



DLR  
Deutsches Zentrum  
für Luft- und Raumfahrt  
German Aerospace Center

# Recent progress and new methods for detecting causal relations in large nonlinear time series datasets

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May 3, 2020

DLR Institute of Data Science



Knowledge for Tomorrow



# Inferring causality: Three strands of modern (Earth) science

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# Inferring causality: Three strands of modern (Earth) science

- Real experiments



Bertini fresco of Galileo Galilei and Doge of Venice



Svante Arrhenius, 1909.  
Print Collector/Getty Images / Getty Images



Earth Science Experiments Class Kit

# Inferring causality: Three strands of modern (Earth) science

- Real experiments
- Earth system simulation models

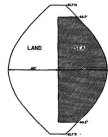


FIG. 1. Cross-continent configuration of the model

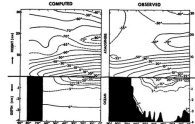


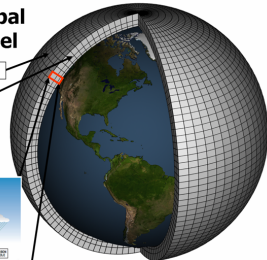
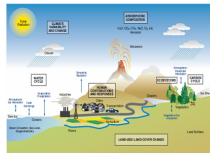
FIG. 2. Total mean temperatures of the joint ocean-atmosphere system, left-hand side. This distribution, which is the average of two distributions, represents the joint mean over two centuries of the period of the final stage of the flow experiment. The right-hand side shows the observed distribution in the North Atlantic. The cross-section represents the geometry of the ocean, and the ocean temperature. The ocean part is based on a cross section for the western North Atlantic from Stenseth et al. (1962).

First coupled climate model: Manabe, S., and K. Bryan, 1969: Climate calculations with a combined ocean-atmosphere model. J. Atmos. Sci., 26, 786–789

## Schematic for Global Atmospheric Model

Horizontal Grid (Latitude-Longitude)

Vertical Grid (Height or Pressure)

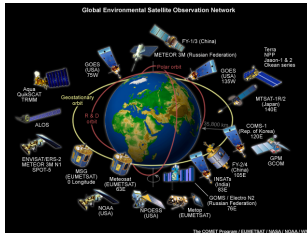


## Inferring causality: Three strands of modern (Earth) science

- Real experiments
- Earth system simulation models
- Observational data analysis

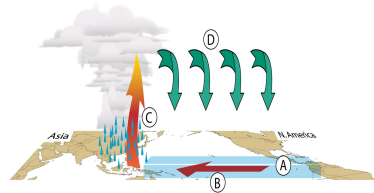
[illegible]<sup>1</sup> Sign omitted is original.

Walker, G. T. 1924. "Correlations in Seasonal Variations of Weather." IX. Mem. Ind. Meteorol. Dept. 24: 53-84.



## Observational (climate) data analysis: 1st attempt

- Walker circulation: Monthly surface pressure anomalies in the West Pacific (WPAC), surface air temperature anomalies in the Central Pacific (CPAC) and East Pacific (EPAC)



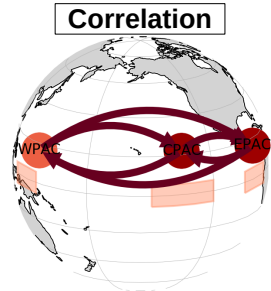
MONTHLY FORECAST																
	December-January				March-May				July-August				September-November			
	Year of data	Yearly income (thousands)	Yearly cost (thousands)	Yearly profit (thousands)	Year of data	Yearly income (thousands)	Yearly cost (thousands)	Yearly profit (thousands)	Year of data	Yearly income (thousands)	Yearly cost (thousands)	Yearly profit (thousands)	Year of data	Yearly income (thousands)	Yearly cost (thousands)	Yearly profit (thousands)
Ireland	12	7.09	2.89	4.20	12	9.70	3.57	6.13	12	11.7	4.05	7.65	12	10.7	3.91	6.79
United Kingdom	12	1.09	0.40	0.69	12	1.11	0.41	0.70	12	1.11	0.41	0.70	12	1.11	0.41	0.70
France	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
Germany	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
Italy	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
Spain	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
United States	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
Japan	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
Canada	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
South America	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
Other	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75	12	1.20	0.45	0.75
Total	12	12.00	4.50	7.50	12	12.00	4.50	7.50	12	12.00	4.50	7.50	12	12.00	4.50	7.50
Percentage	12	100	63.6	36.4	12	100	63.6	36.4	12	100	63.6	36.4	12	100	63.6	36.4
Ratio	12	1.00	0.636	0.364	12	1.00	0.636	0.364	12	1.00	0.636	0.364	12	1.00	0.636	0.364
Forecasting (2-8)	12	1.00	0.636	0.364	12	1.00	0.636	0.364	12	1.00	0.636	0.364	12	1.00	0.636	0.364
Forecast (1-9)	12	1.00	0.636	0.364	12	1.00	0.636	0.364	12	1.00	0.636	0.364	12	1.00	0.636	0.364

1. All figures are subject to revision.

Walker (1924)

# Observational (climate) data analysis: 1st attempt

- Walker circulation: Monthly surface pressure anomalies in the West Pacific (WPAC), surface air temperature anomalies in the Central Pacific (CPAC) and East Pacific (EPAC)
- All three regions are strongly lag-correlated with each other 'in all directions'



Walker (1924)

# Causal inference: 1st attempt

S. Wright, Correlation and Causation, J. of Agricultural Res. 10(7), 1921

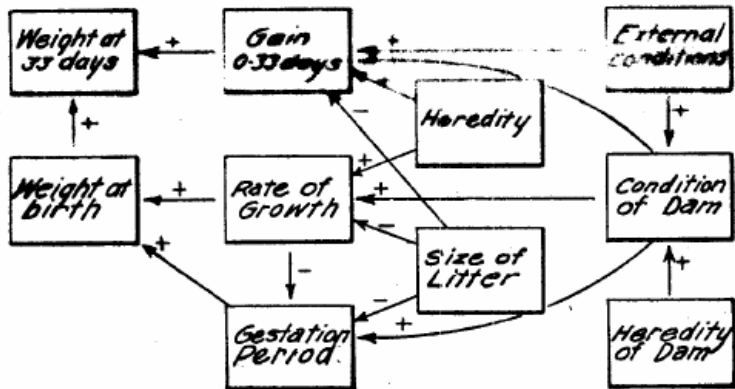


FIG. 1.—Diagram illustrating the interrelations among the factors which determine the weight of guinea pigs at birth and at weaning (33 days).

# Causality and statistics

Karl Pearson's "Grammar of Science" (1911): "Beyond such discarded fundamentals as 'matter' and 'force' lies still another fetish amidst the inscrutable arcana of modern science, namely, the category of cause and effect."



## CONTINGENCY AND CORRELATION 159

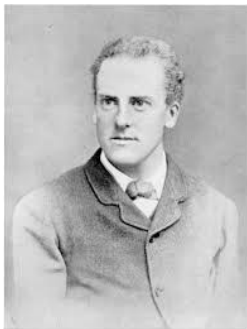
$B_1$  occurs  $n_{11}$ ,  $B_2$  occurs  $n_{12}$  times, and so on. We thus are able to obtain a general distribution of B's for each class of A that we can form, and were we to go through the whole population, N, of A's in this manner we should obtain a table of the following kind:—

TYPE OF A OBSERVED

TYPE OF B OBSERVED	$A_1$	$A_2$	$A_3$	...	$A_p$	...	Total
$B_1$	$n_{11}$	$n_{12}$	$n_{13}$	...	$n_{1p}$	...	$n_{1.}$
$B_2$	$n_{21}$	$n_{22}$	$n_{23}$	...	$n_{2p}$	...	$n_{2.}$
$B_3$	$n_{31}$	$n_{32}$	$n_{33}$	...	$n_{3p}$	...	$n_{3.}$
...	...	...	...	...	...	...	...
$B_r$	$n_{r1}$	$n_{r2}$	$n_{r3}$	...	$n_{rp}$	...	$n_{r.}$
...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...
Total	$n_{.1}$	$n_{.2}$	$n_{.3}$	...	$n_{.p}$	...	N

# Causality and statistics

Karl Pearson's "Grammar of Science" (1911): "Beyond such discarded fundamentals as 'matter' and 'force' lies still another fetish amidst the inscrutable arcana of modern science, namely, the category of cause and effect." **Correlation is not causation!**



## CONTINGENCY AND CORRELATION 159

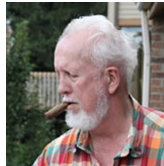
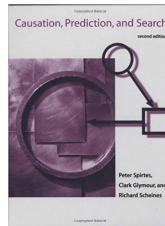
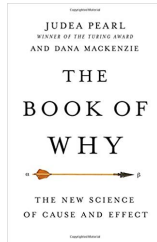
$B_1$  occurs  $n_{11}$ ,  $B_2$  occurs  $n_{12}$  times, and so on. We thus are able to obtain a general distribution of B's for each class of A that we can form, and were we to go through the whole population, N, of A's in this manner we should obtain a table of the following kind:—

TYPE OF A OBSERVED

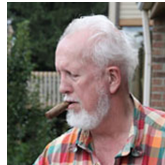
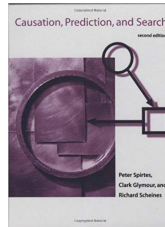
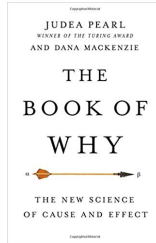
TYPE OF B OBSERVED	TYPE OF A OBSERVED							
	$A_1$	$A_2$	$A_3$	...	...	$A_p$	...	TOTAL
$B_1$	$n_{11}$	$n_{12}$	$n_{13}$	...	...	$n_{1p}$	...	$n_{1.}$
$B_2$	$n_{21}$	$n_{22}$	$n_{23}$	...	...	$n_{2p}$	...	$n_{2.}$
$B_3$	$n_{31}$	$n_{32}$	$n_{33}$	...	...	$n_{3p}$	...	$n_{3.}$
...	...	...	...	...	...	...	...	...
$B_r$	$n_{r1}$	$n_{r2}$	$n_{r3}$	...	...	$n_{rp}$	...	$n_{r.}$
...	...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...	...
TOTAL	$n_{.1}$	$n_{.2}$	$n_{.3}$	...	...	$n_{.p}$	...	N

# Causality and statistics

**Correlation is not causation! Well... not generally, but...**  
**[Pearl, 2000, Pearl and Mackenzie, 2018, Spirtes et al., 2000]**



Causal inference is about identifying assumptions and methods that enable to learn causal relations from observational data



# Table of contents

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2. Causal discovery problem
3. State of the art
4. Challenges for causal inference
5. PCMCI causal discovery framework
6. Application examples
7. Causality benchmark platform

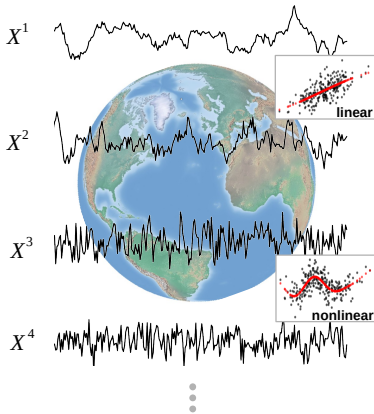
# Causal discovery problem

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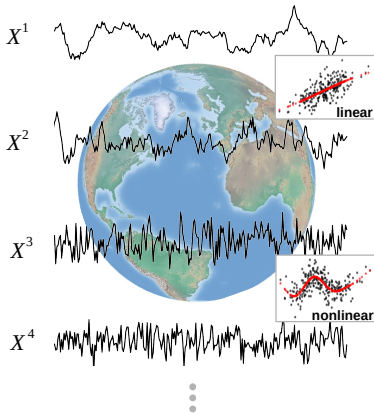
# Causal discovery problem

## Time series dataset



# Causal discovery problem

## Time series dataset



## Causal model

$$X_t^1 = f^1(\mathbf{X}_t^-, \eta_t^1)$$

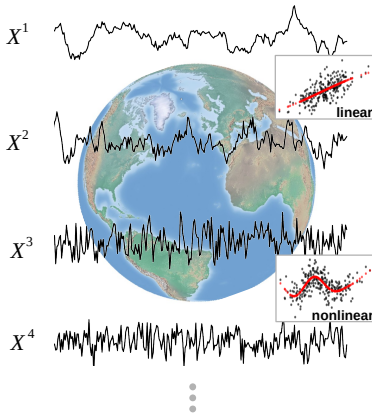


$$\mathbf{X}_t^- = (\mathbf{X}_{t-1}, \mathbf{X}_{t-2}, \dots)$$

Noise  $\eta$

# Causal discovery problem

## Time series dataset



## Causal model

$$X_t^1 = f^1(\mathbf{X}_t^-, \eta_t^1)$$

$$X_t^2 = f^2(\mathbf{X}_t^-, \eta_t^2)$$

$$X_t^3 = f^3(\mathbf{X}_t^-, \eta_t^3)$$

$$X_t^4 = f^4(\mathbf{X}_t^-, \eta_t^4)$$

⋮

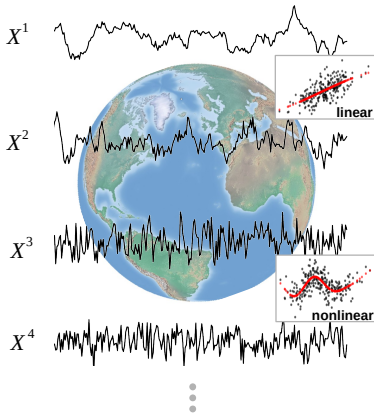
$$\mathbf{X}_t^- = (\mathbf{X}_{t-1}, \mathbf{X}_{t-2}, \dots)$$

Noise  $\eta$



# Causal discovery problem

## Time series dataset



## Causal model

$$X_t^1 = f^1(\mathbf{X}_{t+1}^-, \eta_t^1)$$

$$X_t^2 = f^2(\mathbf{X}_{t+1}^-, \eta_t^2)$$

$$X_t^3 = f^3(\mathbf{X}_{t+1}^-, \eta_t^3)$$

$$X_t^4 = f^4(\mathbf{X}_{t+1}^-, \eta_t^4)$$

⋮

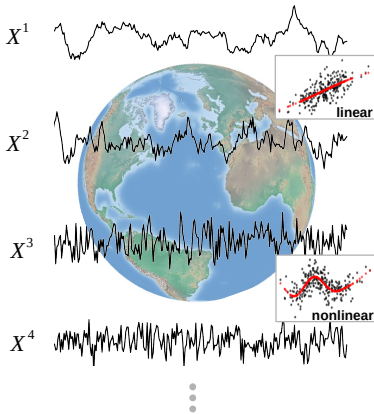
$$\mathbf{X}_{t+1}^- = (\mathbf{X}_t, \mathbf{X}_{t-1}, \dots)$$

Noise  $\eta$



# Causal discovery problem

## Time series dataset



## Causal model

$$X_t^1 = f^1(\mathcal{P}_{X_t^1}, \eta_t^1)$$

$$X_t^2 = f^2(\mathcal{P}_{X_t^2}, \eta_t^2)$$

$$X_t^3 = f^3(\mathcal{P}_{X_t^3}, \eta_t^3)$$

$$X_t^4 = f^4(\mathcal{P}_{X_t^4}, \eta_t^4)$$

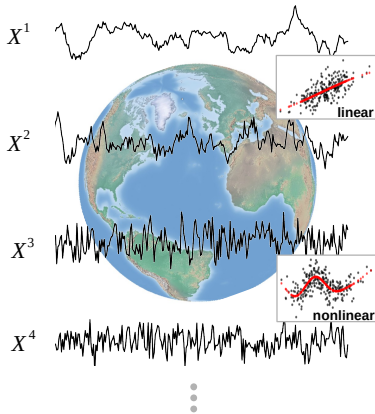
⋮

Parents  $\mathcal{P} \subset \mathbf{X}_{t+1}^-$

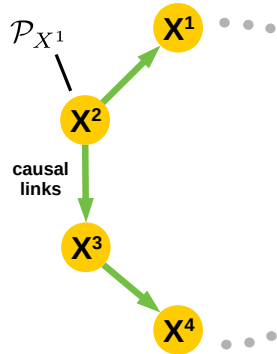
Noise  $\eta$

# Causal discovery problem

Time series dataset

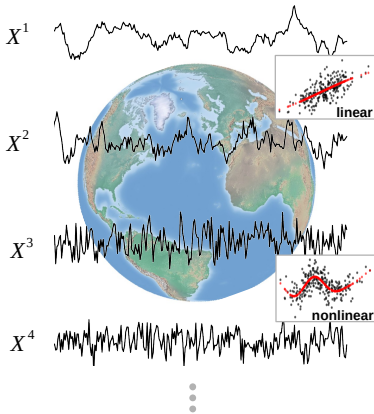


Causal graphical model

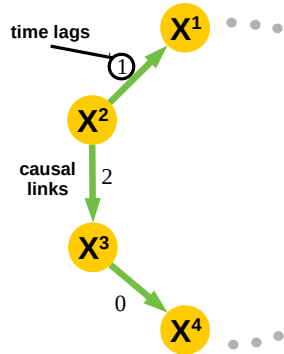


# Causal discovery problem

Time series dataset

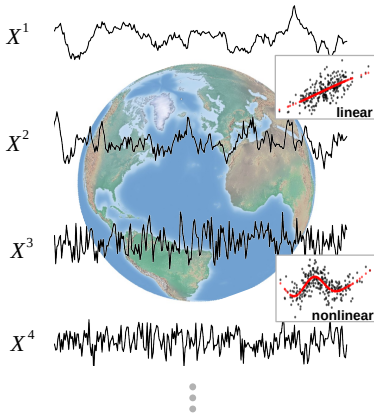


Causal graphical model

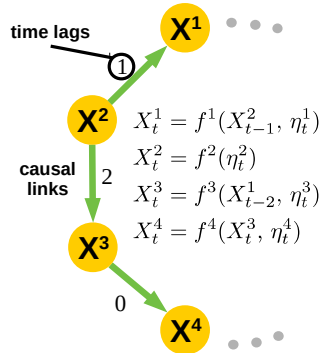


# Causal discovery problem

Time series dataset

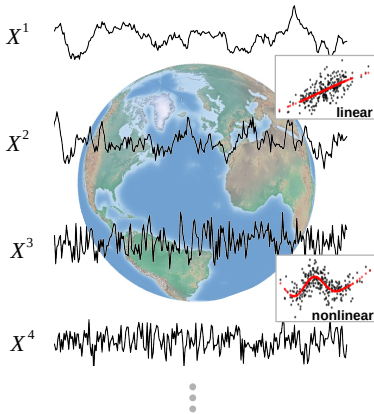


Causal graphical model

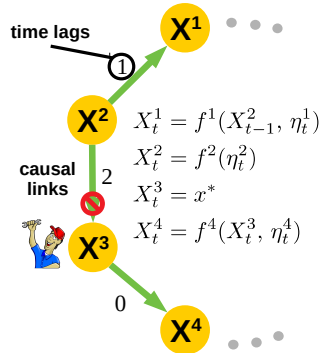


# Causal discovery problem

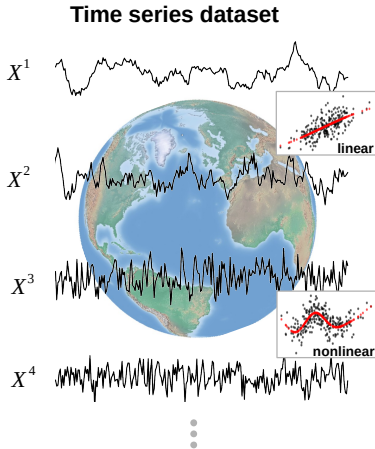
## Time series dataset



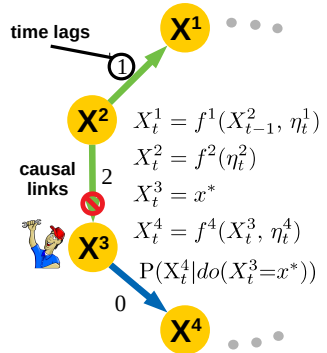
## Causal effect (Pearl)



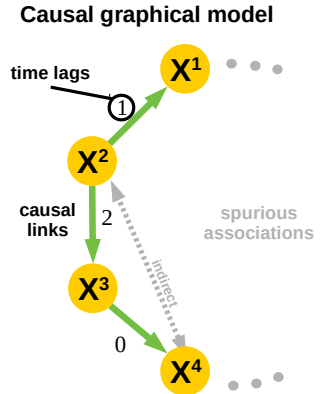
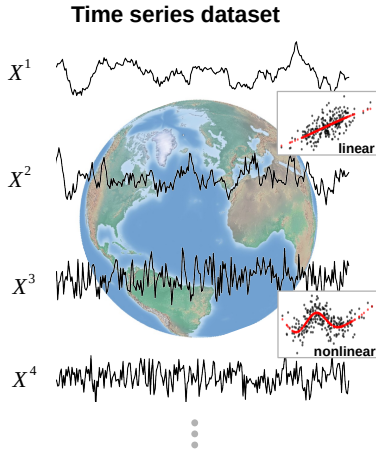
# Causal discovery problem



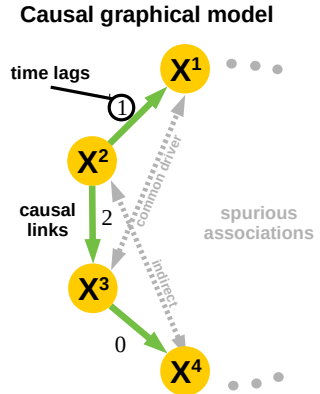
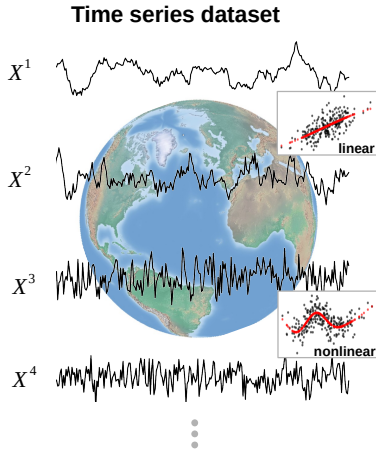
## Causal effect (Pearl)



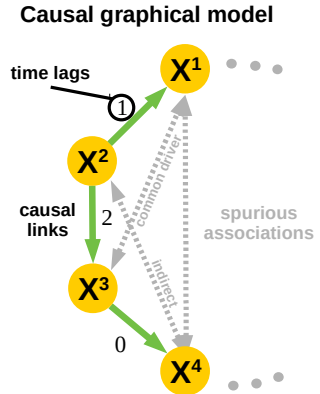
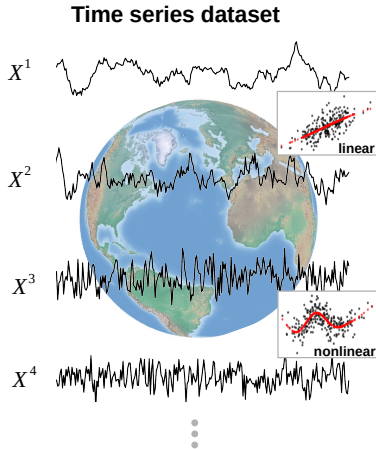
# Causal discovery problem



# Causal discovery problem



# Causal discovery problem



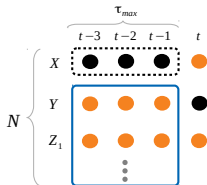
# State of the art

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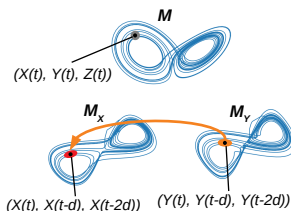


# State of the art: Runge et al., NatComm Perspective 2019

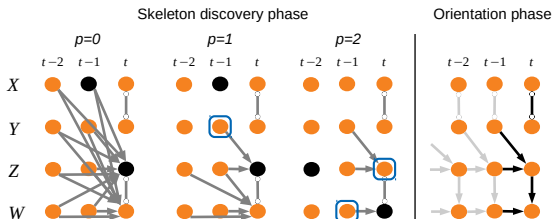
**a** Granger causality



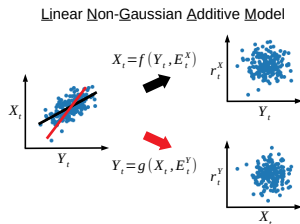
**b** Nonlinear state-space methods



**c** Causal network learning algorithms



**d** Structural causal models



# Challenges for causal inference

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# Challenges for causal inference: Runge et al., NatComm 2019

## Challenges

### Process:

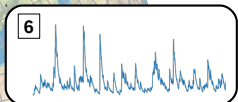
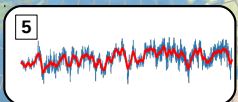
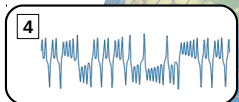
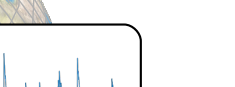
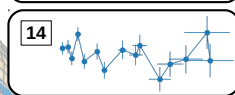
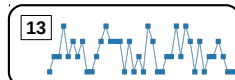
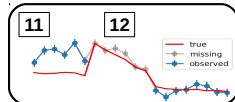
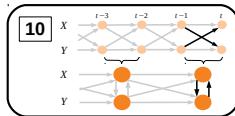
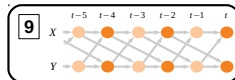
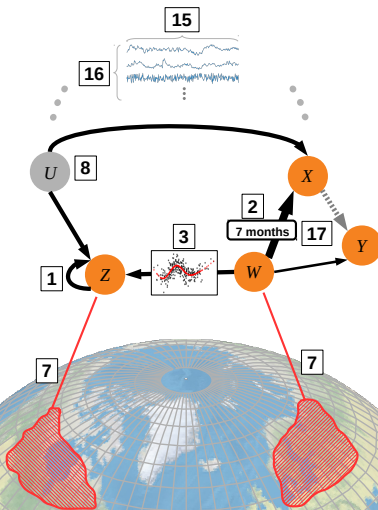
- 1 Autocorrelation
- 2 Time delays
- 3 Nonlinear dependencies
- 4 Chaotic state-dependence
- 5 Different time scales
- 6 Noise distributions

### Data:

- 7 Variable extraction
- 8 Unobserved variables
- 9 Time subsampling
- 10 Time aggregation
- 11 Measurement errors
- 12 Selection bias
- 13 Discrete data
- 14 Dating uncertainties

### Computational / statistical:

- 15 Sample size
- 16 High dimensionality
- 17 Uncertainty estimation



# PCMCI causal discovery framework

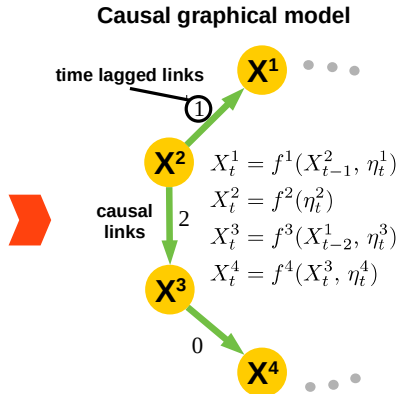
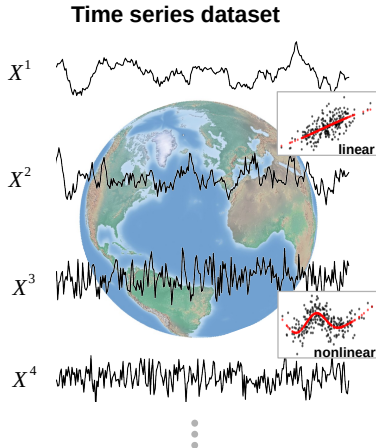
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# PCMCI causal discovery framework

PCMCI: Assumes time-lags (Runge et al. *Science Advances* 2019)

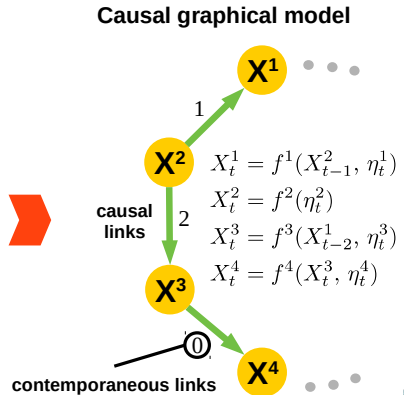
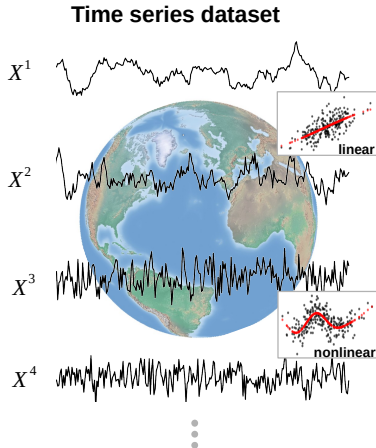
Tigramite 4.2 python package



# PCMCI causal discovery framework

PCMCI+: Allows time-lags and contemporaneous links (Runge (2020))

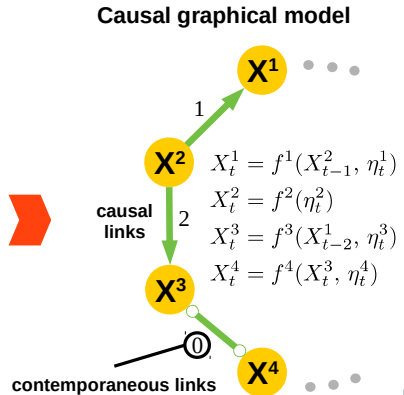
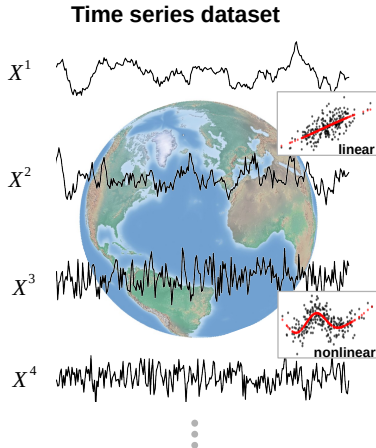
<https://arxiv.org/abs/2003.03685>



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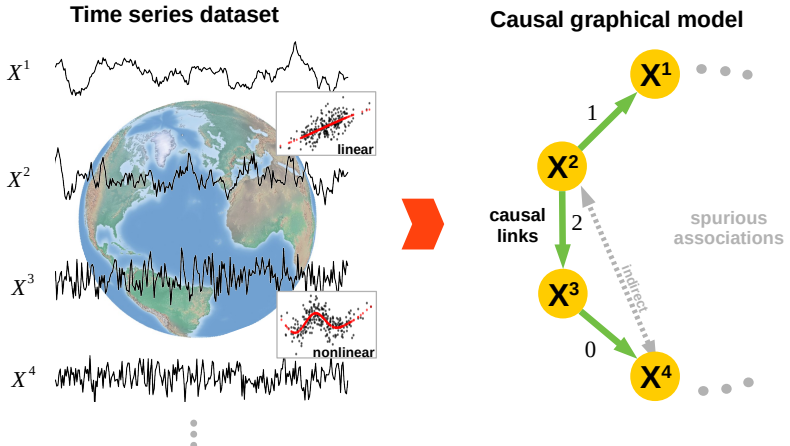
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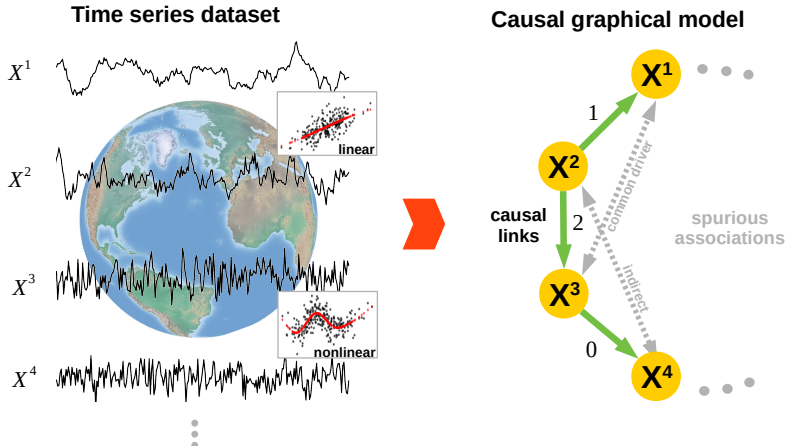
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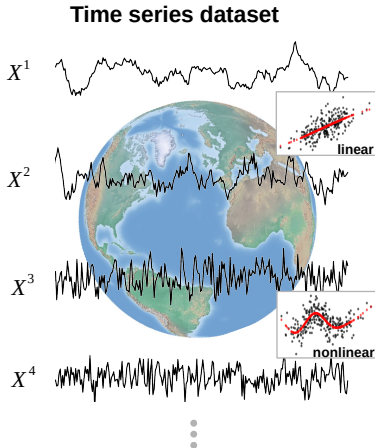
<https://arxiv.org/abs/2003.03685>)



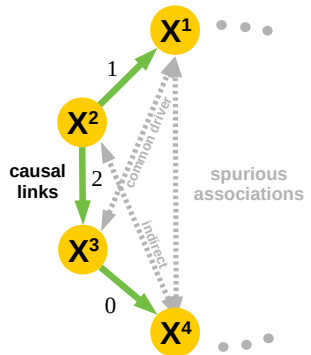
# PCMCI causal discovery framework

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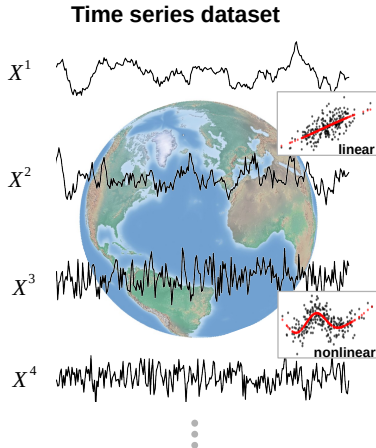
## Causal graphical model



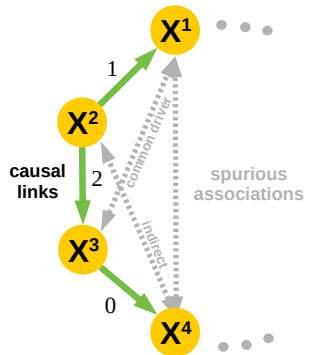
# PCMCI causal discovery framework

PCMCI+: Allows time-lags and contemporaneous links (Runge (2020)  
<https://arxiv.org/abs/2003.03685>)

**Enabling assumptions:** Faithfulness, Markovity, Causal Sufficiency, ~~no~~ contemporaneous effects, and stationarity



**Causal graphical model**

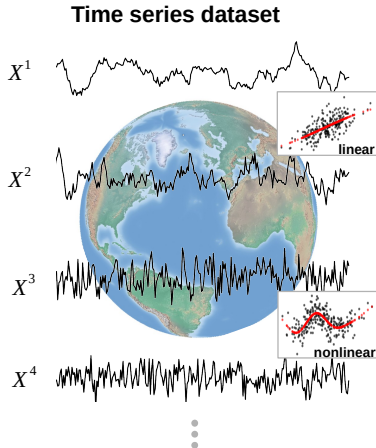


# PCMRI causal discovery framework

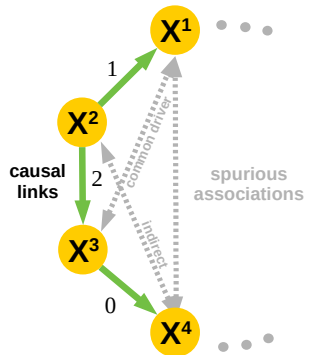
PCMRI+: Allows time-lags and contemporaneous links (Runge (2020)  
<https://arxiv.org/abs/2003.03685>)

**Enabling assumptions:** Faithfulness, Markovity, Causal Sufficiency, ~~no~~ contemporaneous effects, and stationarity

Nonlinearity and noise distributions handled by flexible conditional inde-

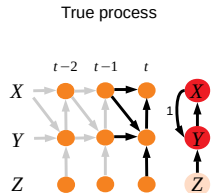
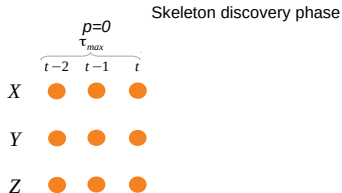


## Causal graphical model



# Problems with PC algorithm

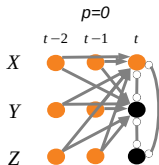
PC algorithm skeleton discovery phase can use different conditional independence (CI) tests: Partial Correlation  $\rho(X; Y|\mathbf{S})$ , Conditional Mutual Information  $I(X; Y|\mathbf{S})$ , etc.



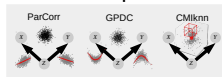
# Problems with PC algorithm

Detection power for detecting  $X \not\perp\!\!\!\perp Y \mid \mathbf{S}$  depends on:  
Sample size

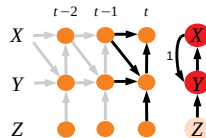
Skeleton discovery phase



Conditional independence tests



True process



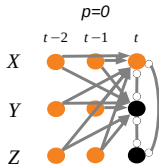
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Detection power for detecting  $X \not\perp\!\!\!\perp Y \mid \mathbf{S}$  depends on:

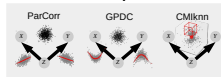
Sample size

Significance level  $\alpha_{PC}$

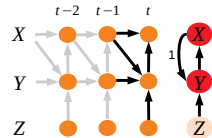
Skeleton discovery phase



Conditional independence tests



True process



# Problems with PC algorithm

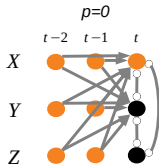
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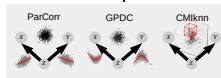
Significance level  $\alpha_{PC}$

Condition dimension, cardinality of  $|\mathbf{S}|$

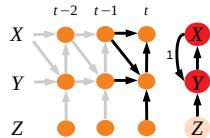
Skeleton discovery phase



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True process



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Detection power for detecting  $X \not\perp\!\!\!\perp Y \mid \mathbf{S}$  depends on:

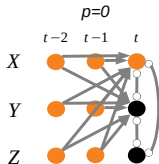
Sample size

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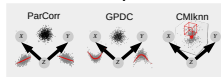
Condition dimension, cardinality of  $|\mathbf{S}|$

Effect size, i.e., magnitude of  $I(X; Y|\mathbf{S})$

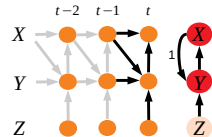
Skeleton discovery phase



Conditional independence tests



True process



# Problems with PC algorithm

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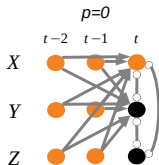
Sample size (given by dataset)

Significance level  $\alpha_{PC}$  (hyperparameter, difficult to tune)

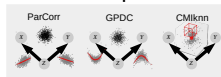
Condition dimension, cardinality of  $|\mathbf{S}|$  (PC optimizes this)

Effect size, i.e., magnitude of  $I(X; Y | \mathbf{S})$  (Problem addressed here)

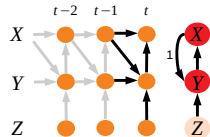
Skeleton discovery phase



Conditional independence tests



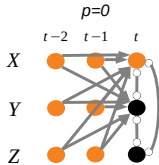
True process



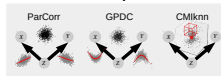
# Problems with PC algorithm

Consider underlying linear model, here  $I(Y_t; Z_t) = \frac{1}{2} \ln \left( 1 + \frac{c\text{Var}(Z)}{\text{Var}(Y)} \right)$

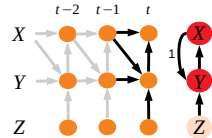
Skeleton discovery phase



Conditional independence tests



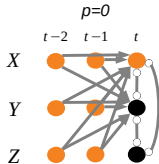
True process



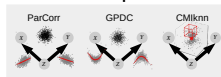
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 $\implies$  Effect size is small if  $\text{Var}(Y) \gg \text{Var}(Z)$ , and lead to false re-  
 moval.

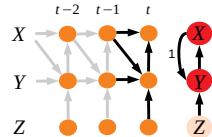
Skeleton discovery phase



Conditional independence tests



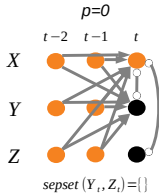
True process



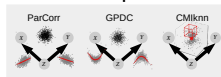
# Problems with PC algorithm

Consider underlying linear model, here  $I(Y_t; Z_t) = \frac{1}{2} \ln \left( 1 + \frac{c\text{Var}(Z)}{\text{Var}(Y)} \right)$   
 $\Rightarrow$  Effect size is small if  $\text{Var}(Y) \gg \text{Var}(Z)$ , and lead to false removal.

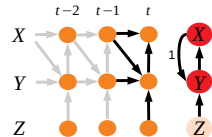
Skeleton discovery phase



Conditional independence tests



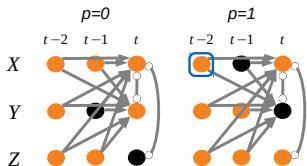
True process



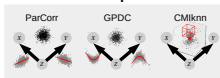
# Problems with PC algorithm

Problem: PC iterates through **all** adjacent conditions **S** and link is removed if  $\min_{\mathbf{S}} I(X; Y | \mathbf{S}) < I_{\alpha_{PC}}$

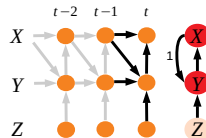
Skeleton discovery phase



Conditional independence tests



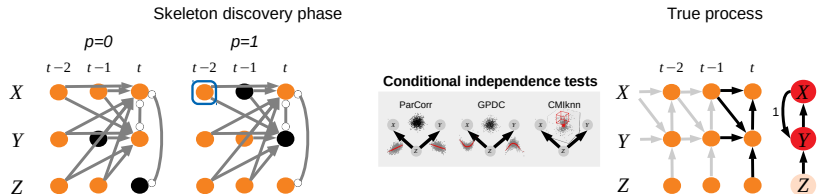
True process



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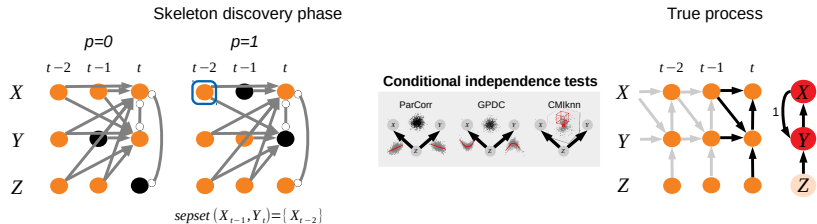
Generally: Effect size for a link  $X_{t-\tau} \rightarrow Y_t$  is small when conditioning on parents of  $X_{t-\tau}$  and large when conditioning on parents of  $Y_t$ , i.e.,  $I(X; Y | \mathcal{P}(X)) \ll I(X; Y | \mathcal{P}(Y))$  [Runge et al., 2012a]



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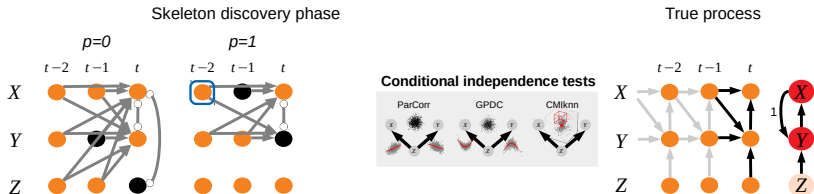
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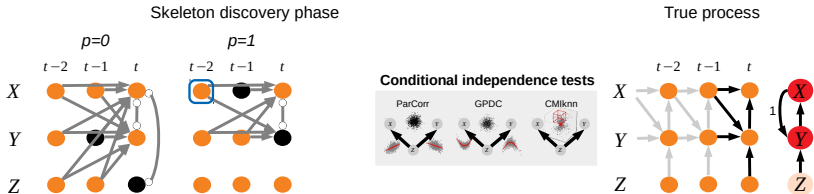


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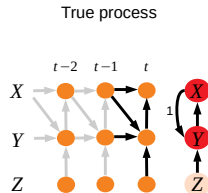
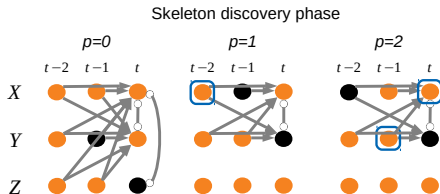
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PC likely iterates through such conditions and removes true links.



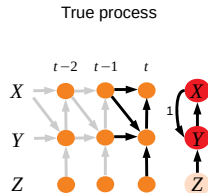
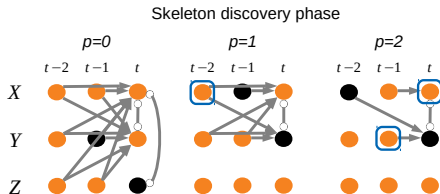
# Problems with PC algorithm

Removed links are not used as conditions for larger  $p$ .



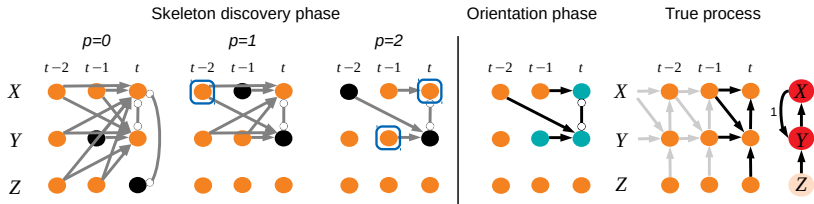
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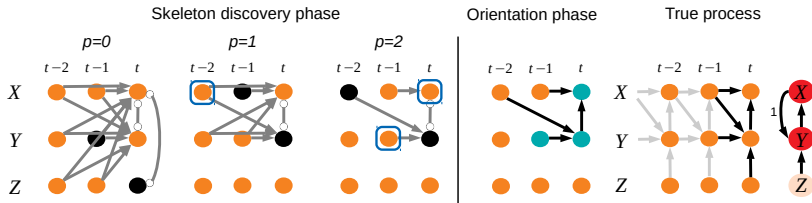
# Problems with PC algorithm

⇒ False positives (incorrect links)! Then orientation phase also suffers from wrong sepsets.



# Problems with PC algorithm

Then orientation phase also suffers from wrong sepsets.



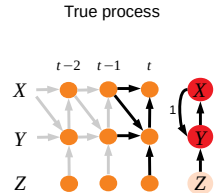
Consider underlying true process graph.

True process



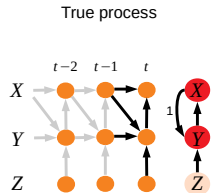
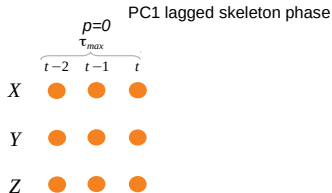
## PCMCI<sup>+</sup> causal discovery

Consider underlying true process graph.  
Associated time series graph.



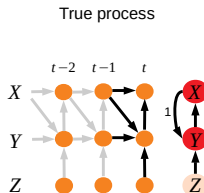
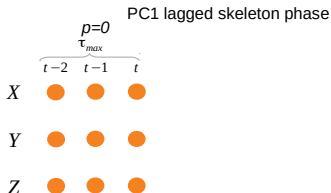
# PCMCI<sup>+</sup> causal discovery

PCMCI<sup>+</sup> has 3 phases: PC<sub>1</sub> lagged phase, MCI contemporaneous phase, Orientation phase.



# PCMCI<sup>+</sup> causal discovery

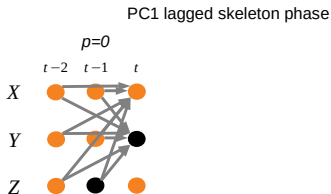
PC<sub>1</sub> lagged phase differs from PC algorithm twofold:



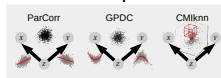
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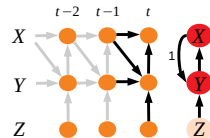
(1) **S** iterates through **lagged** links only,



Conditional independence tests



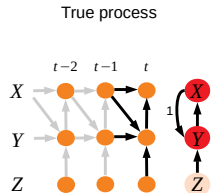
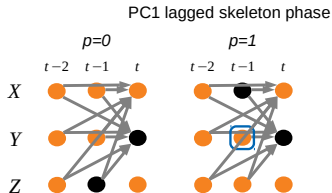
True process



# PCMCI<sup>+</sup> causal discovery

PC<sub>1</sub> lagged phase differs from PC algorithm twofold:

- (1) **S** iterates through **lagged** links only,
- (2) **S** =  $\{\mathcal{A}(X_t^j)\}_{l=1}^p$  for every cardinality  $p$ : lagged conditions with largest association with  $X_t^j$ .

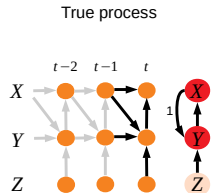
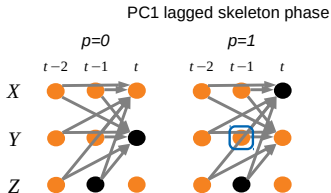


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- (2) **S** =  $\{\mathcal{A}(X_t^j)\}_{l=1}^p$  for every cardinality  $p$ : lagged conditions with largest association with  $X_t^j$ .

⇒ much less likely to condition on “effect-size weakening” parents of  $X_{t-\tau}^i$

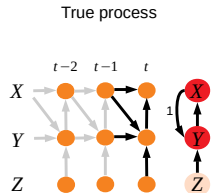
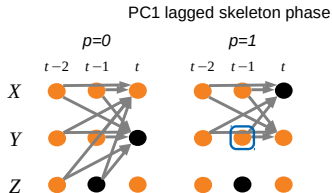


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PC<sub>1</sub> lagged phase differs from PC algorithm twofold:

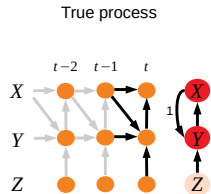
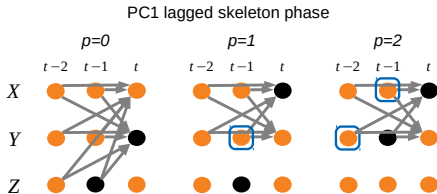
- (1) **S** iterates through **lagged** links only,
- (2) **S** =  $\{\mathcal{A}(X_t^j)\}_{j=1}^p$  for every cardinality  $p$ : lagged conditions with largest association with  $X_t^j$ .

⇒ much less likely to condition on “effect-size weakening” parents of  $X_{t-\tau}^i$



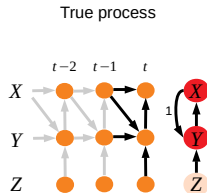
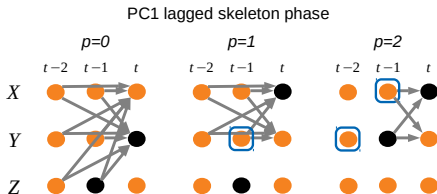
# PCMCI<sup>+</sup> causal discovery

PC<sub>1</sub> converges to lagged parents plus parents of contemporaneous ancestors:  $\widehat{\mathcal{B}}_t^-(X_t^j)$ .



# PCMCI<sup>+</sup> causal discovery

PC<sub>1</sub> converges to lagged parents plus parents of contemporaneous ancestors:  
tensors:  $\hat{\mathcal{B}}_t^-(X_t^j)$ .

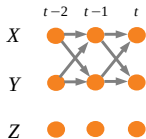


# PCMCI<sup>+</sup> causal discovery

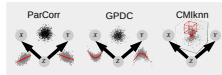
MCI contemporaneous phase is first initialized with lagged links  $\hat{\mathcal{B}}_t^-(X_t^j)$  and all contemporaneous links

Contemp. condition phase w/ MCI

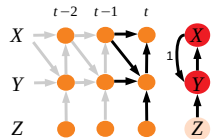
$p=0$



Conditional independence tests



True process

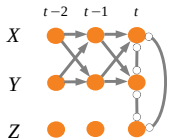


# PCMCI<sup>+</sup> causal discovery

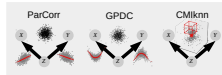
MCI contemporaneous phase is first initialized with lagged links  $\hat{\mathcal{B}}_t^-(X_t^j)$  and all contemporaneous links

Contemp. condition phase w/ MCI

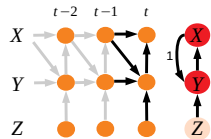
$p=0$



Conditional independence tests



True process

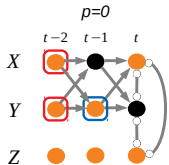


# PCMCI<sup>+</sup> causal discovery

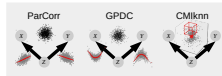
MCI phase iterates through **contemporaneous conditions**  $\mathbf{S} \subseteq \mathcal{A}_t(X_t^j)$  with MCI tests:

$$X_{t-\tau}^i \perp\!\!\!\perp X_t^j \mid \mathbf{S}, \widehat{\mathcal{B}}_t^-(X_t^j) \setminus \{X_{t-\tau}^i\}, \widehat{\mathcal{B}}_{t-\tau}^-(X_{t-\tau}^i)$$

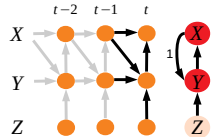
Contemp. condition phase w/ MCI



Conditional independence tests



True process

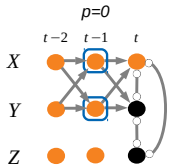


# PCMCI<sup>+</sup> causal discovery

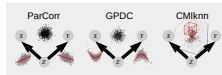
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$$X_{t-\tau}^i \perp\!\!\!\perp X_t^j \mid \mathbf{S}, \widehat{\mathcal{B}}_t^-(X_t^j) \setminus \{X_{t-\tau}^i\}, \widehat{\mathcal{B}}_{t-\tau}^-(X_{t-\tau}^i)$$

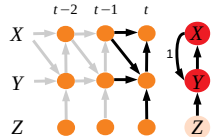
Contemp. condition phase w/ MCI



Conditional independence tests

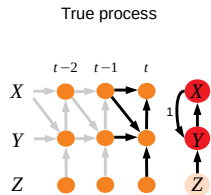
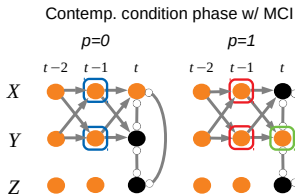


True process



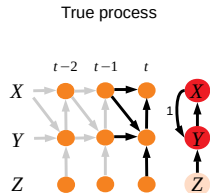
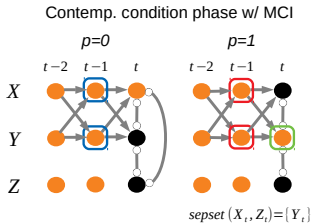
# PCMCI<sup>+</sup> causal discovery

Conditioning on **both**  $\hat{\mathcal{B}}_t^-(X_t^i)$  and  $\hat{\mathcal{B}}_{t-\tau}^-(X_{t-\tau}^i)$  has two important implications: (1) MCI effect size larger than PC effect size, (2) MCI tests well-calibrated (both discussed in paper)



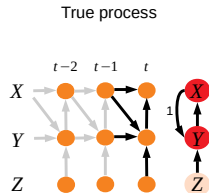
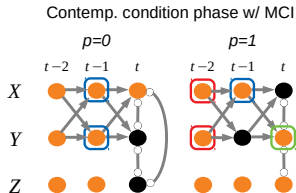
# PCMCI<sup>+</sup> causal discovery

Spurious links due to contemporaneous drivers are removed and sepsets stored; converges much faster than PC algorithm, shorter runtimes.



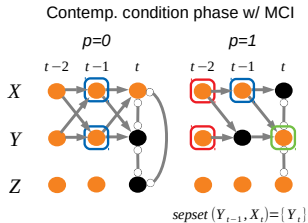
# PCMCI<sup>+</sup> causal discovery

Spurious links due to contemporaneous drivers are removed and sepsets stored; converges much faster than PC algorithm, shorter runtimes.

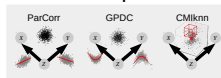


# PCMCI<sup>+</sup> causal discovery

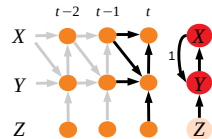
Spurious links due to contemporaneous drivers are removed and sepsets stored; converges much faster than PC algorithm, shorter runtimes.



## Conditional independence tests

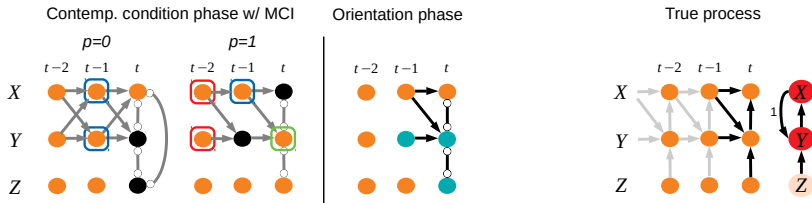


## True process



# PCMCI<sup>+</sup> causal discovery

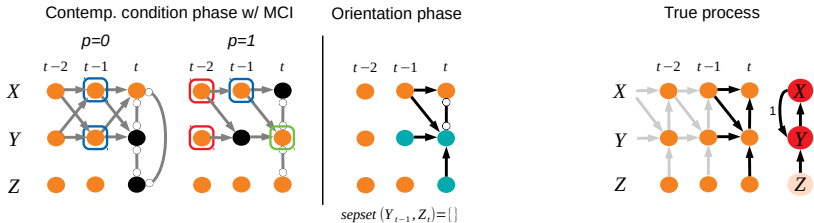
Orientation phase as for PC algorithm.



# PCMCI<sup>+</sup> causal discovery

Orientation phase as for PC algorithm.

Collider/unshielded triple rule:  $Y_t$  is not in  $sepset(Y_{t-1}, Z_t) \implies \text{orient } Z_t \rightarrow Y_t$

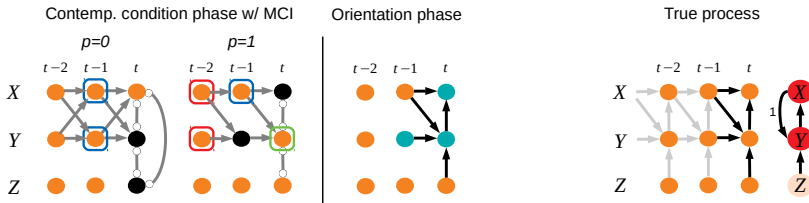


# PCMCI<sup>+</sup> causal discovery

Orientation phase as for PC algorithm.

Collider/unshielded triple rule:  $Y_t$  is not in  $sepset(Y_{t-1}, Z_t) \implies$  orient  $Z_t \rightarrow Y_t$

Rule R1: Orient remaining unshielded trips in other direction



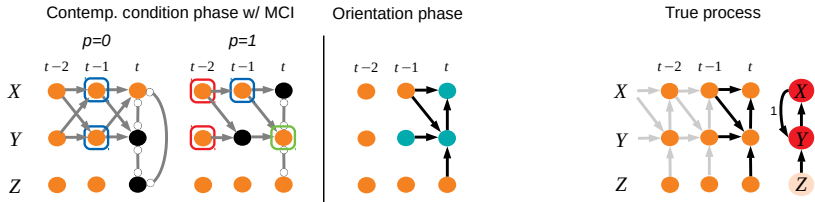
# PCMCI<sup>+</sup> causal discovery

Orientation phase as for PC algorithm.

Collider/unshielded triple rule:  $Y_t$  is not in  $\text{sepset}(Y_{t-1}, Z_t) \implies \text{orient } Z_t \rightarrow Y_t$

Rule R1: Orient remaining unshielded trips in other direction

Further rules that make use of acyclicity assumption (see paper).



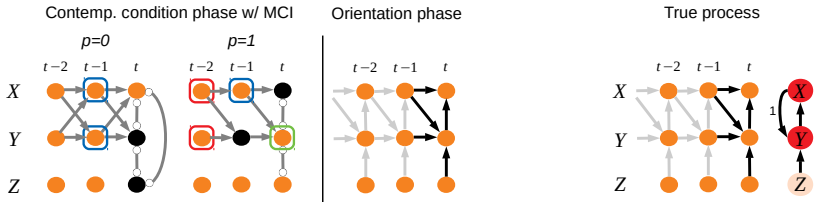
# PCMCI<sup>+</sup> causal discovery

Orientation phase as for PC algorithm.

Collider/unshielded triple rule:  $Y_t$  is not in  $sepset(Y_{t-1}, Z_t) \implies$  orient  $Z_t \rightarrow Y_t$

Rule R1: Orient remaining unshielded trips in other direction

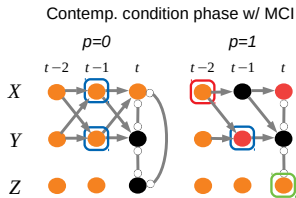
Further rules that make use of acyclicity assumption (see paper). PCMCI<sup>+</sup> converges, links are repeated by assuming stationarity,



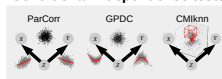
# PCMCI<sup>+</sup> causal discovery

In paper:

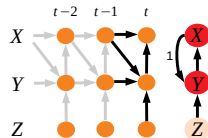
- Asymptotical consistency: PCMCI<sup>+</sup> is sound and complete



## Conditional independence tests



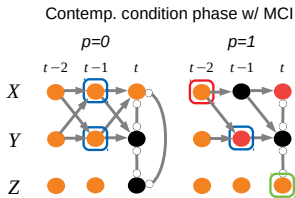
## True process



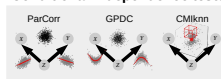
# PCMCI<sup>+</sup> causal discovery

In paper:

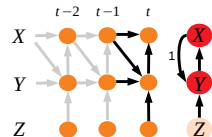
- Asymptotical consistency: PCMCI<sup>+</sup> is sound and complete
- Order independence (with majority rule in collider phase and conflict resolution)



## Conditional independence tests



True process



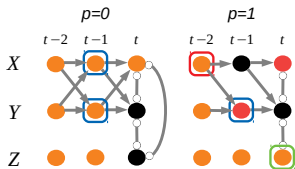
# PCMCI<sup>+</sup> causal discovery

In paper:

- Asymptotical consistency: PCMCI<sup>+</sup> is sound and complete
- Order independence (with majority rule in collider phase and conflict resolution)
- Conjecture: Effect size is always greater than that of PC algorithm

$$\min_{\mathbf{S}} \text{in PCMCI}^+ I(X_{t-\tau}^i ; X_t^j \mid \mathbf{S}, \hat{\mathcal{B}}_j, \hat{\mathcal{B}}_i) > \min_{\mathbf{S}'} \text{in PC} I(X_{t-\tau}^i ; X_t^j \mid \mathbf{S}')$$

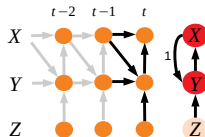
Contemp. condition phase w/ MCI



Conditional independence tests



True process

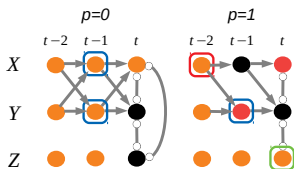


# PCMCI<sup>+</sup> causal discovery

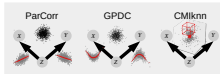
In paper:

- Asymptotical consistency: PCMCI<sup>+</sup> is sound and complete
  - Order independence (with majority rule in collider phase and conflict resolution)
  - Conjecture: Effect size is always greater than that of PC algorithm
- $$\min_{\mathbf{S} \text{ in PCMCI}^+} I(X_{t-\tau}^i ; X_t^j \mid \mathbf{S}, \hat{\mathcal{B}}_j, \hat{\mathcal{B}}_i) > \min_{\mathbf{S}' \text{ in PC}} I(X_{t-\tau}^i ; X_t^j \mid \mathbf{S}')$$
- MCI tests are well-calibrated also for autocorrelated data [Runge et al., 2019b]

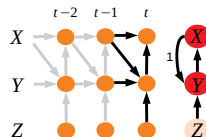
Contemp. condition phase w/ MCI



Conditional independence tests

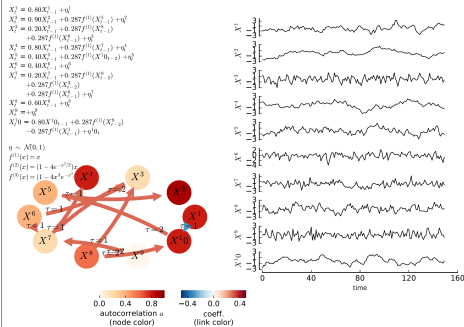


True process



# Numerical experiments

- random coupling topologies, time lags, linear/nonlinear
- 30% contemporaneous links, coefficients  $\pm[0.1..0.5]$
- different autocorrelations for variables
- $\tau_{\max} = 5$ ,  $T = 500$ , varying  $N = 2..40$
- $\alpha_{PC}$  fixed, can be chosen via AIC



# Numerical experiments

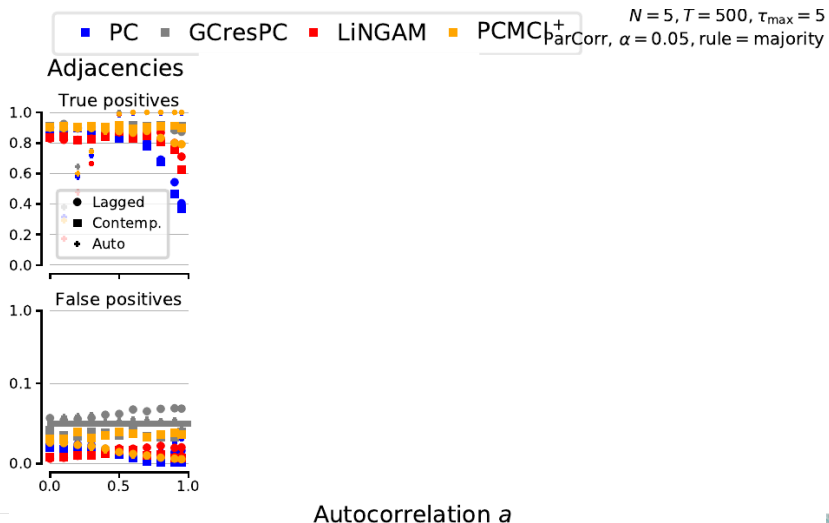
Comparing with PC algo, Granger causality + PC on residuals (GCresPC), LiNGAM

■ PC ■ GCresPC ■ LiNGAM ■ PCMC<sub>ParCorr</sub><sup>+</sup>  $N = 5, T = 500, \tau_{\max} = 5$   
 $\alpha = 0.05, \text{rule} = \text{majority}$

Autocorrelation  $a$

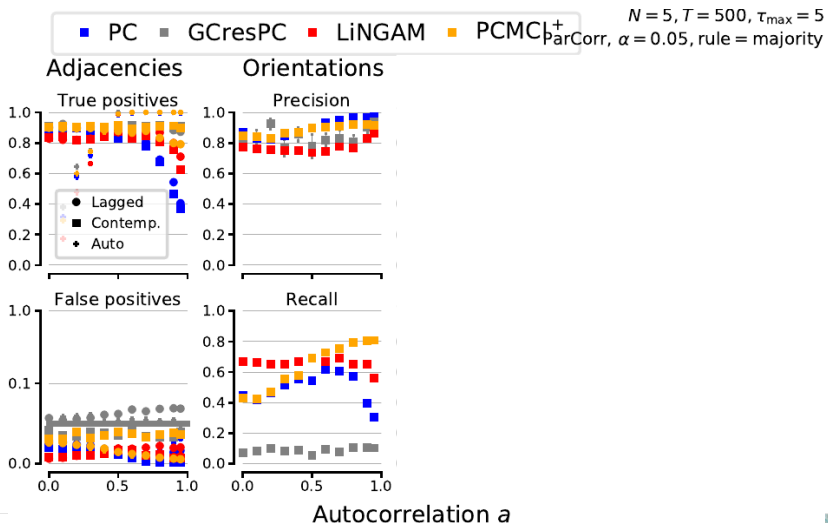
# Numerical experiments

High adjacency detection rate, well-controlled false positives



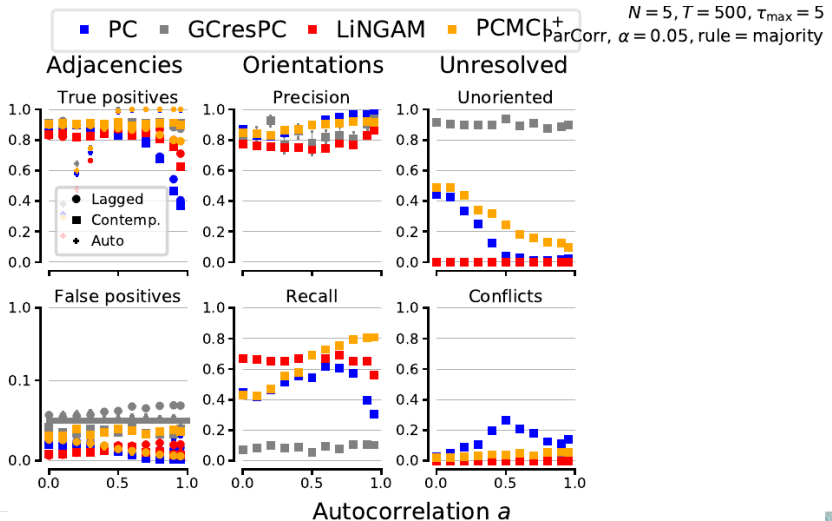
# Numerical experiments

High precision and high recall for strong autocorrelation; LinGAM makes use of non-Gaussianity here, fails for Gaussians



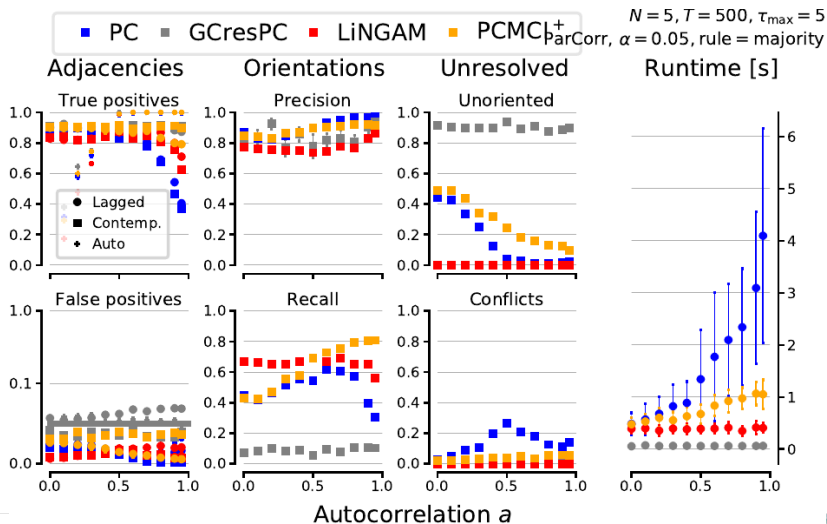
# Numerical experiments

Slightly more unoriented, but also fewer conflicts (majority rule and conflict resolution enabled)



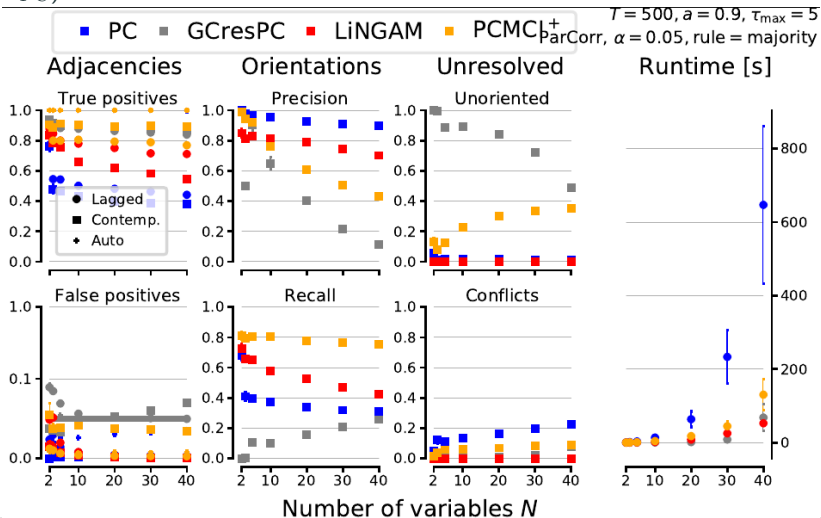
# Numerical experiments

PC takes longer and is more variable



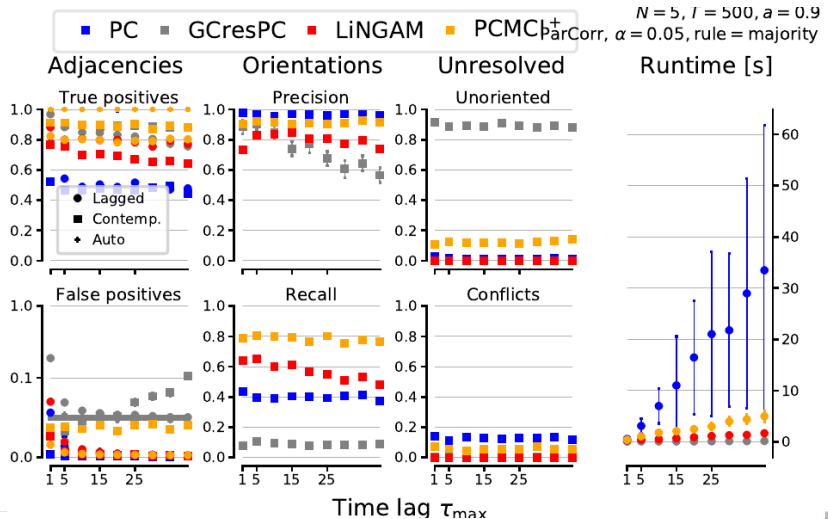
# Numerical experiments

High dimensionality: Still well-calibrated, high recall, less precision (at this  $\alpha_{PC}$ )



# Numerical experiments

Large time lags: Almost no effect on precision and recall

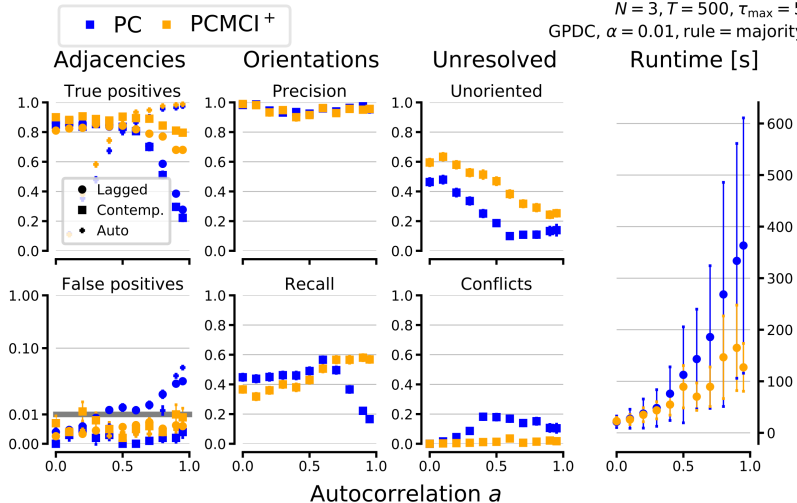


# Numerical experiments

Nonlinear GPDC test: Higher recall than PC for high autocorrelation

$N = 3, T = 500, \tau_{\max} = 5$

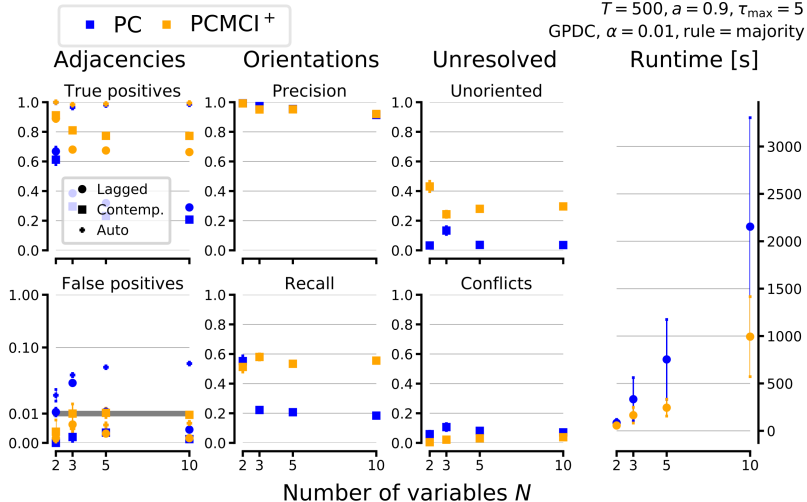
GPDC,  $\alpha = 0.01$ , rule = majority



# Numerical experiments

Nonlinear GPDC test: Higher recall than PC for high dimensionality

$T = 500, a = 0.9, \tau_{\max} = 5$   
GPDC,  $\alpha = 0.01$ , rule = majority



# Application examples

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- Testing causal hypotheses

[Runge et al., 2014, Runge et al., 2015b, Kretschmer et al., 2016, Runge et al., 2019b, Kretschmer et al., 2018, Runge et al., 2018, Runge et al., 2019a, Krich et al., 2019]



# Application cases

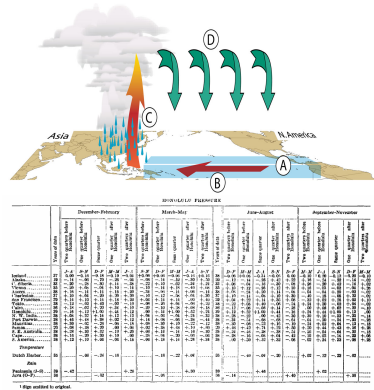
- Testing causal hypotheses  
[Runge et al., 2014, Runge et al., 2015b, Kretschmer et al., 2016, Runge et al., 2019b, Kretschmer et al., 2018, Runge et al., 2018, Runge et al., 2019a, Krich et al., 2019]
- Optimal statistical prediction schemes  
[Runge et al., 2015a, Kretschmer et al., 2017, Di Capua et al., 2019]



- Testing causal hypotheses  
[Runge et al., 2014, Runge et al., 2015b, Kretschmer et al., 2016, Runge et al., 2019b, Kretschmer et al., 2018, Runge et al., 2018, Runge et al., 2019a, Krich et al., 2019]
- Optimal statistical prediction schemes  
[Runge et al., 2015a, Kretschmer et al., 2017, Di Capua et al., 2019]
- Evaluating climate/physical models  
[Schleussner et al., 2014, Nowack et al., 2019]

## Reconstructing Walker Circulation

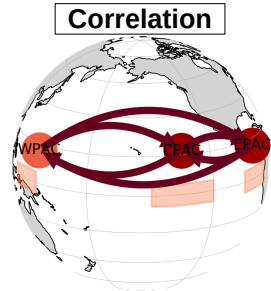
- Monthly surface pressure anomalies in the West Pacific (WPAC), surface air temperature anomalies in the Central Pacific (CPAC) and East Pacific (EPAC)



Runge et al. *Nat. Comm.* (2019)

# Reconstructing Walker Circulation

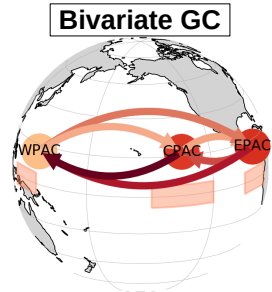
- Monthly surface pressure anomalies in the West Pacific (WPAC), surface air temperature anomalies in the Central Pacific (CPAC) and East Pacific (EPAC)
- Correlation analysis gives a completely connected graph



Runge et al. *Nat. Comm.* (2019)

# Reconstructing Walker Circulation

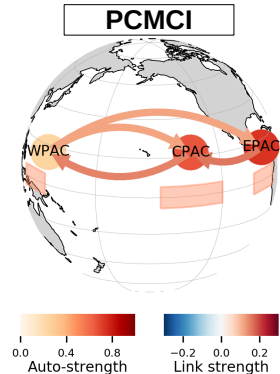
- Monthly surface pressure anomalies in the West Pacific (WPAC), surface air temperature anomalies in the Central Pacific (CPAC) and East Pacific (EPAC)
- Correlation analysis gives a completely connected graph
- Also bivariate Granger Causality cannot remove indirect and common driver links



Runge et al. *Nat. Comm.* (2019)

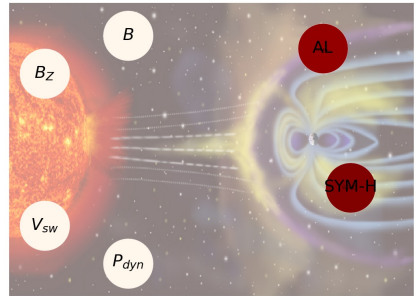
# Reconstructing Walker Circulation

- Monthly surface pressure anomalies in the West Pacific (WPAC), surface air temperature anomalies in the Central Pacific (CPAC) and East Pacific (EPAC)
- Correlation analysis gives a completely connected graph
- Also bivariate Granger Causality cannot remove indirect and common driver links
- PCMCI [Runge et al., 2019b] better identifies the Walker circulation



Runge et al. *Nat. Comm.* (2019)

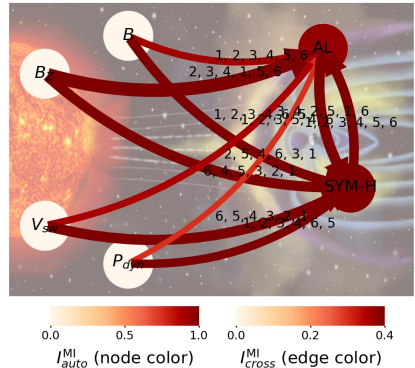
- Hypothesis on interaction between magnetospheric Auroral Electrojet index (AL), magnetospheric ring current strength (SYM-H), and solar wind parameters



Runge et al. *Sci. Rep.* (2018),  $\Delta t = 20\text{min}$   
resolution

- Hypothesis on interaction between magnetospheric Auroral Electrojet index (AL), magnetospheric ring current strength (SYM-H), and solar wind parameters
- Mutual information analysis gives many dependencies

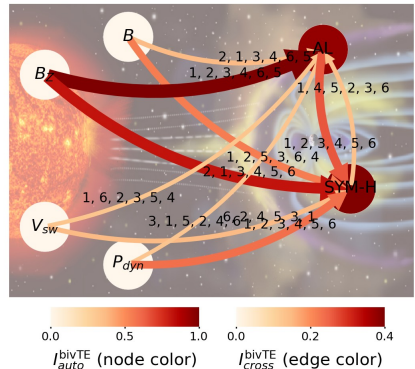
## Mutual information



Runge et al. *Sci. Rep.* (2018),  $\Delta t = 20\text{min}$   
resolution

- Hypothesis on interaction between magnetospheric Auroral Electrojet index (AL), magnetospheric ring current strength (SYM-H), and solar wind parameters
- Mutual information analysis gives many dependencies
- Transfer Entropy cannot remove indirect and common driver links

## Transfer Entropy

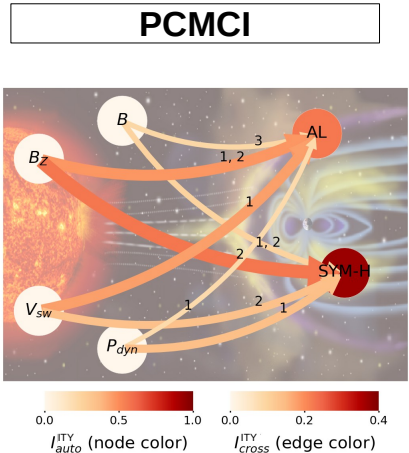


Runge et al. *Sci. Rep.* (2018),  $\Delta t = 20\text{min}$  resolution

# Space physics

- Hypothesis on interaction between magnetospheric Auroral Electrojet index (AL), magnetospheric ring current strength (SYM-H), and solar wind parameters
- Mutual information analysis gives many dependencies
- Transfer Entropy cannot remove indirect and common driver links
- PCMCI yields novel insight that solar wind is common driver of magnetospheric indices

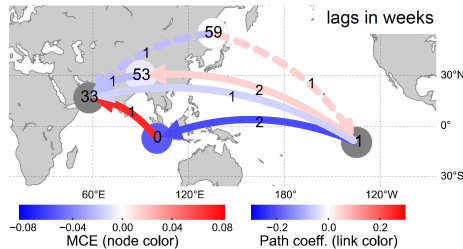
Runge et al. *Sci. Rep.* (2018),  $\Delta t = 20\text{min}$  resolution





## Causal mediation analysis

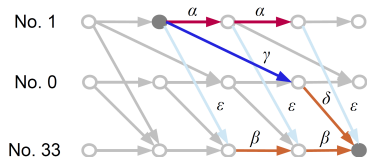
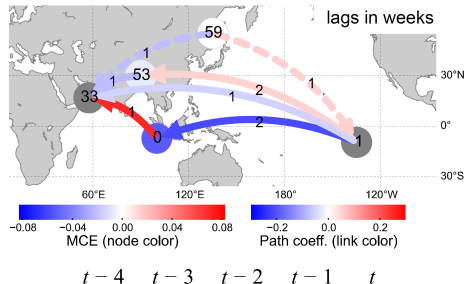
- Pathway mechanisms by which El Nino influences Indian monsoon through sea-level pressure system
- Mediated Causal Effect (MCE) quantifies how much an intermediate variable (node) contributes to a causal effect



Runge et al. *Nat. Comm.* (2015)

# Causal mediation analysis

- Pathway mechanisms by which El Nino influences Indian monsoon through sea-level pressure system
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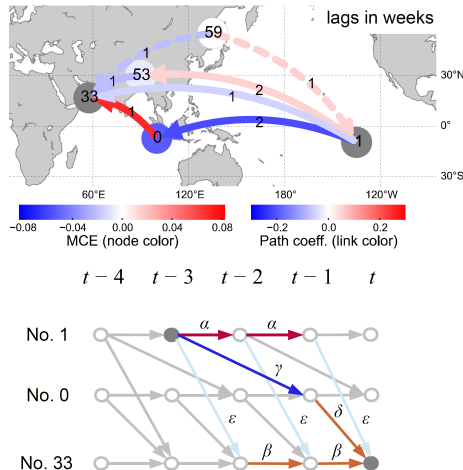


Runge et al. *Nat. Comm.* (2015)

# Causal mediation analysis

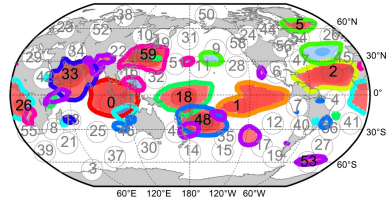
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- Nonlinear extension in Runge *Physical Review E* (2015)

Runge et al. *Nat. Comm.* (2015)



# Causal complex network analysis

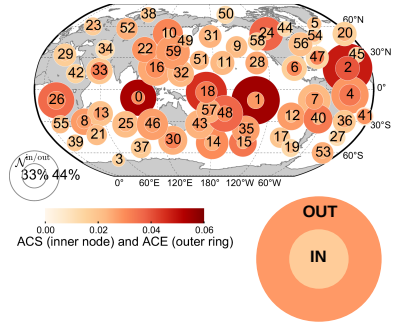
- Complex network measures based on extracted causal network from sea-level pressure system



Runge et al. *Nat. Comm.* (2015)

# Causal complex network analysis

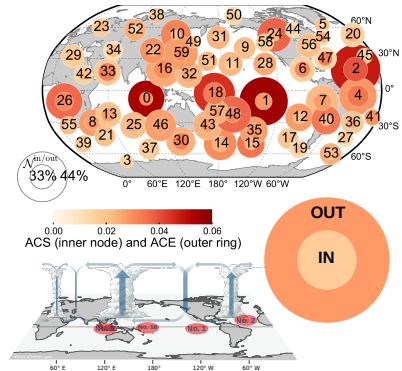
- Complex network measures based on extracted causal network from sea-level pressure system
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Runge et al. *Nat. Comm.* (2015)

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- Complex network measures based on extracted causal network from sea-level pressure system
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- Here well represents tropical atmospheric uplift regions

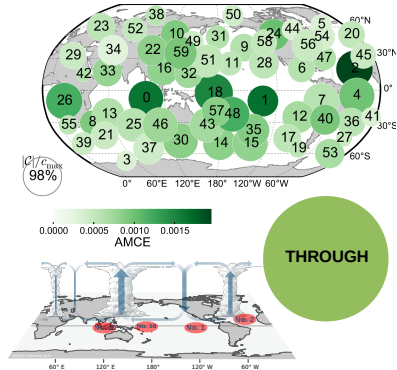


Runge et al. *Nat. Comm.* (2015)

# Causal complex network analysis

- Complex network measures based on extracted causal network from sea-level pressure system
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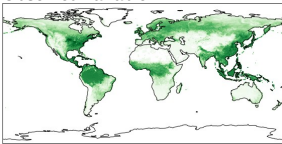
Runge et al. *Nat. Comm.* (2015)



# Causal model evaluation (Nowack et al., 2020)

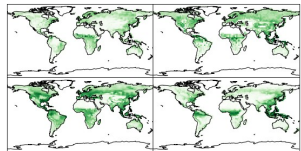
Motivation: Simple statistics (e.g. mean, variance, trends) can be right for the wrong reasons

**Observed variable**



**Real world  
processes**

**Modeled variable**

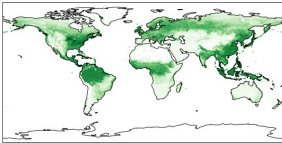


**Modeled  
processes**

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Motivation: Simple statistics (e.g. mean, variance, trends) can be right for the wrong reasons

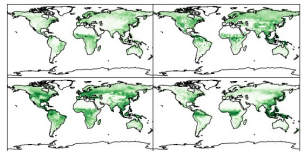
Observed variable



**Real world  
processes**

**Model  
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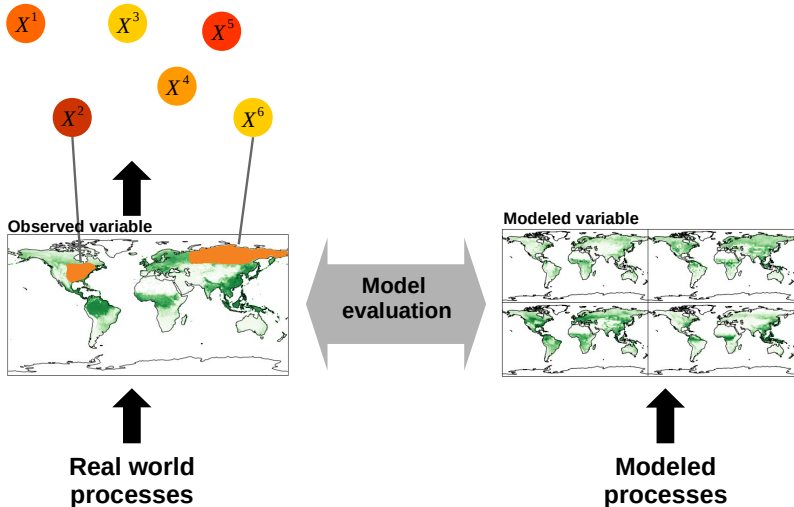
Modeled variable



**Modeled  
processes**

# Causal model evaluation (Nowack et al., 2020)

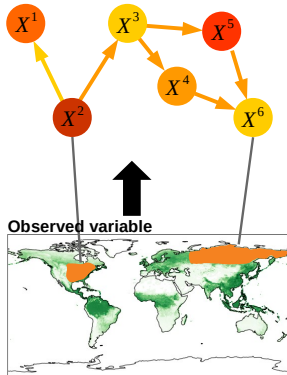
Idea: Compare climate models and observations in terms of causal relationships



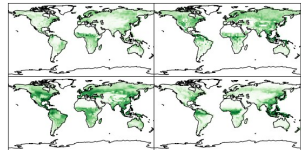
# Causal model evaluation (Nowack et al., 2020)

Idea: Compare climate models and observations in terms of causal relationships

Observed data causal network



Modeled variable



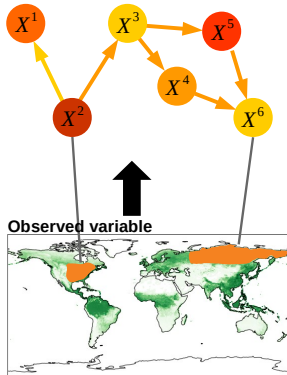
Real world  
processes

Modeled  
processes

# Causal model evaluation (Nowack et al., 2020)

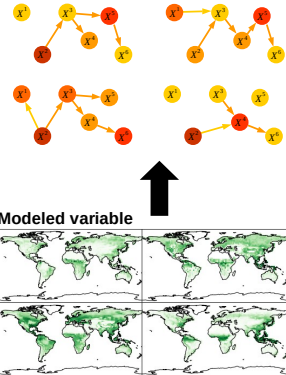
Idea: Compare climate models and observations in terms of causal relationships

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Real world  
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Model data causal networks



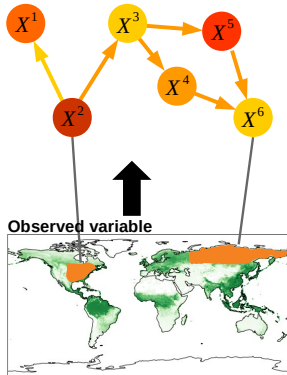
Modeled  
processes

Model  
evaluation

# Causal model evaluation (Nowack et al., 2020)

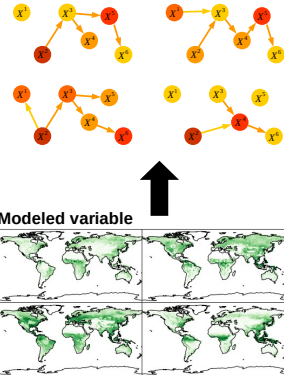
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Causal  
model  
evaluation

Model data causal networks



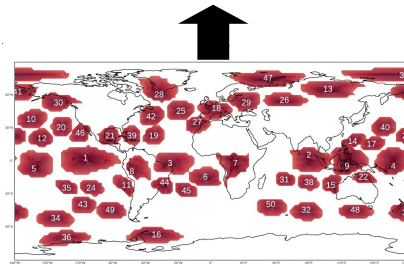
Model  
evaluation

Real world  
processes

Modeled  
processes

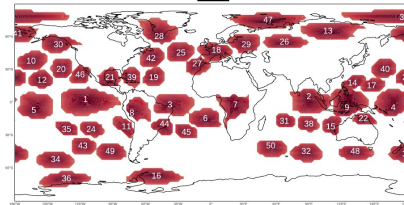
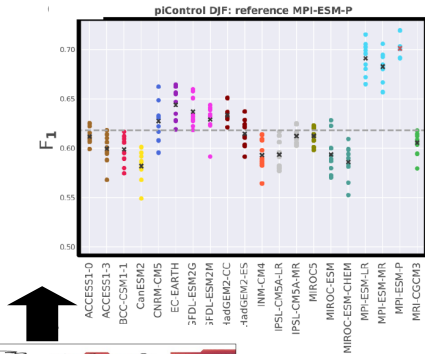
# Causal model evaluation (Nowack et al., 2020)

First results: CMIP5 simulations (historical and preindustrial) vs NCEP/NCAR reanalysis data of regional 3-day-mean sea level pressure



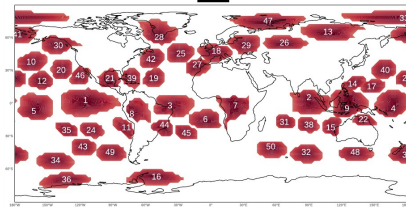
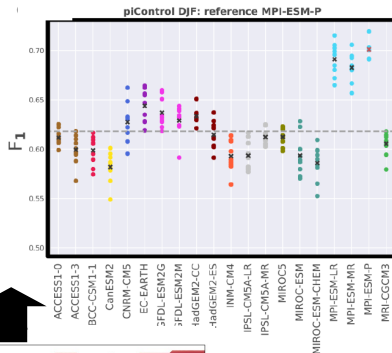
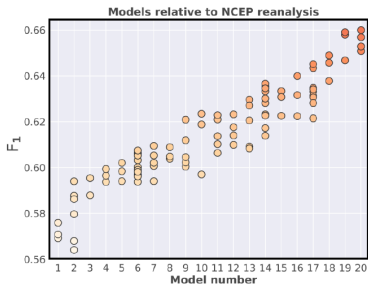
# Causal model evaluation (Nowack et al., 2020)

Validation: Similar climate models have similar causal networks; F-score as network comparison metric



# Causal model evaluation (Nowack et al., 2020)

Model evaluation: Significant differences in comparison to reanalysis



# Causality benchmark platform

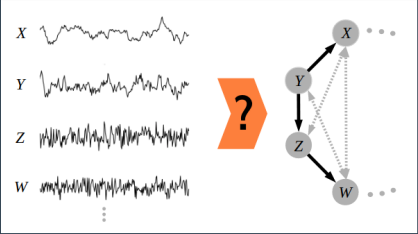
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Joint work with Jordi Munoz-Mari and Gustau Camps-Valls (U Valencia)

**CAUSEME** (BETA)

NEURIPS 2019 COMPETITION   CAUSAL DISCOVERY   HOW IT WORKS   HOW TO CITE   LINKS   LOGIN   SIGN UP   TERMS



**CAUSEME**

A platform to benchmark causal discovery methods

Joint work with Jordi Munoz-Mari and Gustau Camps-Valls (U Valencia)

CAUSEME (BETA)

NEURIPS 2019 COMPETITION

CAUSAL DISCOVERY

HOW IT WORKS

HOW TO CITE

LINKS

LOGIN

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## HOW IT WORKS

**Causeme** currently covers a wide range of synthetic model data mimicking a number of real world challenges. These cover time delays, autocorrelation, nonlinearity, chaotic dynamics, extreme events, measurement error, and will be extended by many more. Method developers can upload their predictions (matrices of causal connections) and the platform evaluates and ranks the methods according to different metrics of performance. After registering and logging in, more information, datasets, and example code snippets are given.

### Challenges

#### Process:

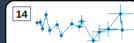
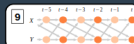
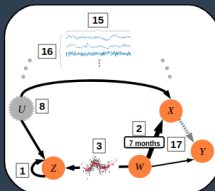
- 1 Autocorrelation
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- 7 Variable extraction
- 8 Unobserved variables
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- 10 Time aggregation
- 11 Measurement errors
- 12 Selection bias
- 13 Discrete data
- 14 Dating uncertainties

#### Computational / statistical:

- 15 Sample size
- 16 High dimensionality
- 17 Uncertainty estimation



Joint work with Jordi Munoz-Mari and Gustau Camps-Valls (U Valencia)

JAKOB RUNGE

DATA AND MODELS

METHODS

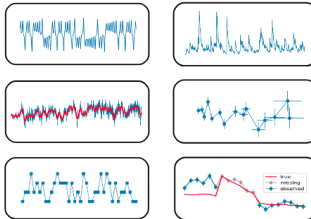
IFRANKING

HOWTO

MY RESULTS

LOGOUT

## DATA AND MODELS



Below you find a list of available datasets. Currently, they come from dynamical model systems featuring different challenges for causal discovery from time series as discussed in the accompanying [Nature Communications Perspective paper](#). At the end of this page you find information on how to contribute real world datasets or model systems. Clicking on the model name will bring you to a description of the model and a list of experimental datasets. Please see the CauseMe workflow description in [HowTo](#) on how to upload your results for these experiments.

You can search through the database by name, description or tags.

Filter models:

Name

Long name

Type

Tags

Joint work with Jordi Munoz-Mari and Gustau Camps-Valls (U Valencia)

JAKOB RUNGE

DATA AND MODELS

METHODS

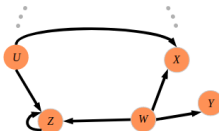
↓ RANKING

HOWTO

MY RESULTS

LOGOUT

## METHODS



Below you find a list of methods applied by users of this platform. Clicking on the name will bring you to a description of the method. You can search through the database by name, user, and tags. Register your own methods on [My Results!](#)

Show  entries

Filter methods:

Name	User	Tags
<a href="#">adaptive-lasso</a>	Jakob runge	Linear, time delays, high-dimensional
<a href="#">correlation</a>	Jakob runge	Linear, time series, non-conditional
<a href="#">distance-correlation</a>	Jakob runge	Time delays, nonlinear, non-conditional
<a href="#">FullCI-CMIkn</a>	Jakob runge	Time delays, nonlinear
<a href="#">FullCI-GPDC</a>	Jakob runge	Time delays, nonlinear
<a href="#">FullCI-BarCorr</a>	Jakob runge	Linear, time delays

## Joint work with Jordi Munoz-Mari and Gustau Camps-Valls (U Valencia)

JAKOB RUNGE

DATA AND MODELS

METHODS

**RANKING**

HOWTO

MY RESULTS

LOGOUT

### RANKING

The table below presents a ranking of methods for different experiments and can be sorted according to the different metrics in columns. Optionally, the table can be filtered by metric values above or below a certain threshold. For example, one can display only methods with a FPR below 6% and sort these by TPR in decreasing order. In addition, the search field can be used on the whole table to select only particular experiments or particular methods (or both). For example, "varmodel N-10 T-150" will list all methods with 'varmodel' in the string and all experiments with N=10 variables and sample length T=150. See [here](#) for a description of metrics: AUC is based on scores, while F-measure, FPR, and TPR are based on binary link predictions by thresholding uploaded p-values at 0.05 (only available if p-values were uploaded). TLR requires lag predictions.

Filter: FPR < 0.06 Go ☐ Paper ☐ Code ☒ Validated

Show 100 entries

Search: linear-VAR\_multirealizations\_N-

Id	User	Experiment	Method (params)	Paper	Code	Valid.	Time	AUC	AUC-PR		F-measure		FPR		TPR		TLR		Boxplot FPR	Boxplot TPR
37	Jakob Runge	linear-VAR_multirealiz	PCMCi-ParCorr (tau_max=5,pc_	✓	✓	✓	2.97	0.98	0.89	0.56	0.05	0.92	0.98							
145	Jakob Runge	linear-VAR_multirealiz	adaptive-lasso (tau_max=5,)	✓	✗	✓	18.99	0.96	0.86	0.75	0.02	0.92	0.99							
215	Jakob Runge	linear-VAR_multirealiz	varmodel (maxlags=5,)	✓	✓	✓	0.48	0.95	0.69	0.50	0.05	0.76	0.98							
249	Jakob Runge	linear-VAR_multirealiz	FullCI-ParCorr (tau_max=5,)	✓	✓	✓	11.24	0.94	0.70	0.51	0.05	0.74	0.98							

Showing 1 to 4 of 4 entries (filtered from 1,604 total entries)

Previous 1 Next

# Discussion and Conclusions

---



- Causal inference = answering causal questions from empirical data



# Discussion

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- Causal inference **methods only give you graph**



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- And to indicate how conclusions are altered for different assumptions

- Causal discovery from observational data is actually possible



# Discussion and Conclusions

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    - Optimal statistical forecast schemes
- [Runge et al., 2015a, Kretschmer et al., 2017, Di Capua et al., 2019]

# Discussion and Conclusions

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[Runge et al., 2015a, Kretschmer et al., 2017, Di Capua et al., 2019]
  - Causal evaluation of physical climate models (Nowack et al., 2020)



# Thank you! Questions?

- PCMCI [Runge et al., 2019b] in Science Advances
- PCMCI<sup>+</sup> Runge (2020) <https://arxiv.org/abs/2003.03685>
- Conditional independence testing based on CMI [Runge, 2018b] in AISTATS
- Nature Comm. Perspective [Runge et al., 2019a]
- My software: [jakobrunge.github.io/tigramite](https://jakobrunge.github.io/tigramite)

## Challenges

### Process:

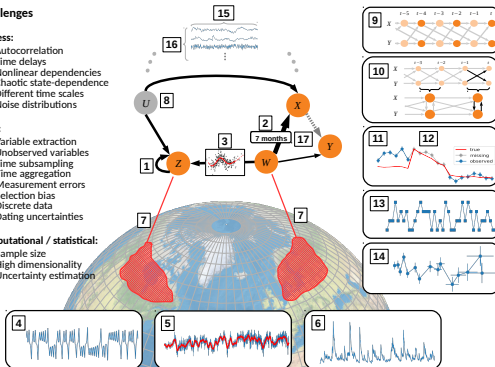
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[Runge et al., 2019b, Runge et al., 2019a, Camps-Valls et al., 2019, Di Capua et al., 2019, Krich et al., 2019, Trifunov et al., 2019a, Trifunov et al., 2019b, Reimers et al., 2019, Runge, 2018b, Boltt et al., 2018, Runge, 2018a, Kretschmer et al., 2018, Tibau et al., 2018, Runge et al., 2018, Kretschmer et al., 2017, Kretschmer et al., 2016, Runge, 2015, Runge et al., 2015a, Runge et al., 2015b, Runge et al., 2014, Schleussner et al., 2014, Runge et al., 2012b, Runge et al., 2012a, Pompe and Runge, 2011]



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Camps-Valls, G., Sejdinovic, D., Runge, J., and Reichstein, M. (2019).

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**The different stratospheric influence on cold-extremes in Eurasia and North America.**

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Kretschmer, M., Coumou, D., Donges, J. F., and Runge, J. (2016).

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Kretschmer, M., Runge, J., and Coumou, D. (2017).

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-  Nowack, P. J., Runge, J., Eyring, V., and Haigh, H. D. (2019).  
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