through mediator(s) M



Causal inference preliminaries

Extended task Given a qualitative causal graph and data: Estimate *conditional causal effect* of X on Y given S

$$p(Y \mid do(X = x), S = s)$$

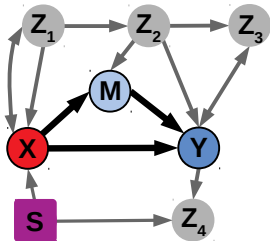


Causal inference preliminaries

Identifiability Effect is *identifiable* if it can be expressed as a function of the observational distribution $p(\mathbf{V})$ [Pearl, 2009]:

$$p(Y \mid do(X = x), S = s) = q(p(\mathbf{V}))$$

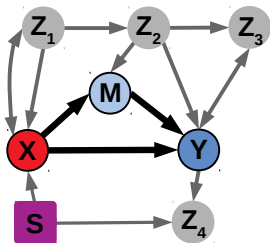
Different approaches: **Backdoor adjustment** / Frontdoor adjustment / General do-calculus



Causal inference preliminaries

Valid backdoor adjustment sets A set \mathbf{Z} for the total causal effect of X on Y is called *valid* relative to (X, Y) if the interventional distribution for setting $do(X = x)$ factorizes as:

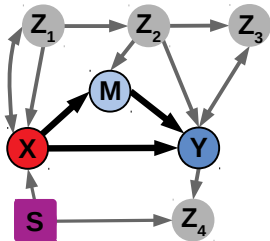
$$p(Y|do(X = x)) = q(p(\mathbf{V})) = \int_{\mathbf{z}} p(Y|x, \mathbf{z})p(\mathbf{z})d\mathbf{z}$$



Causal inference preliminaries

Generalized backdoor criterion [Perković et al., 2018]: With $\text{forb}(X, Y) = X \cup \text{des}(YM)$ a set \mathbf{Z} is valid if:

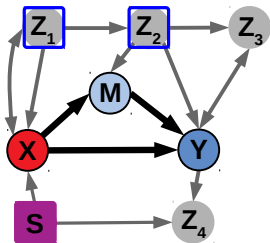
1. $\mathbf{Z} \cap \text{forb} = \emptyset$, and
2. all proper non-causal paths from X to Y are blocked by \mathbf{Z} .



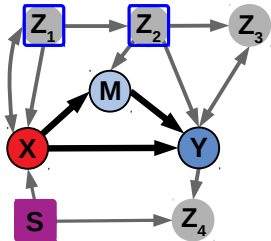
Causal inference preliminaries

Adjust-set [Perković et al., 2018] is valid if and only if a valid set exists:

$$\text{vancs}(X, Y, \mathbf{S}) = \text{an}(XYS) \setminus \text{forb} \quad (1)$$



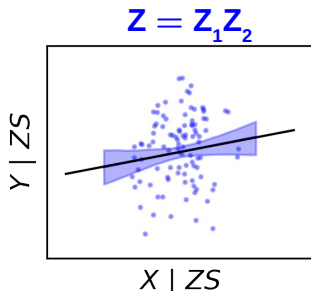
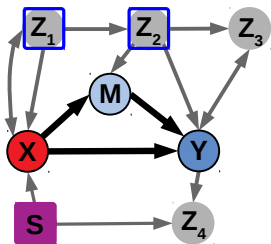
Causal inference preliminaries



Causal inference preliminaries

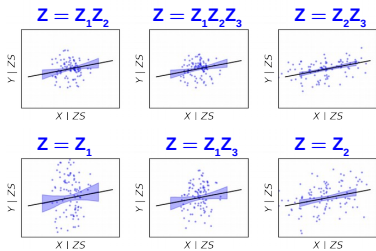
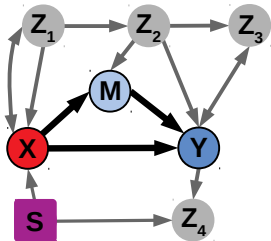
(Linear) total causal effect for $x = x' + 1$ with a valid set \mathbf{Z} is equal to $\beta_{YX \cdot ZS}$ in

$$Y = \boxed{\beta_{YX \cdot ZS}} X + \sum_i \beta_{YZ_i \cdot XS} Z_i + \sum_i \beta_{YS_i \cdot XZ} S_i \quad (1)$$



Problem setting

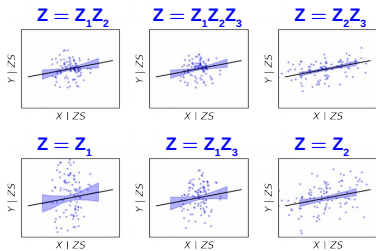
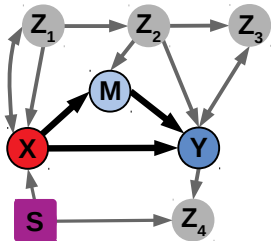
Consider all adjustment sets



Problem setting

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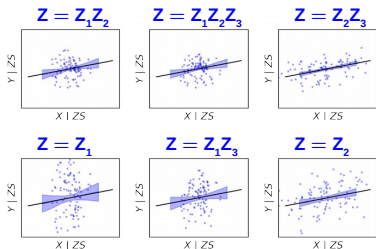
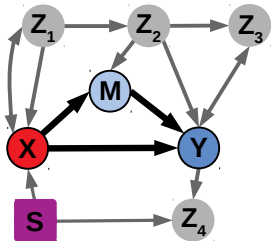
All valid sets lead to estimates with zero bias of $\hat{\beta}_{YX.ZS}$, but variance strongly differs.



Problem setting

Open problem Find valid adjustment set that yields minimal *asymptotic* variance:

$$\mathbf{Z}_{\text{optimal}} \in \operatorname{argmin}_{\mathbf{Z} \in \mathcal{Z}} E[(\Delta_{yxx'|s} - \hat{\Delta}_{yxx'|s,\mathbf{z}})^2]. \quad (2)$$



Information-theoretic optimal adjustment theory

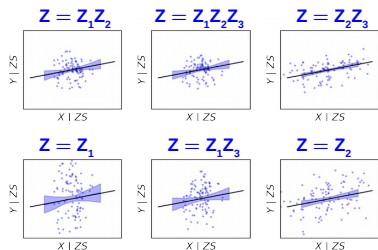
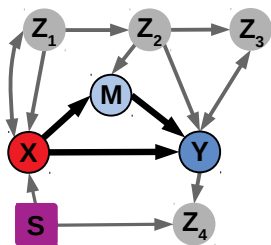
Def.: Conditional mutual information (CMI) for Shannon entropy

$$H_{Y|X} = - \int_{x,y} p(x,y) \ln p(y|x) dx dy$$

$$I_{X;Y|Z} \equiv H_{Y|Z} - H_{Y|ZX} \quad (3)$$

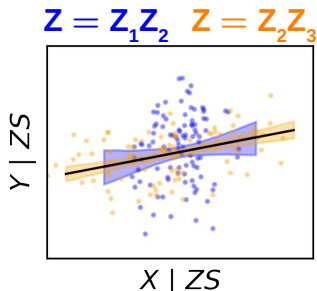
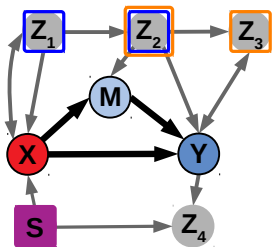
$$\geq 0 \quad (4)$$

$$= 0 \Leftrightarrow X \perp\!\!\!\perp Y | Z \quad (5)$$



Information-theoretic optimal adjustment theory

Compare Adjust set $Z = Z_1Z_2$ vs $O = Z_2Z_3$

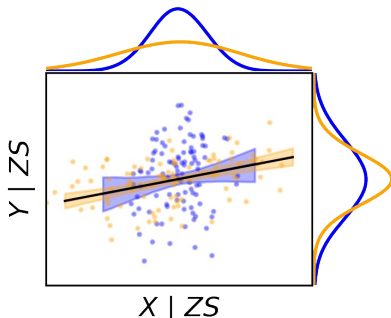
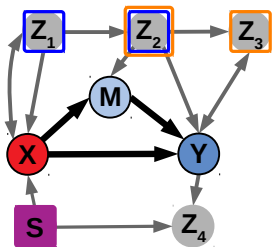


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Compare Adjust set $\mathbf{Z} = Z_1Z_2$ vs $\mathbf{O} = Z_2Z_3$

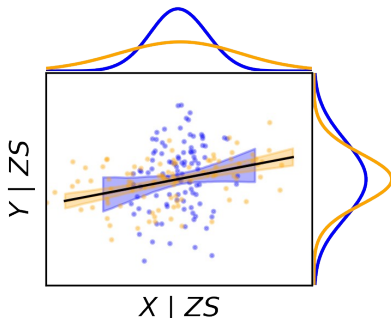
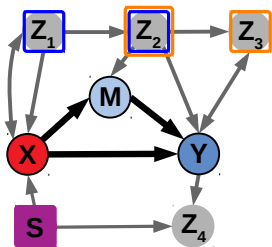
Two reasons for smaller estimator variance:

1. **Larger** residual variance of X
2. **Smaller** residual variance of Y



Information-theoretic optimal adjustment theory

Intuition Choose an adjustment set \mathbf{Z} that maximally constrains Y and minimally constrains X

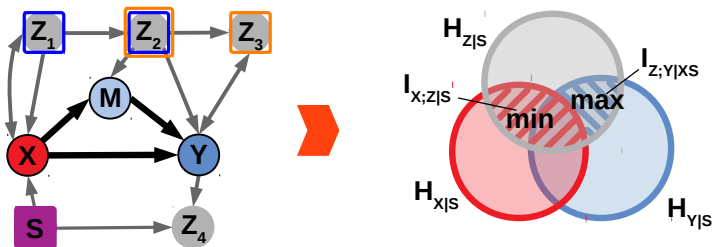


Information-theoretic optimal adjustment theory

Intuition Choose an adjustment set Z that maximally constrains Y and minimally constrains X

Def. 1: Adjustment information

$$J_Z \equiv J_{XY|S,Z} \equiv I_{Z;Y|XS} - I_{X;Z|S} \quad (3)$$

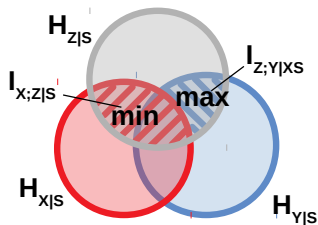
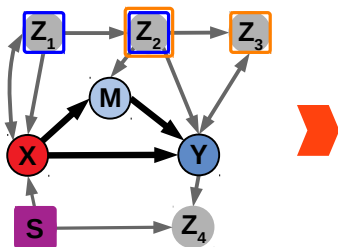


Information-theoretic optimal adjustment theory

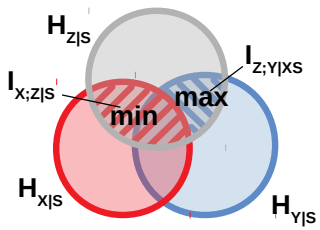
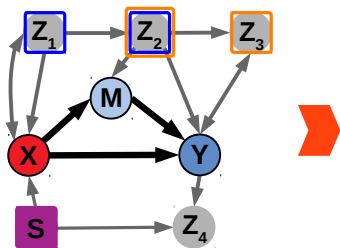
Optimality results are valid for estimators $\hat{\Delta}_{yxx'|s.z}$ that obey

$$\mathbf{Z}_{\text{optimal}} \in \operatorname{argmax}_{\mathbf{Z} \in \mathcal{Z}} J_{\mathbf{Z}} \Rightarrow \operatorname{Var}(\hat{\Delta}_{yxx'|s.z_{\text{optimal}}}) = \min_{\mathbf{Z} \in \mathcal{Z}} \operatorname{Var}(\hat{\Delta}_{yxx'|s.z})$$

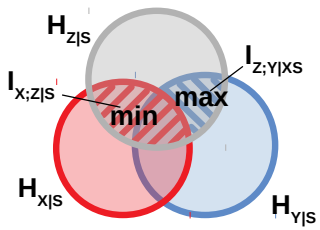
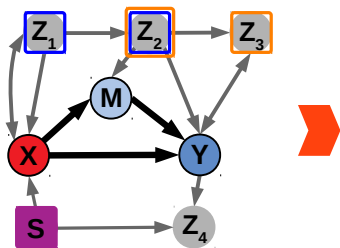
In paper theoretically shown for **OLS**, experimentally also for other estimators.



Information-theoretic optimal adjustment theory

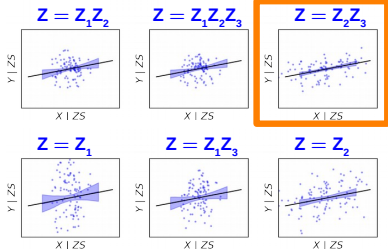
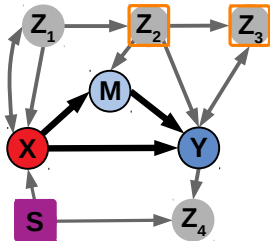


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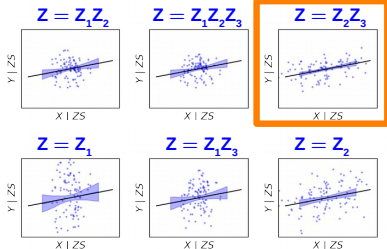
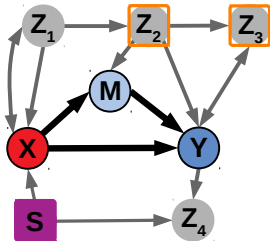
Information-theoretic optimal adjustment theory

Def. 2: Graphical optimality For a tuple (\mathcal{G}, X, Y, S) graphical optimality holds if there is a $\mathbf{Z} \in \mathcal{Z}$ s.t. for all other $\mathbf{Z}' \neq \mathbf{Z} \in \mathcal{Z}$ and all distributions \mathcal{P} consistent with \mathcal{G} we have $J_{\mathbf{Z}} \geq J_{\mathbf{Z}'}$.

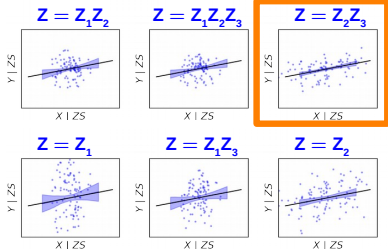
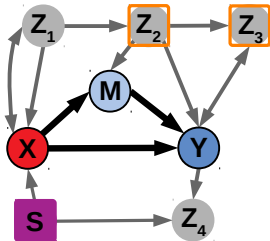


Information-theoretic optimal adjustment theory

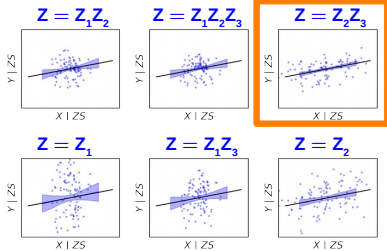
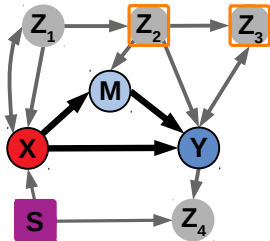
Is there always an optimal adjustment set?



Information-theoretic optimal adjustment theory



Information-theoretic optimal adjustment theory

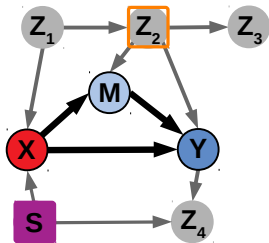


Information-theoretic optimal adjustment theory

Yes for DAGs without hidden variables

([Henckel et al., 2019, Witte et al., 2020, Rotnitzky and Smucler, 2019]):

$$\mathbf{O} = \mathbf{P} = \text{pa}(\mathbf{YM}) \setminus \text{forb}. \quad (3)$$

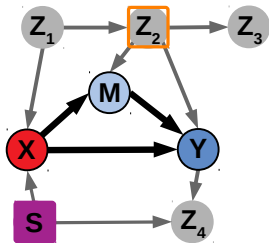


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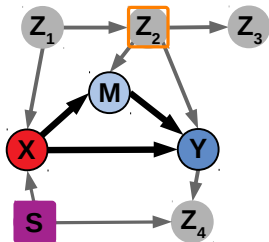


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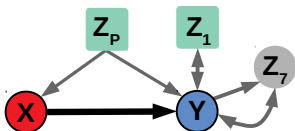
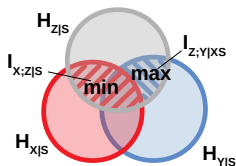
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The optimal adjustment set for ADMGs with hidden variables

Intuition Constraining Y by $pa(YM)$ not enough...

...add spouses since $I(Z_1; Y) > 0$ (as long as $\notin \text{forb}$)...

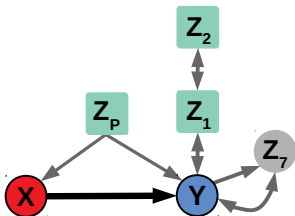
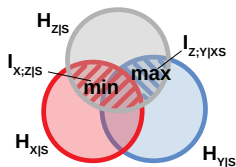


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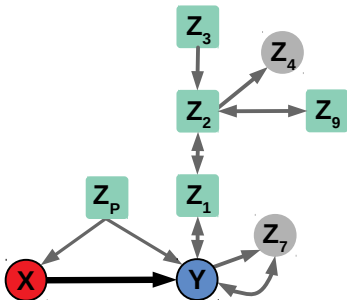
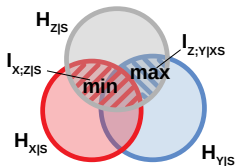
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...until a tail is reached or the path ends...



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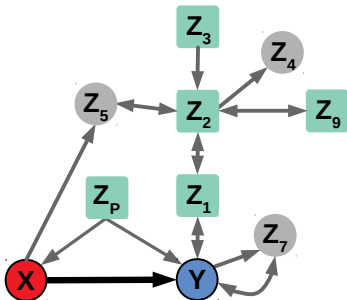
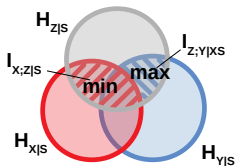
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...exclude collider if $C \not\perp\!\!\!\perp X \mid \mathbf{vancs}$ (avoids non-causal paths)...



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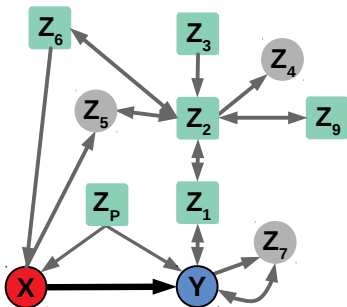
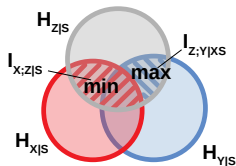
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...until a tail is reached or the path ends...

...exclude collider if $C \not\perp\!\!\!\perp X \mid \mathbf{vancs}$ (avoids non-causal paths)...

...except if $C \in \mathbf{vancs}$ where $\mathbf{vancs} = an(XYS) \setminus \mathbf{forb}$



The optimal adjustment set for ADMGs with hidden variables

Def. O-set: $O(X, Y, S) = P \cup C \cup P_C$ where

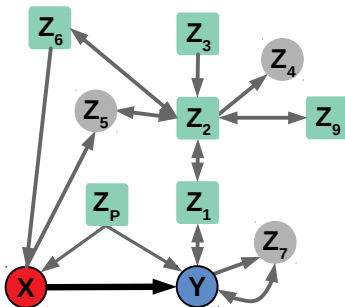
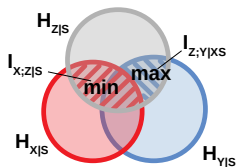
$$P = pa(YM) \setminus \mathbf{forb}$$

C = “valid collider paths from $W \in YM$ ”

$$P_C = pa(C)$$

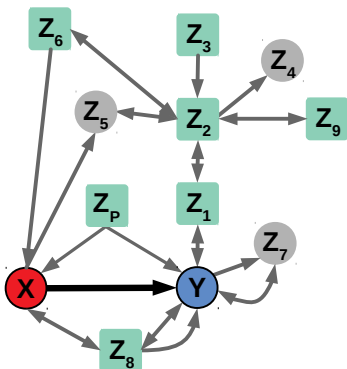
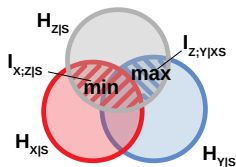
where colliders $C \in C$ fulfill

$$(1) C \notin \mathbf{forb}, \quad \text{and} \quad (2a) C \in \mathbf{vancs} \text{ or } (2b) C \perp\!\!\!\perp X \mid \mathbf{vancs}. \quad (4)$$



The optimal adjustment set for ADMGs with hidden variables

Theorem 1 (Validity) If and only if a valid backdoor adjustment set exists, then \mathbf{O} is a valid adjustment set.

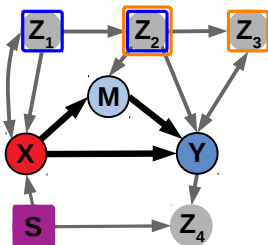


The optimal adjustment set for ADMGs with hidden variables

Theorem 2 (O-set vs Adjust set)

$J_{\mathbf{O}} \geq J_{\text{vancs}}$ for any graph \mathcal{G} (...).

$\implies \text{Var}(\widehat{\Delta}_{yxx'}|_{\mathbf{s.o}}) \leq \text{Var}(\widehat{\Delta}_{yxx'}|_{\mathbf{s.adjust}})$

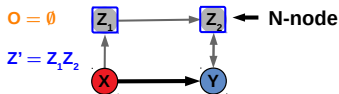


Necessary and sufficient conditions for graphical optimality

Theorem 3 If and only if (...)

(I) for all $N \in \mathbf{N} = sp(\mathbf{YMC}) \setminus (\mathbf{forbOS})$ and all its collider paths i to $W \in \mathbf{YM}$ (...) it holds that $\mathbf{O}_{\pi_i^N} = \mathbf{O}(X, Y, \mathbf{S}' = \mathbf{SN}\pi_i^N)$ is non-valid, and

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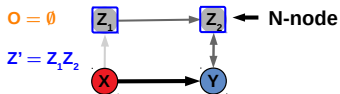


Necessary and sufficient conditions for graphical optimality

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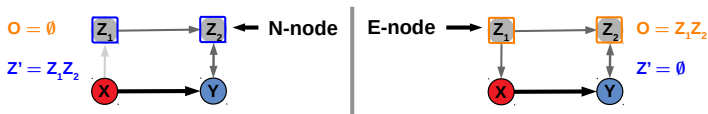


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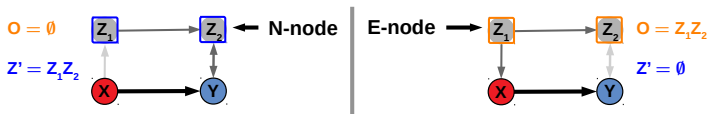


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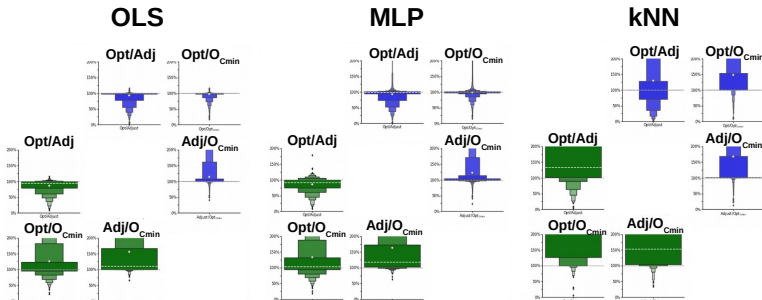
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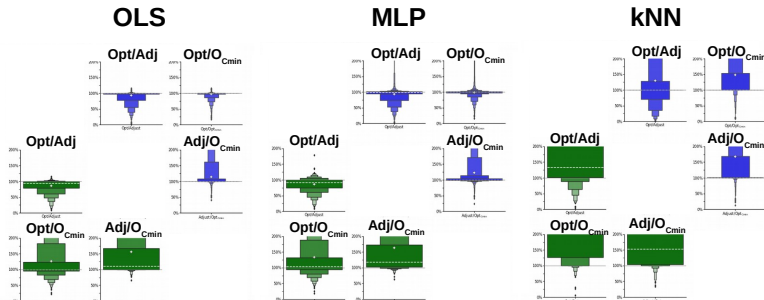
Numerical experiments in paper

- Among 12,000 randomly created configurations **95%** fulfill optimality!



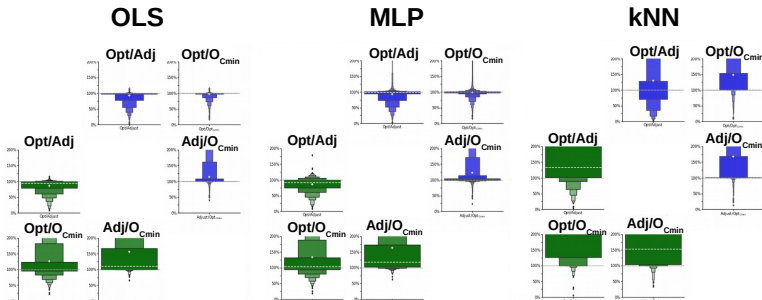
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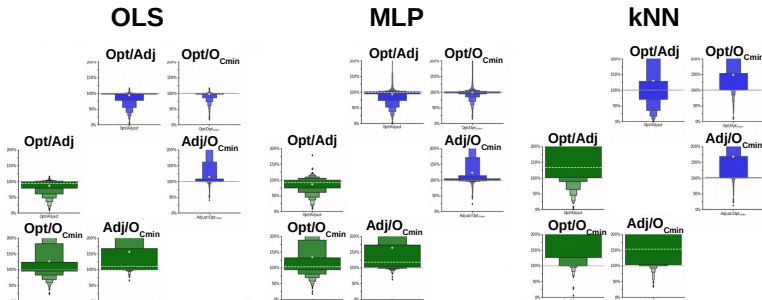
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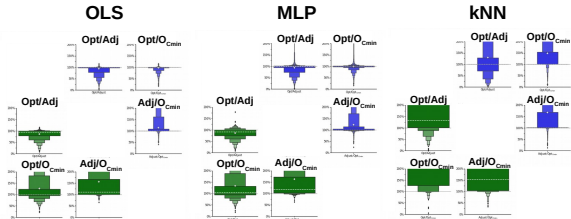
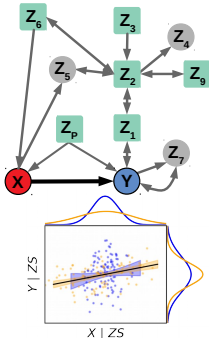
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- **kNN-estimator:** Theory not applicable, but a variant of **O**-set seems to outperform others



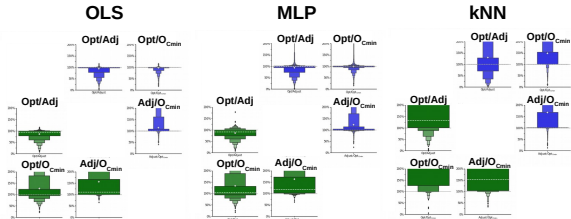
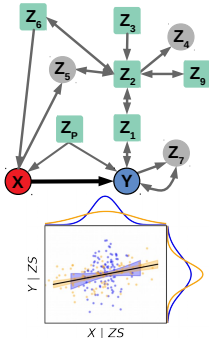
Summary

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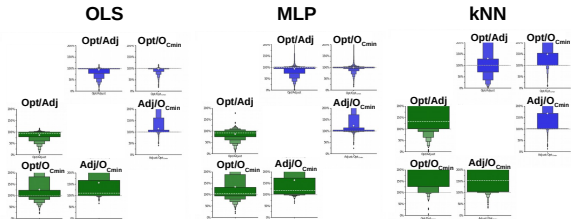
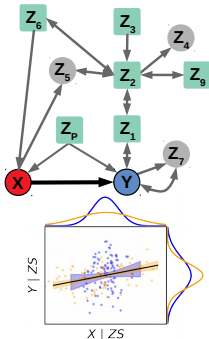
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- **O**-set is valid iff a valid set exists and always better than **Adj**-set
→ natural choice in automated causal inference



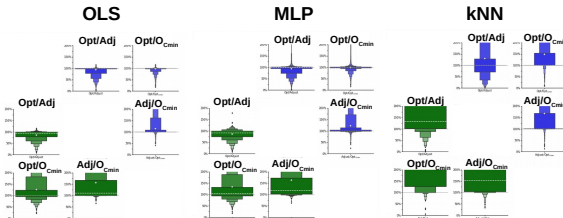
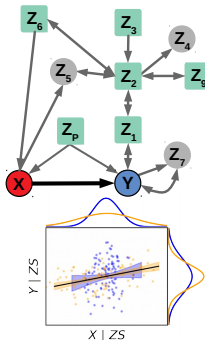
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- Python code: <https://github.com/jakobrunge/tigramite>
- Open questions: Theory for non-parametric estimators, PAGs, ...



Thank you! Questions?

- *Nature Comm.* Perspective on causal discovery in time series [Runge et al., 2019a]
- Causal inference: full theory [Pearl, 2009], primer [Pearl et al., 2016], linear models [Pearl, 2013], popular science book [Pearl and Mackenzie, 2018]
- Causal discovery: general [Spirtes et al., 2000], for time series [Runge, 2018, Runge et al., 2019a]
- Restricted SCMs [Peters et al., 2017]
- PCMCI [Runge et al., 2019b] in *Science Advances*
- PCMCI⁺ [Runge, 2020] in *UAI*
- LPCMCI [Gerhardus and Runge, 2020] in *NeurIPS*
- Optimal adjustment [Runge, 2021] in *NeurIPS*
- My software: jakobrunge.github.io/tigramite



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