



DLR

Deutsches Zentrum  
für Luft- und Raumfahrt  
German Aerospace Center

Imperial College  
London



JAMES S. McDONNELL FOUNDATION

# Causal inference and complex network methods for the geosciences

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Jakob Runge

September 28, 2017

<https://jakobrunge.github.io/tigramite/>

# New research group



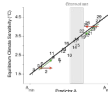
Open PhD and Postdoc positions  
→ [climateinformaticslab.com](http://climateinformaticslab.com)



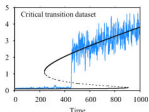
## Climate model evaluation



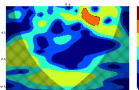
## Climate sensitivity



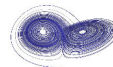
## Extremes prediction



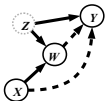
## Time-scale causality



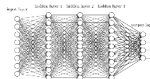
## Data-driven dynamical models



## Causal discovery theory



## Deep learning



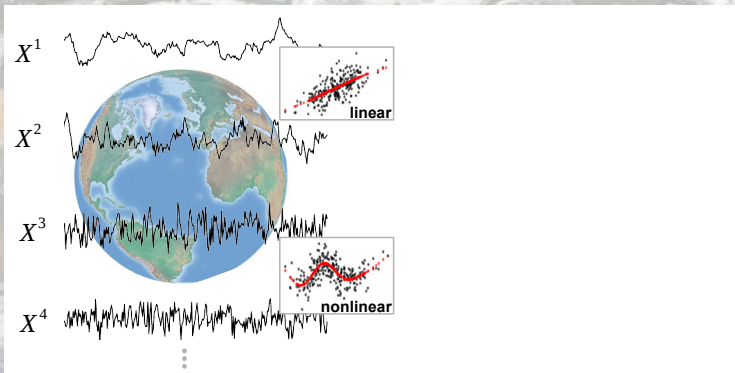
# Problem setting

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## Goal

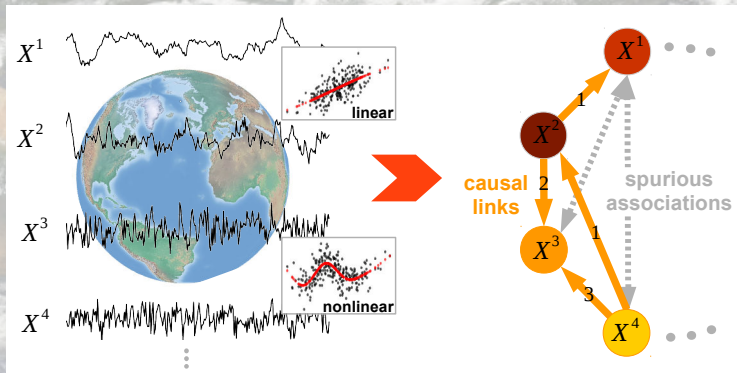
Learn causal interactions from time series of complex dynamical systems



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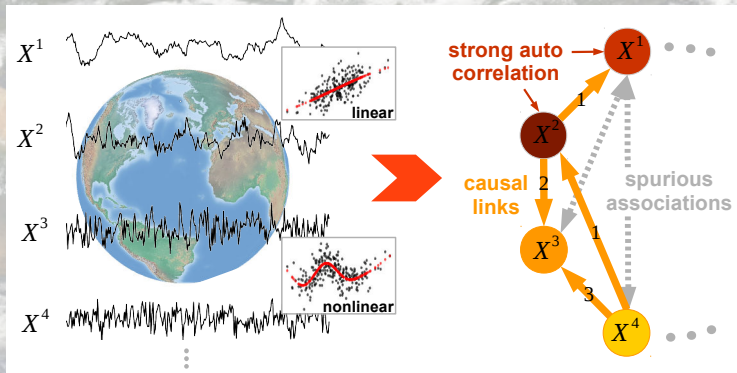
Learn causal interactions from time series of complex dynamical systems



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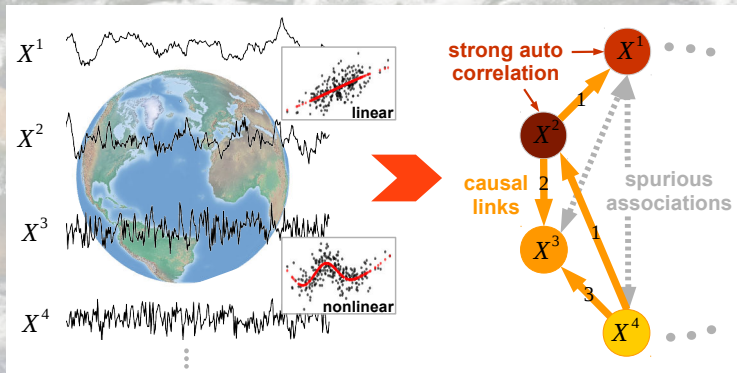
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Learn causal interactions from time series of complex dynamical systems

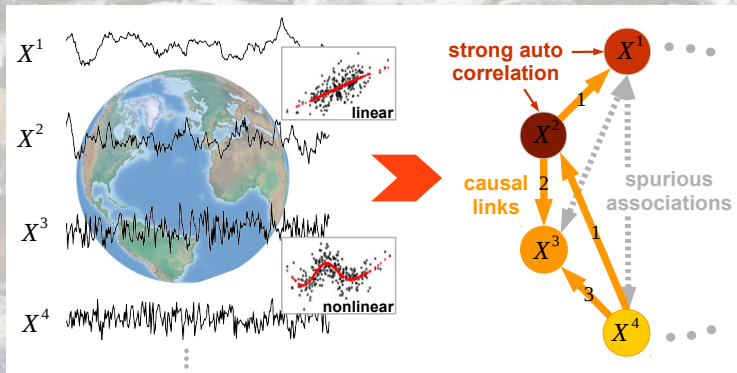


1. How to **formulate** causal inference for complex dynamical systems?

# Problem setting

## Goal

Learn causal interactions from time series of complex dynamical systems



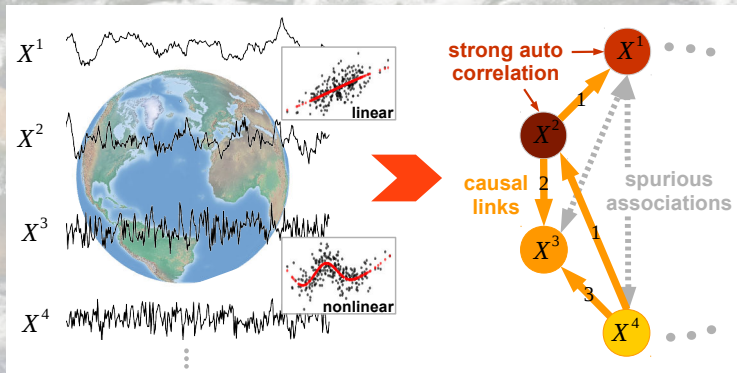
1. How to **formulate** causal inference for complex dynamical systems?
2. How to **detect** causal links?



# Problem setting

## Goal

Learn causal interactions from time series of complex dynamical systems



1. How to **formulate** causal inference for complex dynamical systems?
2. How to **detect** causal links?
3. How to **quantify** causal interactions?

**How to formulate causal  
inference for complex dynamical  
systems?**

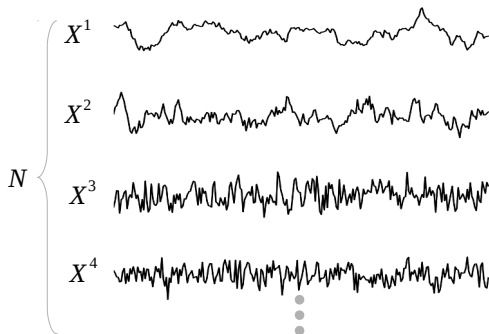
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# Time series graphs

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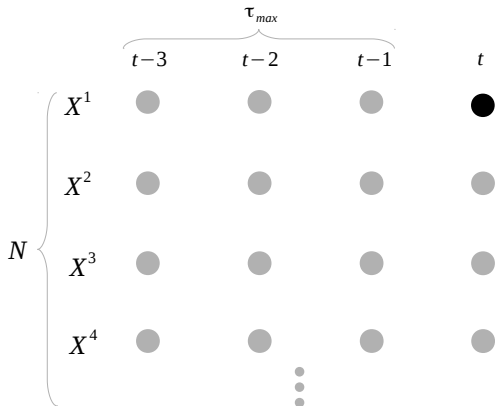
## Definition



[Eichler, 2012]

# Time series graphs

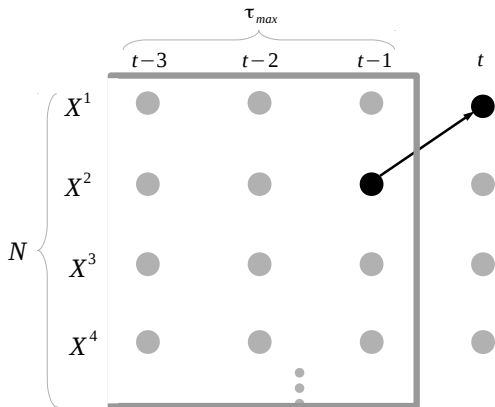
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[Eichler, 2012]

# Time series graphs

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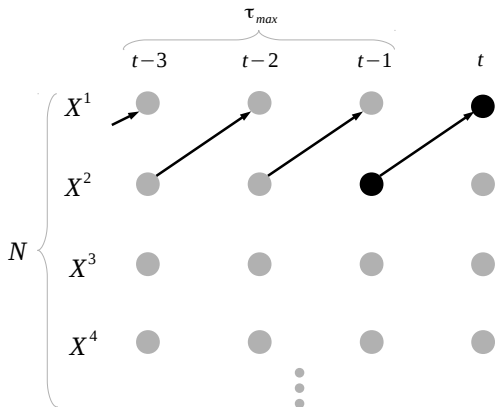


$X_{t-\tau}^i \not\perp X_t^j \mid \mathbf{X}_t^-$   
 $X_{t-\tau}^i$  is *not* independent  
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[Eichler, 2012]

# Time series graphs

## Definition



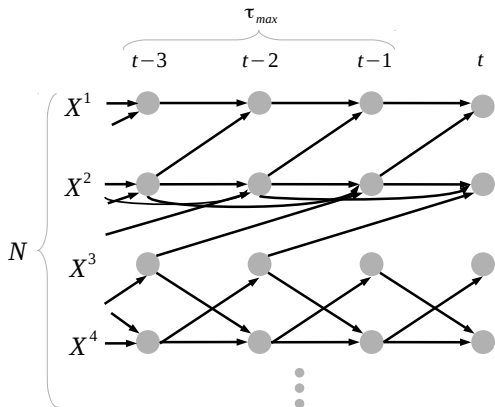
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Assuming stationarity

[Eichler, 2012]

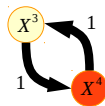
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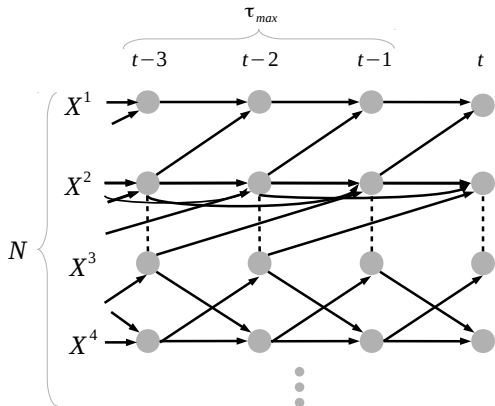


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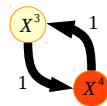
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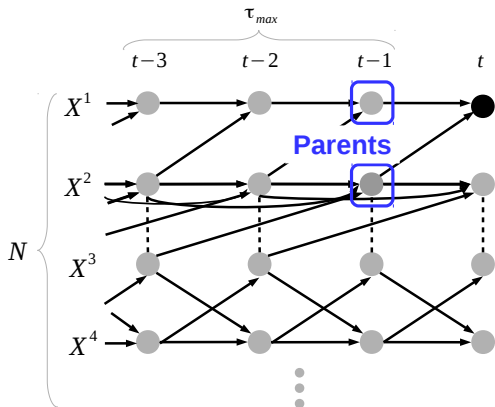
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Contemporaneous links defined as  $X_t^i \not\perp\!\!\!\perp X_t^j \mid \mathbf{X}_t^-$  left *undirected* here  
[Eichler, 2012]

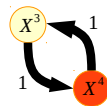
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**How to detect causal links?**

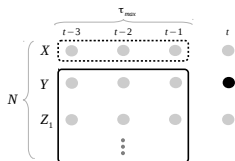
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# Causal discovery

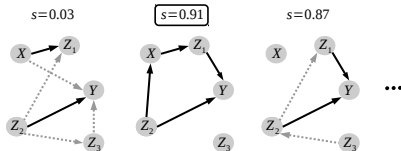
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# Causal discovery overview

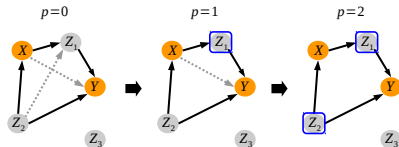
## High-dimensional independence testing / Granger causality



## Score-based / Bayesian network estimation

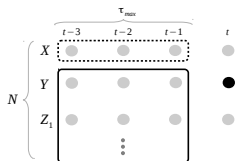


## Constraint-based / PC algorithm



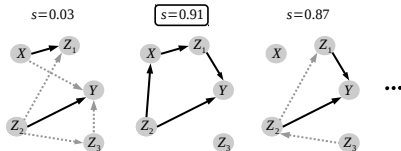
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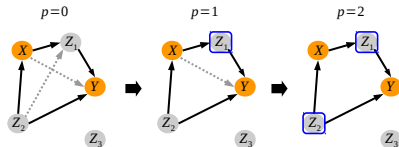


Hybrid-methods

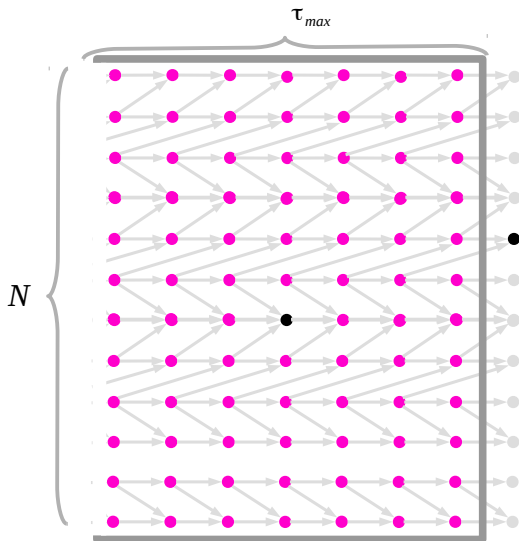
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## Granger causality

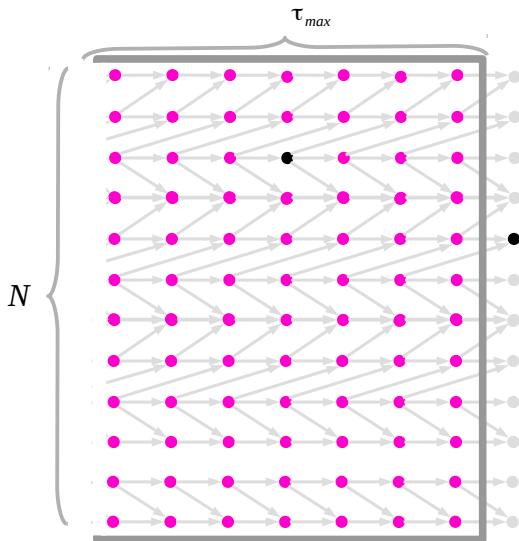


## Lag-specific Granger causality:

$$X_{t-\tau}^i \not\perp\!\!\!\perp X_t^j \mid \mathbf{X}_t^-$$

here implemented with  
ParCorr based on OLS /  
Ridge / Lasso,  
non-parametric Gaussian  
processes test  $\rightarrow$  paper

## Granger causality



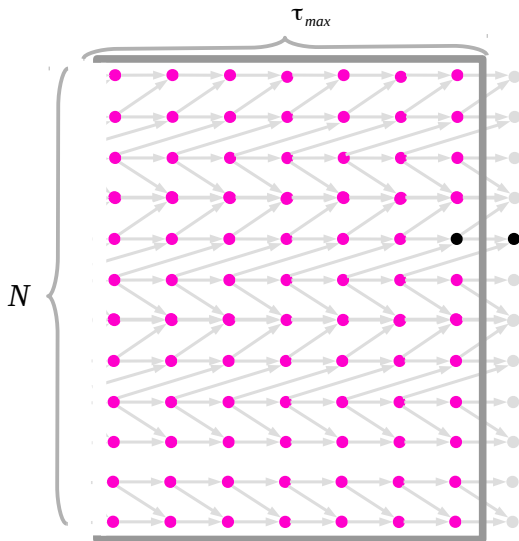
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## Granger causality



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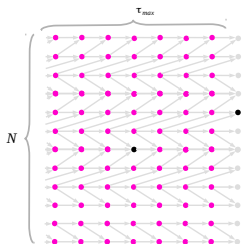
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# PCMCI = $PC_1$ -condition selection + MCI test

## 1. Condition selection (Markov blanket)

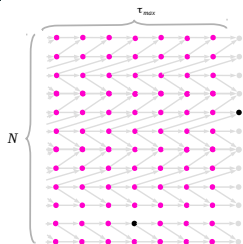
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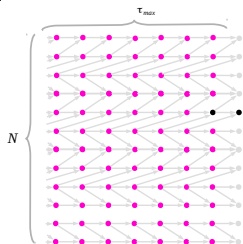
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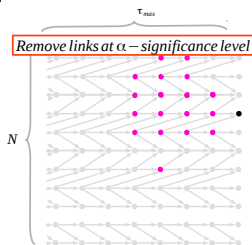
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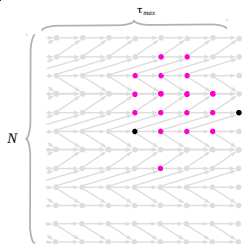
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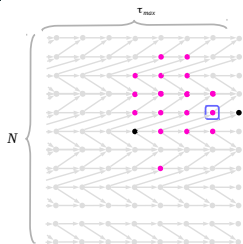
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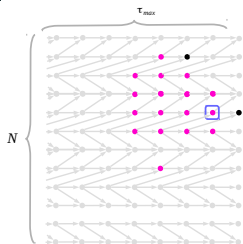
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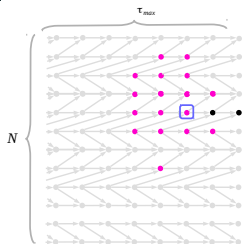




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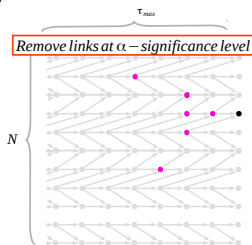
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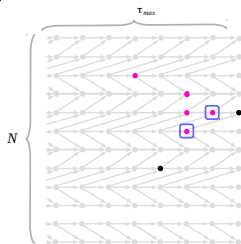
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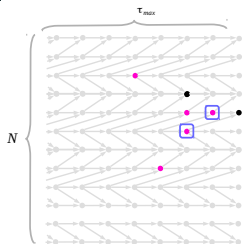
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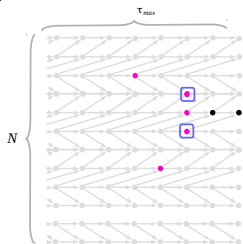
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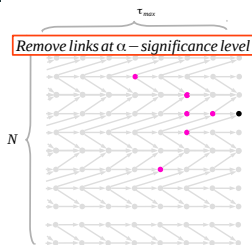
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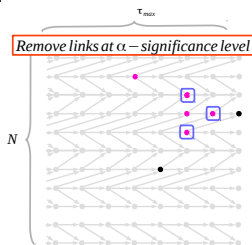
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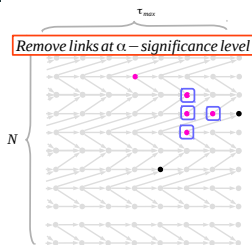
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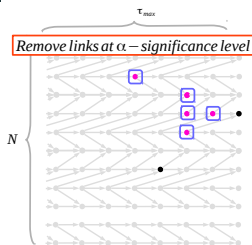




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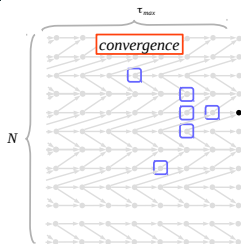
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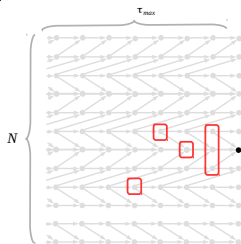
For  $j \in \{1, \dots, N\}$ : Estimate superset of parents  $\tilde{\mathcal{P}}(X_t^j)$  such that  $X_t^j \perp\!\!\!\perp \mathbf{X}_t^- \setminus \tilde{\mathcal{P}}(X_t^j) \mid \tilde{\mathcal{P}}(X_t^j)$  with iterative  $PC_1$  algorithm: **tuned to high power with liberal  $\alpha$ , false pos. control in next step!**



# PCMCI = PC<sub>1</sub>-condition selection + MCI test

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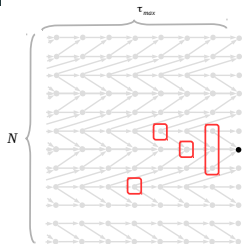
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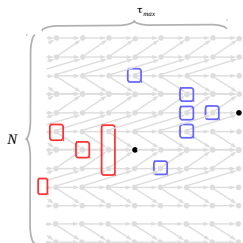
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## 2. Momentary conditional independence (MCI) test

For  $i, j \in \{1, \dots, N\}$  and  $0 \leq \tau \leq \tau_{\max}$ :  
Test

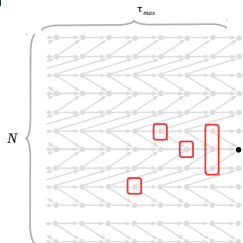
$$\text{MCI: } X_{t-\tau}^i \perp\!\!\!\perp X_t^j \mid \tilde{\mathcal{P}}(X_t^j), \tilde{\mathcal{P}}(X_{t-\tau}^i)$$



# PC<sub>1</sub> = PC<sub>1</sub>-condition selection + MCI test

## 1. Condition selection (Markov blanket)

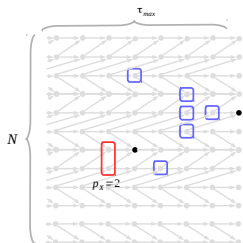
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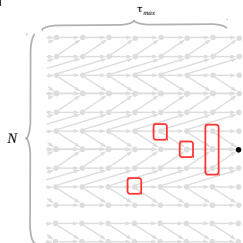
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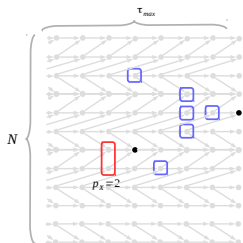
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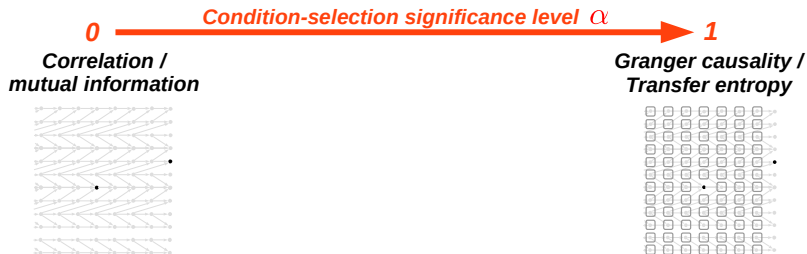
## Flexible regarding conditional independence tests

here ParCorr (OLS), Gaussian processes  $\rightarrow$  paper

PCMCI =  $PC_1$ -condition selection + MCI test

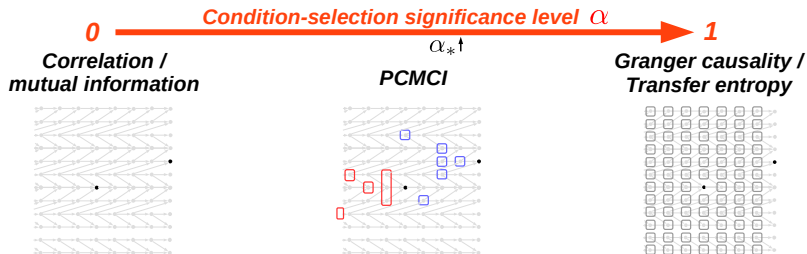
*0*  *1*  
*Condition-selection significance level  $\alpha$*

# PCMCI = PC<sub>1</sub>-condition selection + MCI test

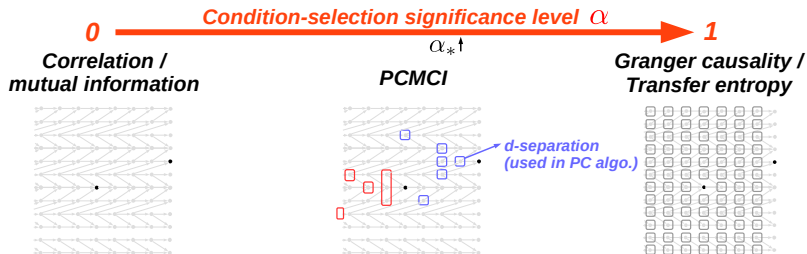




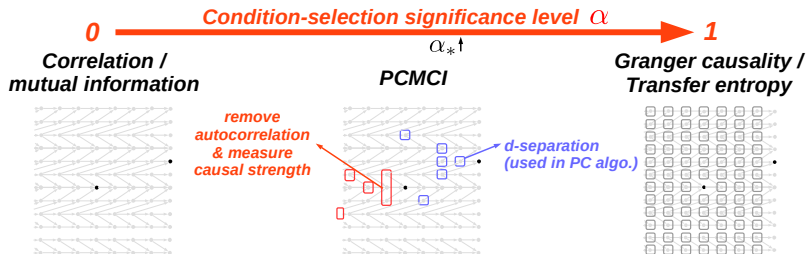
# PCMCI = PC<sub>1</sub>-condition selection + MCI test



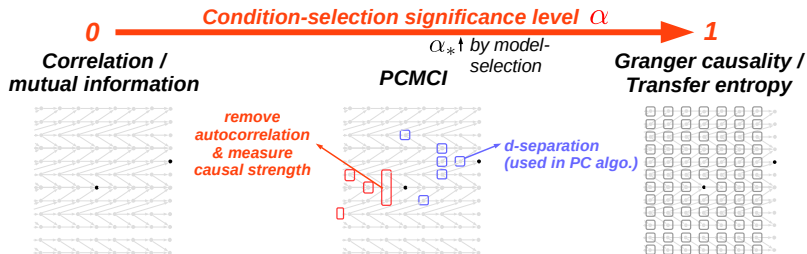
# PCMCI = $PC_1$ -condition selection + MCI test



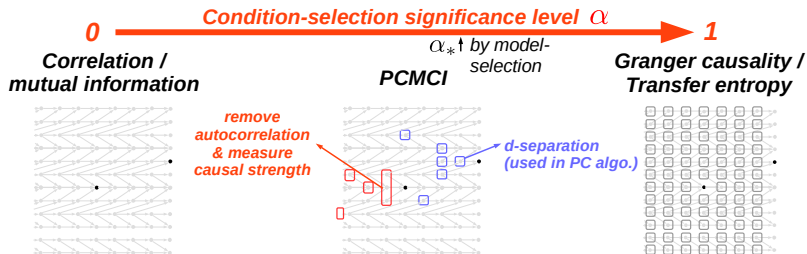
# PCMCI = PC<sub>1</sub>-condition selection + MCI test



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# PCMCI = PC<sub>1</sub>-condition selection + MCI test



## More theory in paper:

If PC<sub>1</sub> identifies parents, then

- MCI has unbiased detection power for linear links in additive models

$$I_{X \rightarrow Y}^{\text{MCI}} = I(\eta_{t-\tau}^X; c\eta_{t-\tau}^X + \eta_t^Y)$$

- MCI is well-calibrated also for autocorrelated data
- effect size of MCI is larger than GC  $\rightarrow$  more power also for low dimensions

## Conditional independence tests

---

## Assuming linear model: Partial correlation (ParCorr)

1. Regress out influence of  $Z$  with OLS

$$X = Z\beta_X + \epsilon_X$$

$$Y = Z\beta_Y + \epsilon_Y$$

Ridge and Lasso implemented with `scikit-learn` on standardized time series

- Ridge regularization: LOO-cross-validated regularization parameter  $\alpha \in \{0.1, 1, 2, \dots, 500\}$
  - Lasso regularization: multi-task lasso,  $\alpha \in \{0.0001, 0.001, 0.01, 0.1, 1\}$  using 5-fold cross-validation, max. iterations = 100
2. Test independence of residuals with  $t$ -test
    - OLS:  $T - D_Z - 2$  degrees of freedom

## Assuming nonlinear additive Gaussian: GPDC

1. Regress out influence of  $Z$  with Gaussian process assuming

$$X = f_X(Z) + \epsilon_X$$

$$Y = f_Y(Z) + \epsilon_Y$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

GP regression implemented using `sklearn`

- Radial Basis Function (RBF) + White Noise kernel
  - bandwidth estimated with MLE
2. Test independence of uniformized residuals with *distance correlation coefficient* [Székely et al., 2007]

$$\mathcal{R}(r_X, r_Y)$$

using pre-computed null distribution (for every  $T$ )



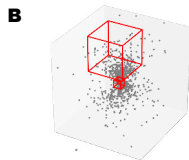
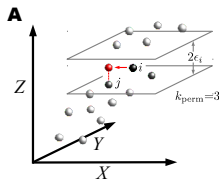
# Conditional independence tests $X \perp\!\!\!\perp Y \mid Z$

## General: Conditional mutual information (CMI)

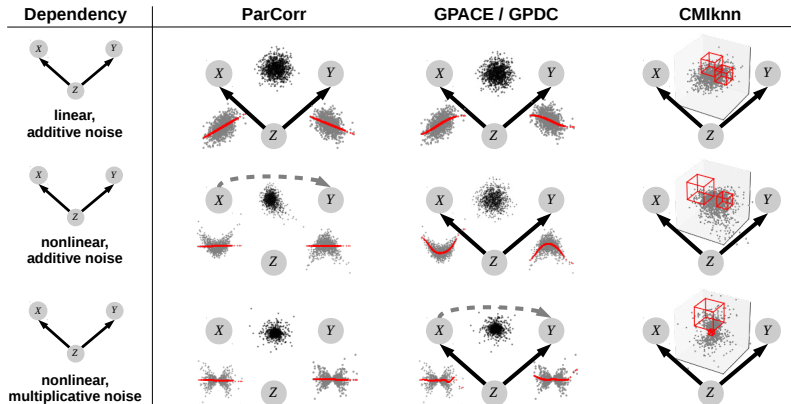
$$I(X; Y|Z) = \int dz p(z) \int \int dx dy p(x, y|z) \log \frac{p(x, y|z)}{p(x|z) \cdot p(y|z)}$$

Estimated with  $k$ NN-estimator  
[Kraskov et al., 2004,  
Frenzel and Pompe, 2007]

**Free parameter:** number of  
nearest neighbors  $k \sim$  locally  
adaptive bandwidth



# Conditional independence tests $X \perp\!\!\!\perp Y \mid Z$



# Causal assumptions

**Causal interpretation assumes [Spirtes et al., 2000]:**

- **Causal Markov Condition:** “All the relevant probabilistic information that can be obtained from the system is contained in its direct causes”
- **Causal Sufficiency:** Measured variables include all of the common causes
- **Faithfulness / Stableness:** “Independencies in data arise not from incredible coincidence, but rather from causal structure”; violated by purely deterministic dependencies

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More discussion → appendix

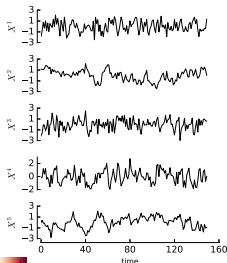
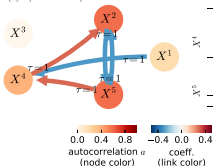
## Numerical experiments

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# Numerical experiments

## Model setup

$$\begin{aligned}X_1^t &= 0.20X_1^{t-1} + \eta_t^1 \\X_2^t &= 0.60X_2^{t-1} - 0.287f^{(1)}(X_2^{t-1}) \\&\quad + 0.287f^{(1)}(X_2^{t-1}) + \eta_t^2 \\X_3^t &= +\eta_t^3 \\X_4^t &= 0.40X_4^{t-1} - 0.287f^{(1)}(X_4^{t-1}) \\&\quad + 0.287f^{(1)}(X_4^{t-1}) + \eta_t^4 \\X_5^t &= 0.60X_5^{t-1} - 0.287f^{(1)}(X_5^{t-1}) + \eta_t^5 \\ \eta &\sim \mathcal{N}(0,1) \\ f^{(1)}(x) &= x \\ f^{(2)}(x) &= (1 - 4e^{-x^2/2})x \\ f^{(3)}(x) &= (1 - 4x^3e^{-x^2/2})x\end{aligned}$$



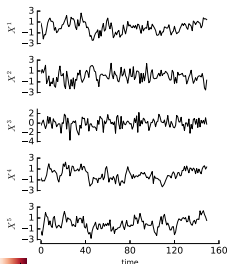
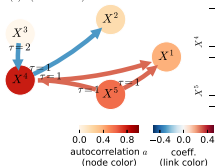
- random coupling topologies, time lags, linear
- fixed link strength within each network
- different autocorrelations for variables
- $\tau_{\max} = 5$ ,  $T = 150$ , varying  $N = 5..60 \rightarrow N \cdot \tau_{\max} > T$

# Numerical experiments

## Model setup

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$\eta \sim \mathcal{N}(0,1)$   
 $f^{(1)}(x) = x$   
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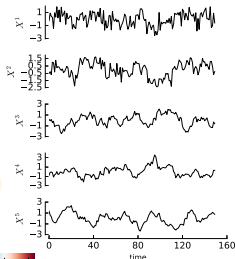
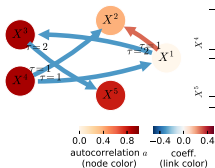


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## Model setup

$$\begin{aligned}
 X_1^1 &= -0.287f^{(1)}(X_{t-1}^1) + \eta_t^1 \\
 X_2^1 &= 0.40X_{t-1}^2 - 0.287f^{(1)}(X_{t-1}^2) \\
 &\quad + 0.287f^{(1)}(X_{t-1}^1) + \eta_t^2 \\
 X_3^1 &= 0.90X_{t-1}^3 - 0.287f^{(1)}(X_{t-1}^3) + \eta_t^3 \\
 X_4^1 &= 0.90X_{t-1}^4 + \eta_t^4 \\
 X_5^1 &= 0.80X_{t-1}^5 - 0.287f^{(1)}(X_{t-1}^5) + \eta_t^5 \\
 \eta &\sim \mathcal{N}(0,1) \\
 f^{(1)}(x) &= x \\
 f^{(2)}(x) &= (1 - 4e^{-x^2/2})x \\
 f^{(3)}(x) &= (1 - 4x^3e^{-x^2/2})x
 \end{aligned}$$



- random coupling topologies, time lags, linear
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# Numerical experiments

## Model setup

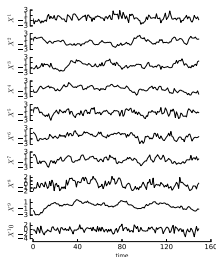
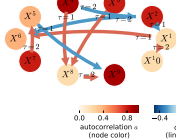
$$\begin{aligned}
 X_1^t &= 0.30X_1^{t-1} - 0.287f^{(1)}(X_2^{t-1}) + \eta_t^1 \\
 X_2^t &= 0.80X_2^{t-1} - 0.287f^{(1)}(X_1^{t-1}) + \eta_t^2 \\
 X_3^t &= 0.80X_3^{t-1} + \eta_t^3 \\
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 X_6^t &= 0.80X_6^{t-1} + \eta_t^6 \\
 X_7^t &= 0.30X_7^{t-1} + 0.287f^{(1)}(X_2^{t-1}) \\
 &\quad + 0.287f^{(1)}(X_3^{t-1}) + \eta_t^7 \\
 X_8^t &= 0.90X_8^{t-1} + 0.287f^{(1)}(X_7^{t-1}) \\
 &\quad - 0.287f^{(1)}(X_2^{t-1}) + \eta_t^8 \\
 X_9^t &= 0.30X_9^{t-1} + 0.287f^{(1)}(X_2^{t-1}) + \eta_t^9
 \end{aligned}$$

$$\eta \sim \mathcal{N}(0, 1)$$

$$f^{(1)}(x) = x$$

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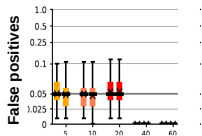
$$f^{(3)}(x) = (1 - 4e^{-x^2})x^2$$



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## Similarly well-calibrated tests

GC

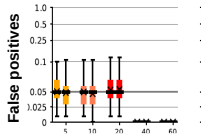


Number of variables  $N$

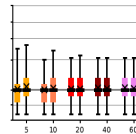
# Numerical experiments

## Similarly well-calibrated tests

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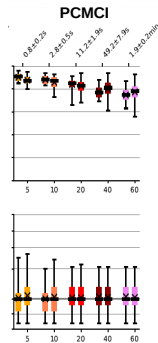
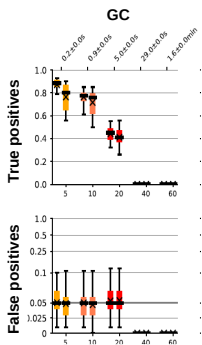
PCMCI



Number of variables  $N$

# Numerical experiments

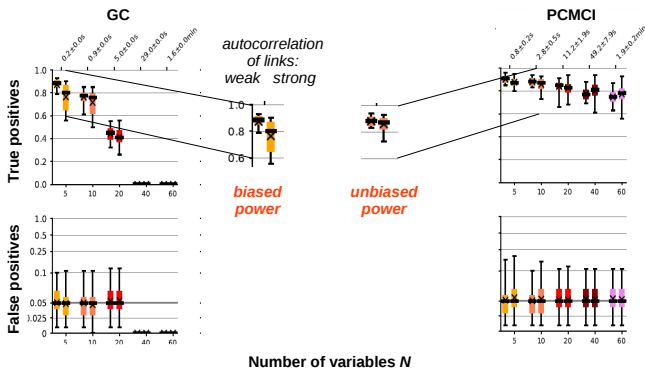
## GC suffers from curse of dimensionality and power bias



Number of variables  $N$

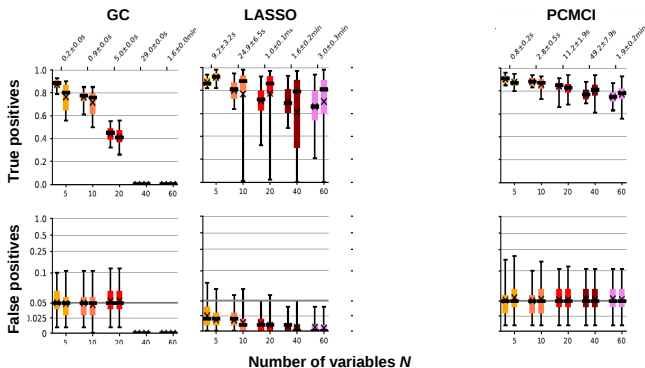
# Numerical experiments

## GC suffers from curse of dimensionality and power bias



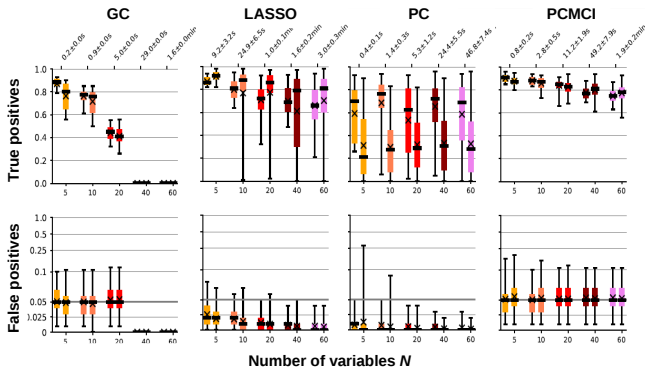
# Numerical experiments

## Lasso not well-calibrated and power bias



# Numerical experiments

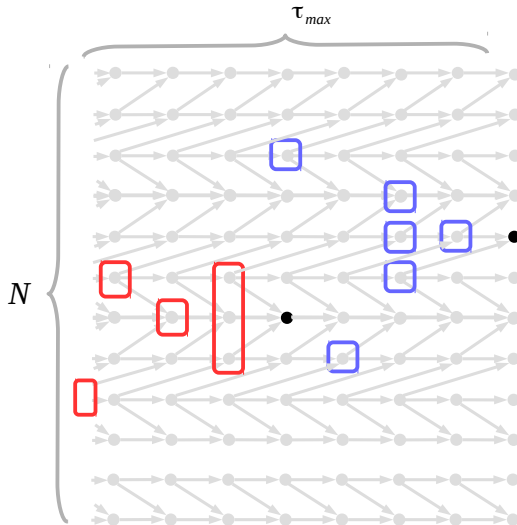
## PC algorithm also low and biased power





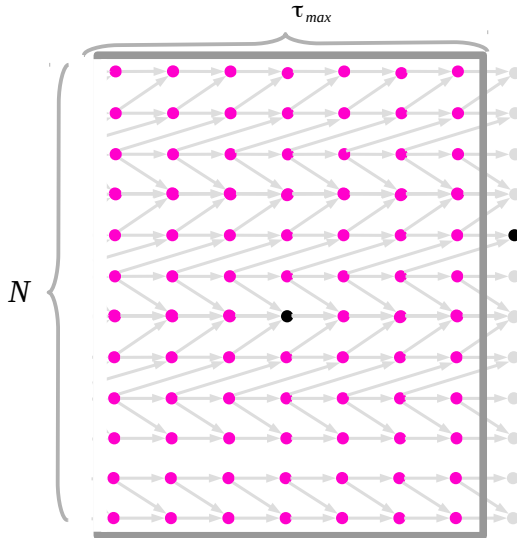
# Numerical experiments

Key idea again



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Key idea again



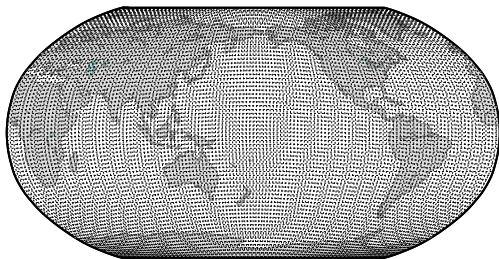
# Applications

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- **Causal hypothesis testing**  
[Runge et al., 2014, Runge et al., 2015c, Kretschmer et al., 2016]
- **Variable selection** for model building
- ...or **prediction schemes**  
[Runge et al., 2015a, Kretschmer et al., 2017]
- **Pathway analysis** [Runge et al., 2015b, Runge, 2015]

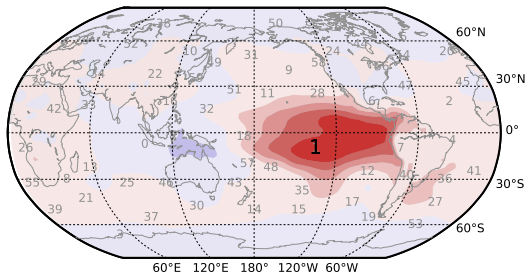
# Global sea-level pressure interactions

## Sea-level pressure system [Kalnay et al., 1996]



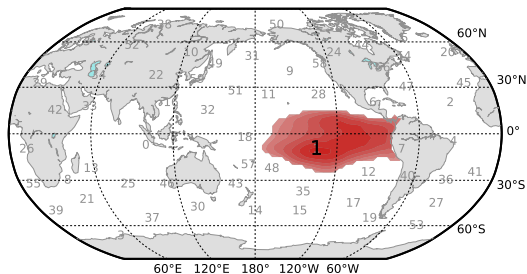
- detrended, anomalized, winter-only (DJF) of 1981–2012
- dimension reduction using Varimax-rotated PCA [Vejmelka et al., 2014]
- time resolution: 3-days,  $\tau_{\max} = 3$  weeks

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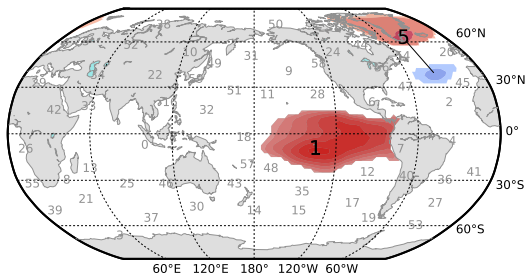
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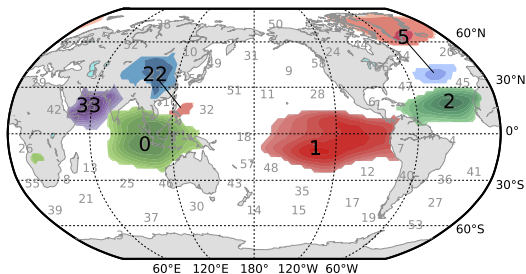
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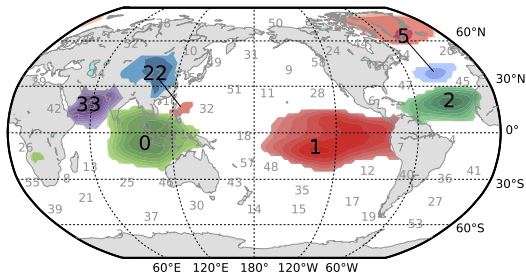


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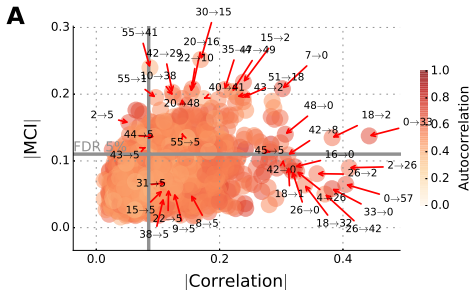
- detrended, anomalized, winter-only (DJF) of 1981–2012
- dimension reduction using Varimax-rotated PCA [Vejmelka et al., 2014]
- time resolution: 3-days,  $\tau_{\max} = 3$  weeks

## Sea-level pressure system [Kalnay et al., 1996]



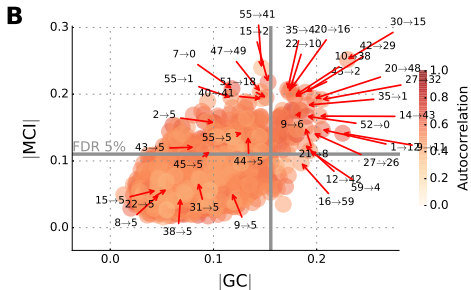
- detrended, anomalized, winter-only (DJF) of 1981–2012
- dimension reduction using Varimax-rotated PCA [Vejmelka et al., 2014]
- time resolution: 3-days,  $\tau_{\max} = 3$  weeks
- $N_{\tau_{\max}} = 60 \cdot 7 = 420$  with a comparably small sample size of about 950 samples and partially strong autocorrelations

## Spurious correlation vs MCI



- even strong correlations are spurious

## Granger causality vs MCI



- many even strong causal links overlooked with GC

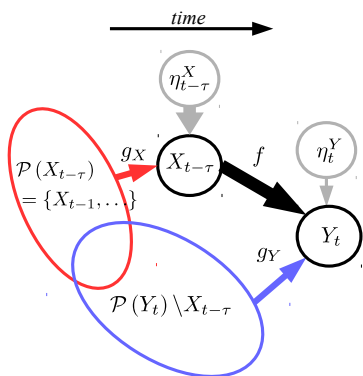
## **How to quantify causal interactions?**

---

## Causal strength

---

## Defining causal strength



$$X_{t-\tau} = g_X(\mathcal{P}(X_{t-\tau})) + \eta_{t-\tau}^X$$

$$Y_t = g_Y(\mathcal{P}(Y_t) \setminus \{X_{t-\tau}\}) + \tilde{\eta}_t^Y$$

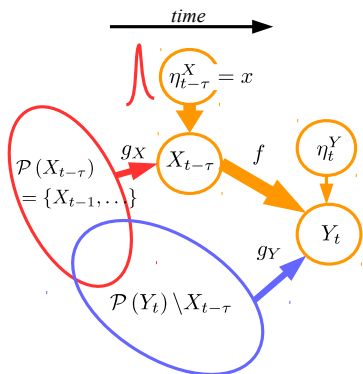
with link  $X_{t-\tau} \rightarrow Y_t$  represented as  
 $\tilde{\eta}_t^Y = f(X_{t-\tau}) + \eta_t^Y$

## Causal strength

$$I(\eta_{t-\tau}^X; \tilde{\eta}_t^Y | \mathcal{P}(X_{t-\tau}))$$

measures "momentary" dependence in  $\tilde{\eta}_t^Y$  on  $X_{t-\tau}$  that does not come through the parents of  $X_{t-\tau}$

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# MCI and causal strength

## Definition

$$\text{MCI: } X_{t-\tau} \perp\!\!\!\perp Y_t \mid \mathcal{P}(Y_t) \setminus \{X_{t-\tau}\}, \mathcal{P}(X_{t-\tau}) \quad (1)$$

## Definition

$$I_{X \rightarrow Y}^{\text{MCI}}(\tau) = I(X_{t-\tau} ; Y_t \mid \mathcal{P}(Y_t) \setminus \{X_{t-\tau}\}, \mathcal{P}(X_{t-\tau})) \quad (1)$$

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## 1. MCI measures causal strength

$$\begin{aligned} I_{X \rightarrow Y}^{\text{MCI}} &= I(g_X(\mathcal{P}_{X_{t-\tau}}) + \eta_{t-\tau}^X; g_Y(\mathcal{P}_{Y_t} \setminus \{X_{t-\tau}\}) + \tilde{\eta}_t^Y \mid \dots) \\ &= I(\eta_{t-\tau}^X; \tilde{\eta}_t^Y \mid \mathcal{P}_{X_{t-\tau}}) \quad \square \end{aligned}$$

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### 2. MCI has unbiased detection power for linear links

$$\begin{aligned} \tilde{\eta}_t^Y &= cX_{t-\tau} + \eta_t^Y = c(g_X(\mathcal{P}_{X_{t-\tau}}) + \eta_{t-\tau}^X) + \eta_t^Y \\ \implies I_{X \rightarrow Y}^{\text{MCI}} &= I(\eta_{t-\tau}^X; c\eta_{t-\tau}^X + \eta_t^Y) \end{aligned}$$

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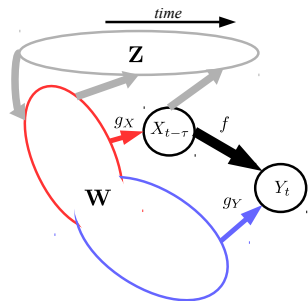
$$\begin{aligned} \tilde{\eta}_t^Y &= cX_{t-\tau} + \eta_t^Y = c(g_X(\mathcal{P}_{X_{t-\tau}}) + \eta_{t-\tau}^X) + \eta_t^Y \\ \implies I_{X \rightarrow Y}^{\text{MCI}} &= I(\eta_{t-\tau}^X; c\eta_{t-\tau}^X + \eta_t^Y) \end{aligned}$$

### 3. MCI leads to well-calibrated test

$$\tilde{\eta}_t^Y = \eta_t^Y \implies I_{X \rightarrow Y}^{\text{MCI}} = I(\eta_{t-\tau}^X; \eta_t^Y) = 0$$

## 1. Generally: $GC \leq MCI$ ( $\rightarrow$ GC has lower power)

$$I_{X \rightarrow Y}^{GC}(\tau) = I(X_{t-\tau}; Y_t | \mathbf{X}_t^- \setminus \{X_{t-\tau}\})$$



$$\begin{aligned} I((X, Z); Y | W) &= \underbrace{I(X; Y | W)}_{\text{MCI}} + \underbrace{I(Z; Y | W, X)}_{=0 \text{ (Markov)}} \\ &= \underbrace{I(Z; Y | W)}_{\geq 0} + \underbrace{I(X; Y | WZ)}_{\text{GC}} \\ \implies I_{X \rightarrow Y}^{\text{MCI}}(\tau) &\geq I_{X \rightarrow Y}^{\text{GC}}(\tau) \quad \square \end{aligned}$$

2. Single PC test has more power, but is non-iid

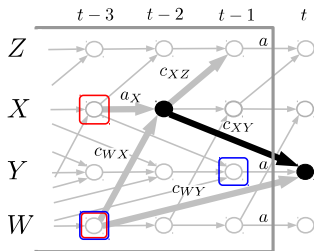
$$\begin{aligned}
 I_{X \rightarrow Y}^{\text{PC}}(\tau) &= I(X_{t-\tau}; Y_t | \mathcal{P}(Y_t) \setminus \{X_{t-\tau}\}) \\
 &= I(\eta_{t-\tau}^X, \mathcal{P}(X_{t-\tau}); Y_t | \mathcal{P}(Y_t) \setminus \{X_{t-\tau}\}) \\
 &= \underbrace{I(\mathcal{P}(X_{t-\tau}); Y_t | \mathcal{P}(Y_t) \setminus \{X_{t-\tau}\})}_{\text{typically non-iid}} \\
 &\quad + \underbrace{I(\eta_{t-\tau}^X; Y_t | \mathcal{P}(Y_t) \setminus \{X_{t-\tau}\}, \mathcal{P}(X_{t-\tau}))}_{\text{MCI}}
 \end{aligned}$$

$$\implies I_{X \rightarrow Y}^{\text{MCI}}(\tau) \leq I_{X \rightarrow Y}^{\text{PC}}(\tau)$$

# MCI and causal strength

## Effect size analysis for simple model

**A**

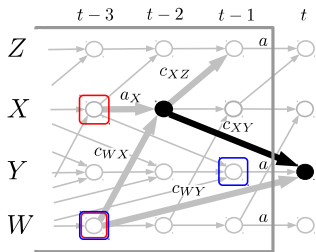




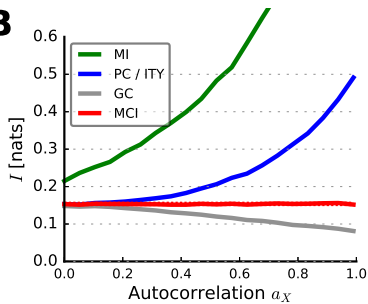
# MCI and causal strength

## Effect size analysis for simple model

**A**



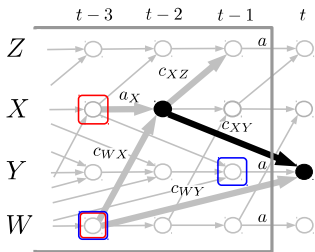
**B**



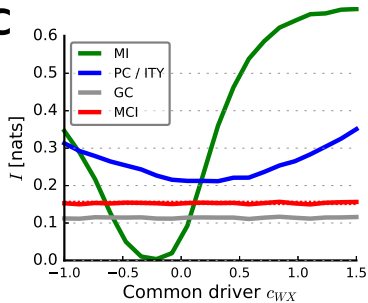
# MCI and causal strength

## Effect size analysis for simple model

**A**

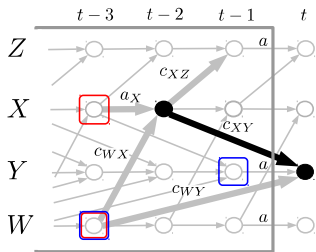
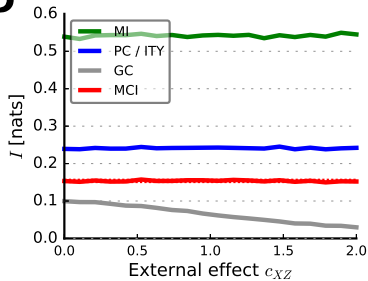


**C**



# MCI and causal strength

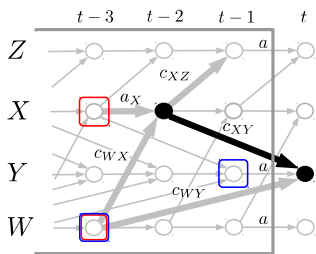
## Effect size analysis for simple model

**A****D**

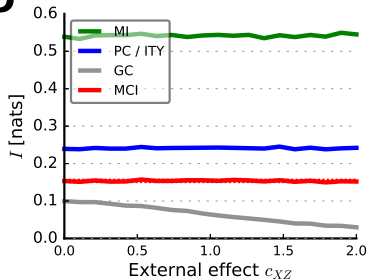
# MCI and causal strength

## Effect size analysis for simple model

**A**



**D**



General proof for 'unbiased' detection power → paper

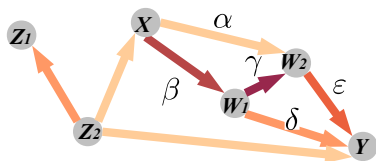
# Quantifying causal pathways

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# Quantifying causal pathways

## Linear approach: Mediated Causal Effect (MCE)

$$Y_t = f(\vec{\mathcal{P}}_Y) + \text{error} = \vec{\mathcal{P}}_Y \cdot \vec{B} + \text{error}$$

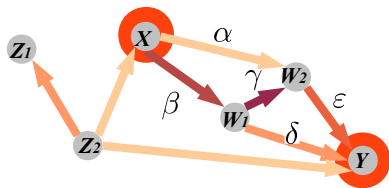


- Direct links: path coefficients  $\alpha, \beta, \gamma, \delta, \epsilon$

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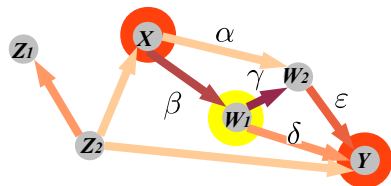


- Direct links: path coefficients  $\alpha, \beta, \gamma, \delta, \epsilon$
- Indirect causal effect:

$$CE_{X \rightarrow Y} = \alpha\epsilon + \beta\delta + \beta\gamma\epsilon$$

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- Mediated causal effect:

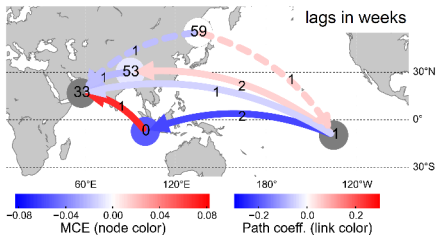
$$MCE_{X \rightarrow Y|W_1} = \beta\delta + \beta\gamma\epsilon$$



# Quantifying causal pathways

## Climate application: East Pacific → Monsoon pathway

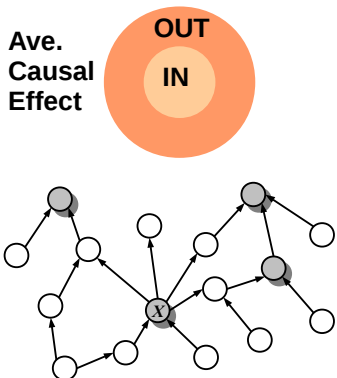
Here whole year analysis [Runge et al., 2015b]



- causal approach to atmospheric teleconnections

## Climate application

Here whole year analysis [Runge et al., 2015b]



- Average Causal Effect (ACE)

$$ACE(i) = \frac{1}{N-1} \sum_{j \neq i} CE_{i \rightarrow j}^{\max}$$

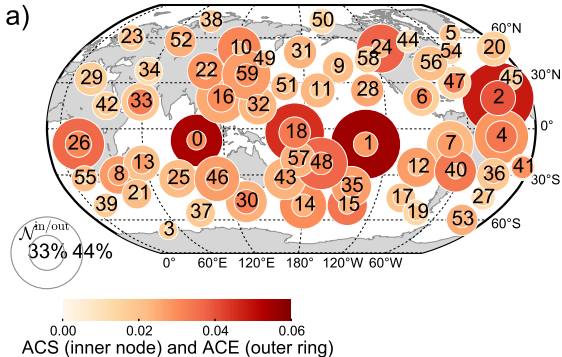
- Average Causal Susceptibility

$$ACS(j) = \frac{1}{N-1} \sum_{i \neq j} CE_{i \rightarrow j}^{\max}$$

# Network analysis

## Climate application

Here whole year analysis [Runge et al., 2015b]



- uplifts over tropical oceans are major drivers

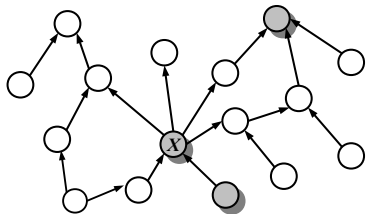
# Network analysis

## Climate application

Here whole year analysis [Runge et al., 2015b]

Ave.  
Mediated  
Causal  
Effect

THROUGH



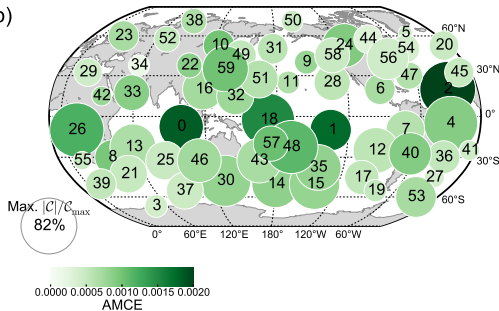
- Average Mediated Causal Effect (AMCE)

$$\text{AMCE}(i) = \frac{1}{|\mathcal{C}_k|} \sum_{(i,j) \in \mathcal{C}_k} \max_{\tau} |\text{MCE}_{i \rightarrow j|k}(\tau)|$$

## Climate application

Here whole year analysis [Runge et al., 2015b]

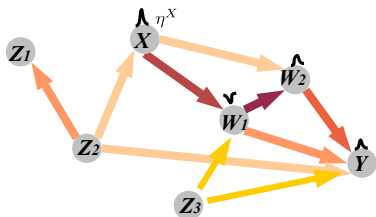
b)



- uplifts over tropical oceans also major mediators

# Quantifying causal pathways

## Information-theoretic approach [Runge, 2015]



$$I(X; Y|Z) =$$

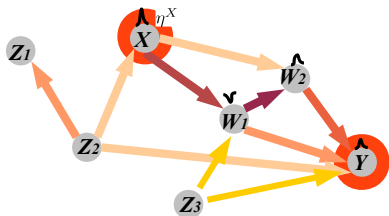
$$\int dz p(z) \iint dx dy p(x, y|z) \log \frac{p(x, y|z)}{p(x|z) \cdot p(y|z)}$$

- Direct links: Momentary information transfer (MIT)

$$I_{X \rightarrow Y}^{\text{MIT}} = I(X; Y | \mathcal{P}_Y, \mathcal{P}_X)$$

# Quantifying causal pathways

## Information-theoretic approach [Runge, 2015]



$$X_t = f(\mathcal{P}_X) + \eta_t^X$$

$$I_{X \rightarrow Y}^{\text{MITP}} = I(\eta_{t-3}^X ; Y_t | \mathcal{P}_{\text{paths}})$$

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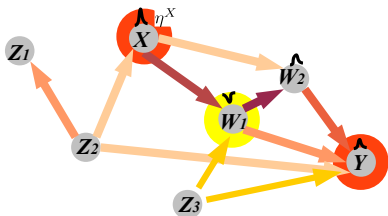
$$I_{X \rightarrow Y}^{\text{MIT}} = I(X; Y | \mathcal{P}_Y, \mathcal{P}_X)$$

- Indirect paths: Momentary information transfer along paths (MITP)

$$I_{X \rightarrow Y}^{\text{MITP}}(\tau) = I(X; Y | \mathcal{P}_{\text{paths}})$$

# Quantifying causal pathways

## Information-theoretic approach [Runge, 2015]



$$X_t = f(\mathcal{P}_X) + \eta_t^X$$

$$I_{X \rightarrow Y}^{\text{MITP}} = I(\eta_{t-3}^X; Y_t | \mathcal{P}_{\text{paths}})$$

$$\mathcal{I}_{X \rightarrow Y|W_1}^{\text{MII}} = \mathcal{I}(\eta_{t-3}^X; W_{1,t-2}; Y_t | \mathcal{P}_{\text{paths}})$$

$$I(X; Y|Z) =$$

$$\int dz p(z) \iint dx dy p(x, y|z) \log \frac{p(x, y|z)}{p(x|z) \cdot p(y|z)}$$

- Direct links: Momentary information transfer (MIT)

$$I_{X \rightarrow Y}^{\text{MIT}} = I(X; Y | \mathcal{P}_Y, \mathcal{P}_X)$$

- Indirect paths: Momentary information transfer along paths (MITP)

$$I_{X \rightarrow Y}^{\text{MITP}}(\tau) = I(X; Y | \mathcal{P}_{\text{paths}})$$

- Mediation: Momentary interaction information (MII)

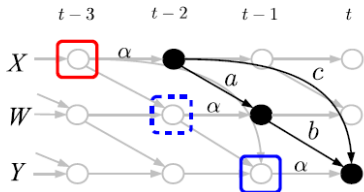
$$\mathcal{I}_{X \rightarrow Y|W}^{\text{MII}}(\tau) = I_{X \rightarrow Y}^{\text{MITP}}(\tau)$$

$$- \underbrace{I(X; Y | \mathcal{P}_{\text{paths}}, \mathbf{W})}_{\text{MITP conditioned on } \mathbf{W}}$$

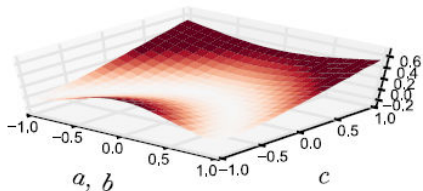


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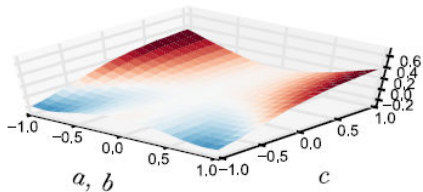
## Information-theoretic approach [Runge, 2015]



MITP



MII



## **Discussion and conclusion**

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## Discussion and conclusion

- framework for **reliable** large-scale time-lagged causal discovery

**Python code** on <https://jakobrunge.github.io/tigramite/>

**Paper:** J. Runge, D. Sejdinovic, S. Flaxman (2017):  
<https://arxiv.org/abs/1702.07007>

## Discussion and conclusion

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- **flexible** regarding (non-parametric) conditional independence tests  
→ nodes can be multivariate, variables discrete, ...

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→ ranking causal links in large-scale analyses

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- Causal complex **network measures** [Nature Comm. 2015]
- Optimal **prediction** [PRE May 2015]

**Python code** on <https://jakobrunge.github.io/tigramite/>

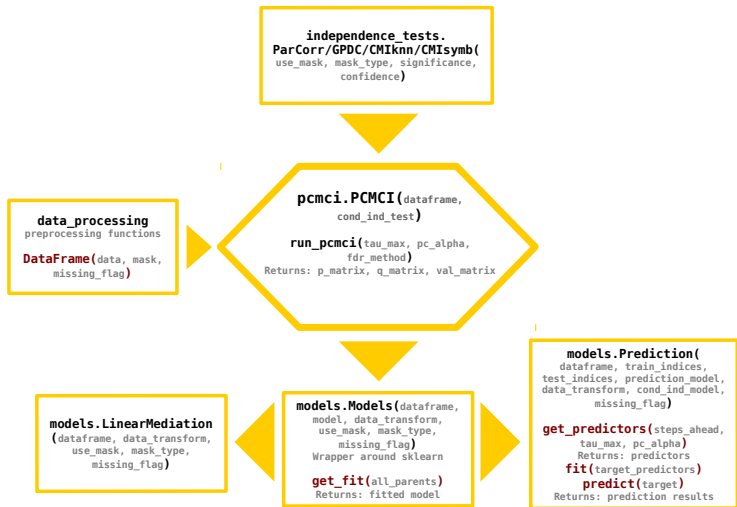
**Paper:** J. Runge, D. Sejdinovic, S. Flaxman (2017):  
<https://arxiv.org/abs/1702.07007>



# Tigramite

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<https://jakobrunge.github.io/tigramite/>



# New research group



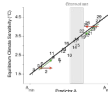
Open PhD and Postdoc positions  
→ [climateinformaticslab.com](http://climateinformaticslab.com)



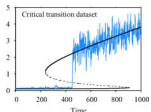
## Climate model evaluation



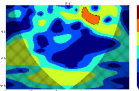
## Climate sensitivity



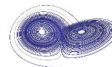
## Extremes prediction



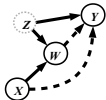
## Time-scale causality



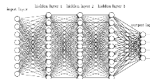
## Data-driven dynamical models



## Causal discovery theory



## Deep learning



Thank you !!!





Eichler, M. (2012).

**Graphical modelling of multivariate time series.**


*Probability Theory and Related Fields*, 153(1):233–268.



Frenzel, S. and Pompe, B. (2007).

**Partial mutual information for coupling analysis of multivariate time series.**

*Physical Review Letters*, 99(20):204101.

-  Kalnay, E., Kanamitsu, M., Kistler, R., Collins, W., Deaven, D., Gandin, L., Iredell, M., Saha, S., White, G., Woollen, J., Zhu, Y., Chelliah, M., Ebisuzaki, W., Higgins, W., Janowiak, J., Mo, K. C., Ropelewski, C., Wang, J., Leetmaa, A., Reynolds, R., Jenne, R., and Joseph, D. (1996).




**The NCEP/NCAR 40-year reanalysis project.**

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-  Kraskov, A., Stögbauer, H., and Grassberger, P. (2004).

**Estimating mutual information.**

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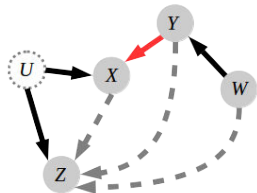
-  Vejmelka, M., Pokorná, L., Hlinka, J., Hartman, D., Jajcay, N., and Paluš, M. (2014).

**Non-random correlation structures and dimensionality reduction in multivariate climate data.**

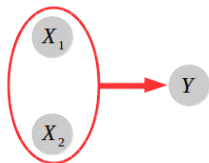
*Climate Dynamics*, 44(9-10):2663–2682.

# Causal discovery challenges

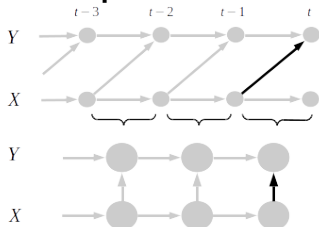
## Latent variables



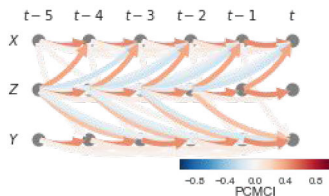
## Synergistic dependencies



## Contemporaneous effects



## Long-range memory



## Causal assumptions

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# Causal assumptions

**Causal interpretation assumes [Spirtes et al., 2000]:**

- **Causal Markov Condition:** “All the relevant probabilistic information that can be obtained from the system is contained in its direct causes”
- **Causal Sufficiency:** Measured variables include all of the common causes
- **Faithfulness / Stableness:** “Independencies in data arise not from incredible coincidence, but rather from causal structure”; violated by purely deterministic dependencies

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- **Stationarity:** time series case
- **Parametric assumptions** of independence tests

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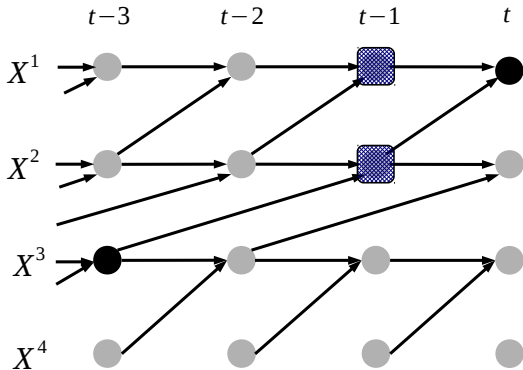
More discussion → appendix

# Causal assumptions

## Causal Markov Condition

“All the relevant probabilistic information that can be obtained from the system is contained in its direct causes”

Formally: Upon specifying a complete graph that contains all common causes: separation in graph entails *at least* implied conditional independencies in process



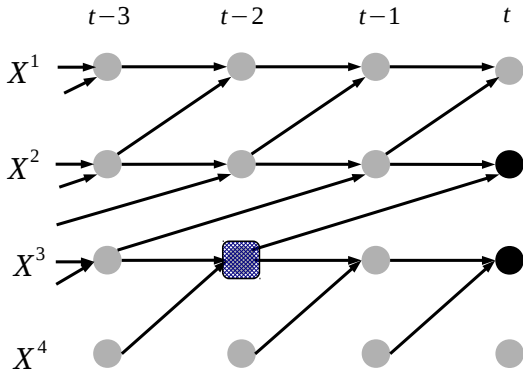


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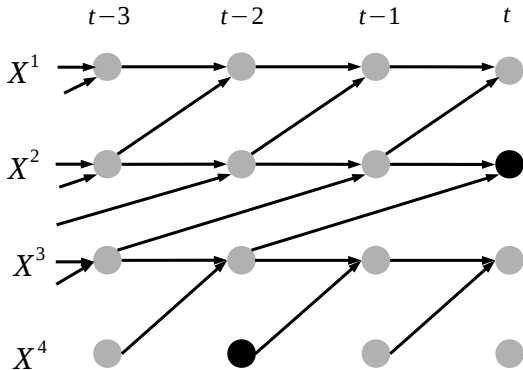


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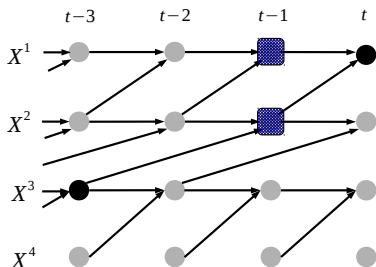


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Structural equation modeling framework:

$$X_t^j = f(\mathbf{X}_t^-, \eta_t^j) \quad \eta_t^j \perp\!\!\!\perp \mathbf{X}_{t+1}^- \setminus X_t^j$$

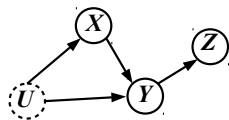
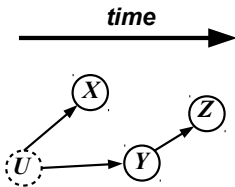
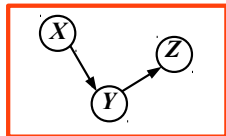
# Causal assumptions

## Causal Sufficiency

R. Scheines: "Theory of causal inference is about the inferential effect of a variety of assumptions far more than it is an endorsement of particular assumptions"

Given estimates  $X \perp\!\!\!\perp Z \mid Y$  and no other independencies. Assuming only Markov condition and faithfulness allows for several different graphs:

**Assuming sufficiency**

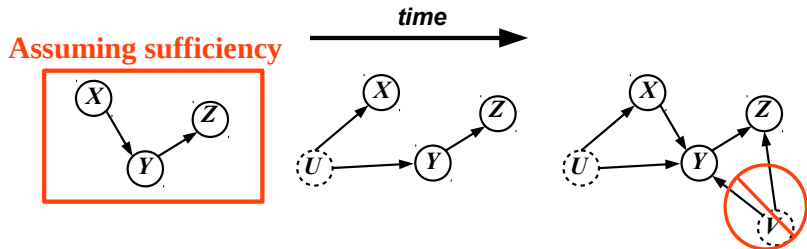


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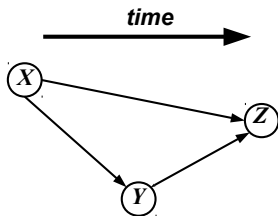
# Causal assumptions

## Faithfulness

*If there are any independence relations in the population that are not a consequence of the Causal Markov condition (or d-separation), then the population is unfaithful.*

For example, given three variables and assuming the Causal Markov and Sufficiency Conditions, suppose we measure these (in-)dependencies:

$$\begin{array}{ll} X \perp\!\!\!\perp Z & X \not\perp\!\!\!\perp Z \mid Y \\ X \not\perp\!\!\!\perp Y & (X \not\perp\!\!\!\perp Y \mid Z) \\ Y \not\perp\!\!\!\perp Z & Y \not\perp\!\!\!\perp Z \mid X \end{array}$$



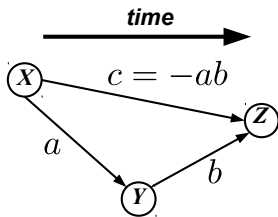
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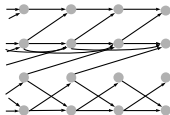
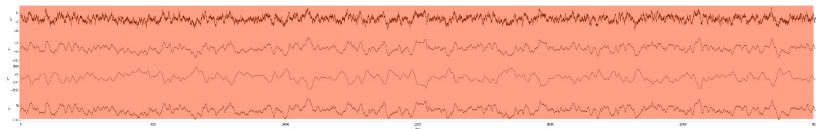
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# Causal assumptions

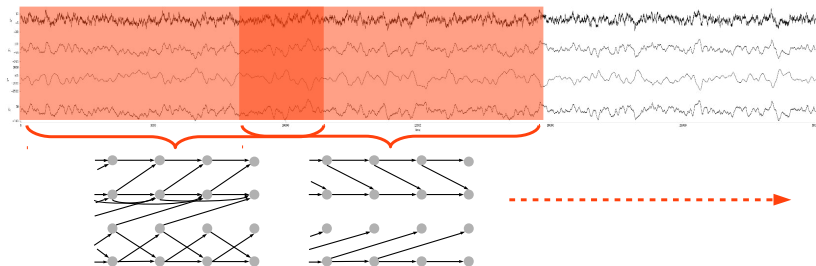
## Stationarity of causal structure



**structurally stationary for all samples**

# Causal assumptions

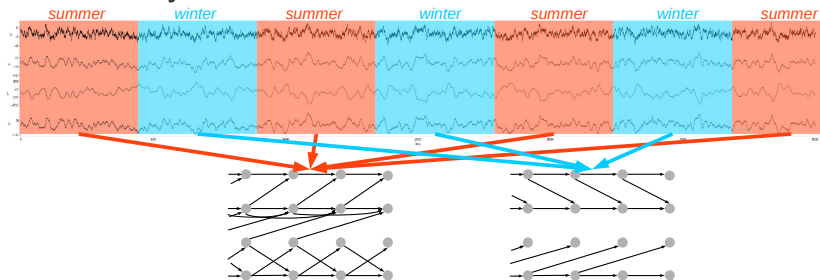
## Stationarity of causal structure



structurally stationary within sliding windows

# Causal assumptions

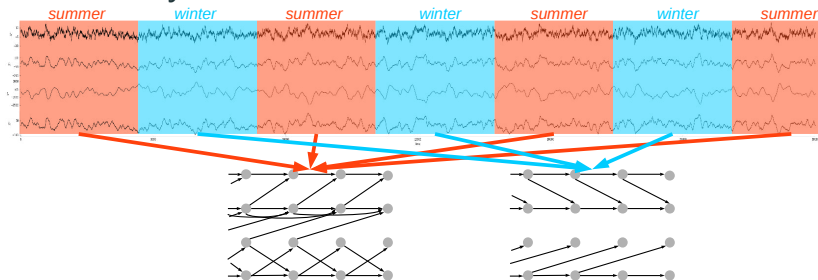
## Stationarity of causal structure



periodically structurally stationary

# Causal assumptions

## Stationarity of causal structure

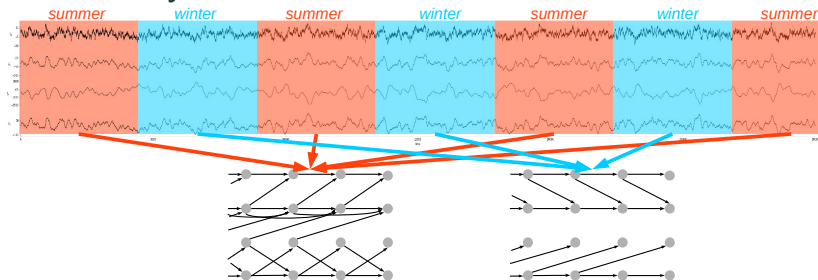


### periodically structurally stationary

- structurally, *not necessarily* same strength / parameters

# Causal assumptions

## Stationarity of causal structure



### periodically structurally stationary

- structurally, *not* necessarily same strength / parameters
- *masking* implemented in Tigramite