Deutsches Zentrum
für Luft- und Raumfahrt
German Aerospace Center

Causal discovery in time series with unobserved confounders

Andreas Gerhardus*

March 17, 2021

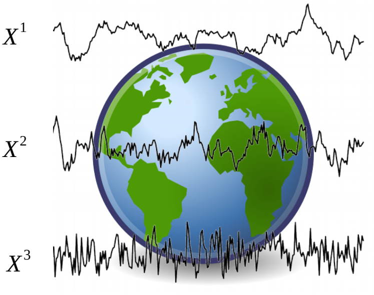
Joint IS-ENES3/ESiWACE2 Virtual Workshop on New Opportunities for ML and AI in Weather and Climate Modelling

*Climate Informatics Group
DLR-Institute of Data Science
Jena, Germany

Introduction

Motivation: Complex dynamics of the climate system

System of interest:



Goal:

Contribute to a better understanding of Earth's complex weather and climate system.

Approach of the Climate Informatics Group @DLR Jena

Climate Informatics in general:

Use modern tools of machine learning, statistics, and data science to aid climate and Earth system sciences.

Approach of the Climate Informatics Group @DLR Jena

Climate Informatics in general:
Use modern tools of machine learning, statistics, and data science to aid climate and Earth system sciences.

Focus of the Climate Informatics Group @DLR Jena*:

- Development of methods
- Provisioning of open-source software implementations† for application by domain scientists
- Methods based on the modern **causal inference** framework

*www.climateinformaticslab.com
†https://github.com/jakobrunge/tigramite

Causal inference

Causal inference and causal discovery

Causal inference:

- Defines notions of *cause* and *effect* in a mathematical framework.
- Casts causal questions within this framework.
- Specifies assumptions and develops methods for answering these questions.

Causal inference and causal discovery

Causal inference:

- Defines notions of *cause* and *effect* in a mathematical framework.
- Casts causal questions within this framework.
- Specifies assumptions and develops methods for answering these questions.

Sub-field: Causal discovery

- Specifies assumptions and develops methods for learning cause and effect relationships from observational data.

On the notion of causation

Correlation is not causation:

Statistical dependencies in observational data do not by themselves imply causal relationships.

$\Rightarrow$ Need assumptions to connect stat. dependencies and causation

On the notion of causation

Correlation is not causation:

Statistical dependencies in observational data do not by themselves imply causal relationships.

$\Rightarrow$ Need assumptions to connect stat. dependencies and causation

Working definition of causality:

Variable X causes variable Y if an experimental manipulation that changes X (and only X) leads to a change of Y.

$\Rightarrow$ experimental mode of inferring causation

On the notion of causation

Correlation is not causation:

Statistical dependencies in observational data do not by themselves imply causal relationships.

$\Rightarrow$ Need assumptions to connect stat. dependencies and causation

Working definition of causality:

Variable X causes variable Y if an experimental manipulation that changes X (and only X) leads to a change of Y.

$\Rightarrow$ experimental mode of inferring causation

A theory of causality:

Framework of causal inference, largely developed and popularized by Judea Pearl, Peter Spirtes, Clark Glymour, Richard Scheines.

Textbooks: [Pearl, 2000, Spirtes et al., 2000, Peters et al., 2017].

Modelling causal relationships: Structural causal models

Intuition:

A structural causal model (SCM) specifies the functional causal relationships between a set of random variables.

Example (scientifically oversimplied, for illustration only):

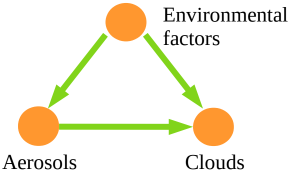
Structural causal model:

$$X_{\text{clouds}} := f_{\text{clouds}}(X_{\text{aerosols}},\, X_{\text{env. facs.}},\, \eta_{\text{clouds}})$$

$$X_{\text{aerosols}} := f_{\text{aerosols}}(X_{\text{env. facs.}},\, \eta_{\text{aerosols}})$$

$$X_{\text{env. facs.}} := f_{\text{env. facs.}}(\eta_{\text{env. facs.}})$$

Causal graph:



Causal graph:

Specifies the *direct causes* of each variable.

Modelling causal relationships: Structural causal models

Intuition:

A structural causal model (SCM) specifies the functional causal relationships between a set of random variables.

Example (scientifically oversimplied, for illustration only):

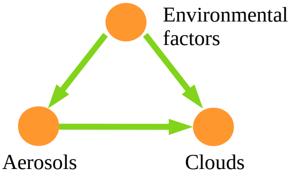
Structural causal model:

$$X_{\text{clouds}} := f_{\text{clouds}}(X_{\text{aerosols}}, X_{\text{env. facs.}}, \eta_{\text{clouds}})$$

$$X_{\text{aerosols}} := f_{\text{aerosols}}(X_{\text{env. facs.}}, \eta_{\text{aerosols}})$$

$$X_{\text{env. facs.}} := f_{\text{env. facs.}}(\eta_{\text{env. facs.}})$$

Causal graph:



Causal graph:

Specifies the *direct causes* of each variable.

Modelling causal relationships: Structural causal models

Intuition:
A structural causal model (SCM) specifies the functional causal relationships between a set of random variables.

Example (scientifically oversimplied, for illustration only):

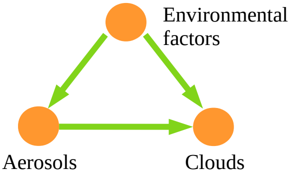
Structural causal model:

$$X_{\text{clouds}} := f_{\text{clouds}}(X_{\text{aerosols}}, X_{\text{env. facs.}}, \eta_{\text{clouds}})$$

$$X_{\text{aerosols}} := f_{\text{aerosols}}(X_{\text{env. facs.}}, \eta_{\text{aerosols}})$$

$$X_{\text{env. facs.}} := f_{\text{env. facs.}}(\eta_{\text{env. facs.}})$$

Causal graph:



Causal graph:
Specifies the *direct causes* of each variable.

Modelling causal relationships: Structural causal models

Intuition:

A structural causal model (SCM) specifies the functional causal relationships between a set of random variables.

Example (scientifically oversimplied, for illustration only):

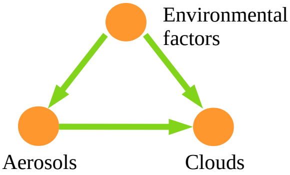
Structural causal model:

$X_{\text{clouds}} := f_{\text{clouds}}(X_{\text{aerosols}}, X_{\text{env. facs.}}, \eta_{\text{clouds}})$

$X_{\text{aerosols}} := f_{\text{aerosols}}(X_{\text{env. facs.}}, \eta_{\text{aerosols}})$

$X_{\text{env. facs.}} := f_{\text{env. facs.}}(\eta_{\text{env. facs.}})$

Causal graph:



Causal graph:

Specifies the *direct causes* of each variable.

Modelling causal relationships: Structural causal models

Intuition:

A structural causal model (SCM) specifies the functional causal relationships between a set of random variables.

Example (scientifically oversimplied, for illustration only):

Structural causal model:

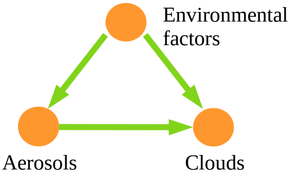
$$X_{\text{clouds}} := f_{\text{clouds}}(X_{\text{aerosols}},\, X_{\text{env. facs.}},\, \eta_{\text{clouds}})$$

$$X_{\text{aerosols}} := f_{\text{aerosols}}(X_{\text{env. facs.}},\, \eta_{\text{aerosols}})$$

$$X_{\text{env. facs.}} := f_{\text{env. facs.}}(\eta_{\text{env. facs.}})$$

Dynamical noise

Causal graph:



Causal graph:

Specifies the *direct causes* of each variable.

Modelling causal relationships: Structural causal models

Intuition:
A structural causal model (SCM) specifies the functional causal relationships between a set of random variables.

Example (scientifically oversimplied, for illustration only):

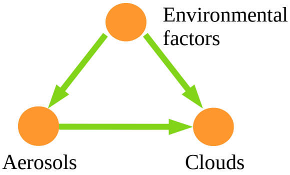
Structural causal model:

$$X_{\text{clouds}} := f_{\text{clouds}}(X_{\text{aerosols}}, X_{\text{env. facs.}}, \eta_{\text{clouds}})$$

$$X_{\text{aerosols}} := f_{\text{aerosols}}(X_{\text{env. facs.}}, \eta_{\text{aerosols}})$$

$$X_{\text{env. facs.}} := f_{\text{env. facs.}}(\eta_{\text{env. facs.}})$$

Causal graph:



Causal graph:
Specifies the *direct causes* of each variable.

Why is causal knowledge important?

Scientific understanding:

Knowledge of cause and effect relationships is an essential part of the physical understanding of natural processes.

Why is causal knowledge important?

Scientific understanding:

Knowledge of cause and effect relationships is an essential part of the physical understanding of natural processes.

Robust prediction & forecasting:

Predictive systems consistent with the underlying causal structures are thought to be more robust under changing environmental conditions.

Why is causal knowledge important?

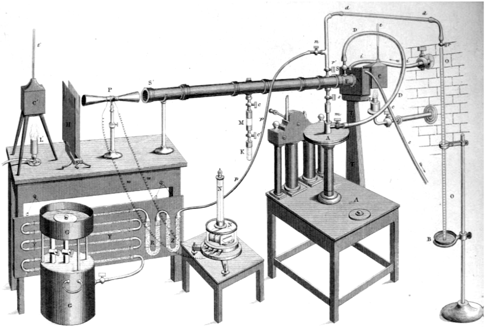
Scientific understanding:
Knowledge of cause and effect relationships is an essential part of the physical understanding of natural processes.

Robust prediction & forecasting:
Predictive systems consistent with the underlying causal structures are thought to be more robust under changing environmental conditions.

Attribution:
Questions of the type *Why did this event happen?* or *Is this due to climate change?* are of causal nature.

How to obtain causal knowledge?

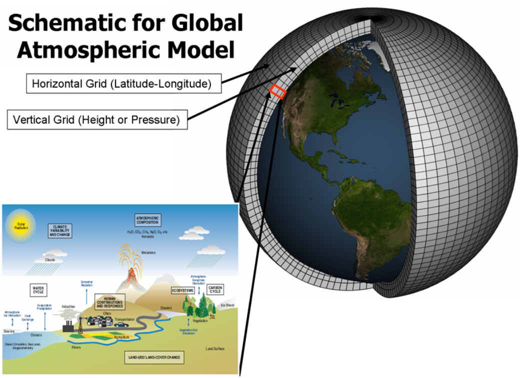
1. **Experimentation:**
Deliberately manipulate the system and observe the consequences.



How to obtain causal knowledge?

2. Simulation:

Experimentation inside a simulated version of the system.



How to obtain causal knowledge?

3. Causal discovery:

Learn from observational data, given certain assumptions.

Causal discovery

Learning causal relationships from statistical independencies

Today's approach to causal discovery:

Learn causal graph from statistical tests of (conditional) independencies* in observational data

$\Rightarrow$ *CI-based* causal discovery

***Conditional independence:**

For random variables X, Y, and Z with distribution p: X and Y are conditionally independent Z, denoted as $X \perp\!\!\!\perp Y \mid Z$, if $p(x|y,z) = p(x|z)$ for all x, y, z.

Learning causal relationships from statistical independencies

Today's approach to causal discovery:

Learn causal graph from statistical tests of (conditional) independencies* in observational data

$\Rightarrow$ *CI-based* causal discovery

Enabling assumptions:

1. Observational data is generated by a structural causal model (this true SCM is unknown)
2. No *accidental* independencies $\Rightarrow$ more on this later
3. Optional: No unobserved confounders $\Rightarrow$ more on this later

***Conditional independence:**

For random variables X, Y, and Z with distribution p: X and Y are conditionally independent Z, denoted as $X \perp\!\!\!\perp Y \mid Z$, if $p(x|y,z) = p(x|z)$ for all x, y, z.

Causal graphs and (conditional) independencies

Fact:

The structure of the causal graph often has observable implications in terms of (conditional) independencies in the observed data.

Intuition:

- Statistical dependencies derive from causal relationships
- Conditioning can block and open the *flow of information*

Causal graphs and (conditional) independencies

Example:

- X influences Y: $X \not\perp\!\!\!\perp Y$
- Y influences Z: $Y \not\perp\!\!\!\perp Z$
- X influences Z through Y: $X \not\perp\!\!\!\perp Z$

Causal graphs and (conditional) independencies

Example:

- X influences Y: $X \not\perp\!\!\!\perp Y$
- Y influences Z: $Y \not\perp\!\!\!\perp Z$
- X influences Z through Y: $X \not\perp\!\!\!\perp Z$
- Knowing Y, X does not say more about Z: $X \perp\!\!\!\perp Z \mid Y$

Causal graphs and (conditional) independencies

Example:

- X influences Y: $X \not\perp\!\!\!\perp Y$
- Y influences Z: $Y \not\perp\!\!\!\perp Z$
- X influences Z through Y: $X \not\perp\!\!\!\perp Z$
- Knowing Y, X does not say more about Z: $X \perp\!\!\!\perp Z \mid Y$

General rule: d-separation

Graphical criterion to read off all (conditional) independencies implied by the structure of a given causal graph [Pearl, 1985, Pearl, 1988].

No accidental independencies:

There are no independencies beyond those implied by the causal graph.

CI-based causal discovery without unobserved confounders

Idea:

- Perform statistical tests of (conditional) independence in observational data
- Use test results to constrain the structure of the causal graph

CI-based causal discovery without unobserved confounders

Idea:

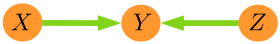
- Perform statistical tests of (conditional) independence in observational data
- Use test results to constrain the structure of the causal graph

Example 1:

Test decisions:

- $X \not\perp\!\!\!\perp Y$
- $Y \not\perp\!\!\!\perp Z$
- $X \perp\!\!\!\perp Z$

Possible causal graphs:



CI-based causal discovery without unobserved confounders

Idea:

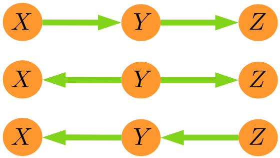
- Perform statistical tests of (conditional) independence in observational data
- Use test results to constrain the structure of the causal graph

Example 2:

Test decisions:

- $X \not\perp\!\!\!\perp Y$
- $Y \not\perp\!\!\!\perp Z$
- $X \not\perp\!\!\!\perp Z$
- $X \perp\!\!\!\perp Z \mid Y$

Possible causal graphs:

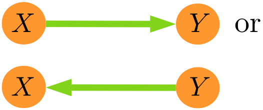


observationally equivalent graphs

Unobserved confounders make causal discovery more difficult

Without unobserved confounders:

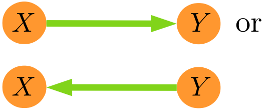
$X \not\perp\!\!\!\perp Y \qquad \Rightarrow$



Unobserved confounders make causal discovery more difficult

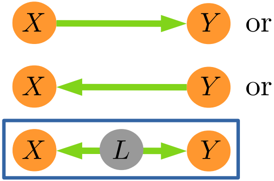
Without unobserved confounders:

$X \not\perp\!\!\!\perp Y \qquad \Rightarrow$



With unobserved confounders:

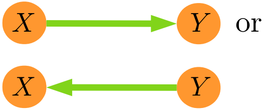
$X \not\perp\!\!\!\perp Y \qquad \Rightarrow$



Unobserved confounders make causal discovery more difficult

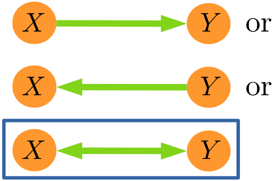
Without unobserved confounders:

$X \not\perp\!\!\!\perp Y \qquad \Rightarrow$



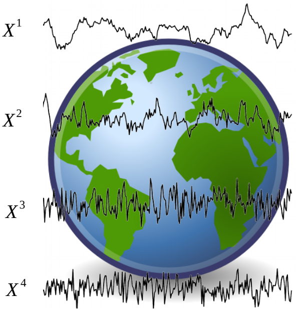
With unobserved confounders:

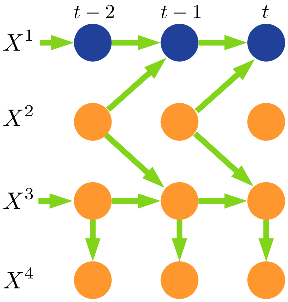
$X \not\perp\!\!\!\perp Y \qquad \Rightarrow$



Our research:
Causal discovery for time series

CI-based causal discovery for time series

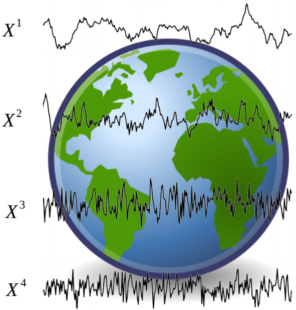


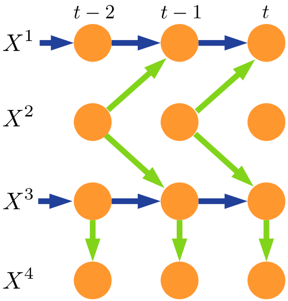


Particularities:

- Variables are resolved in time

CI-based causal discovery for time series

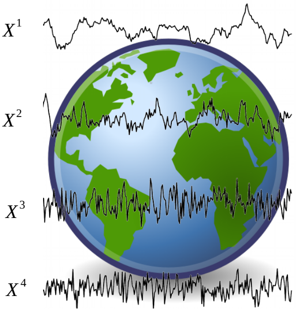


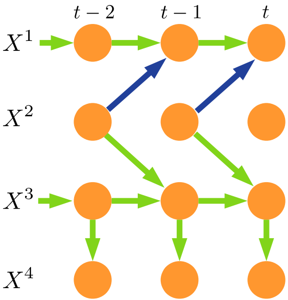


Particularities:

- Variables are resolved in time
- Autocorrelation

CI-based causal discovery for time series





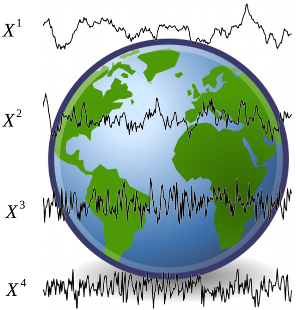
Particularities:

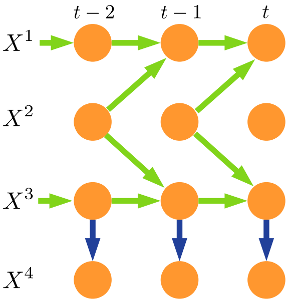
- Variables are resolved in time
- Autocorrelation

Additional assumption:

- Stationary causal structure

CI-based causal discovery for time series





Particularities:

- Variables are resolved in time
- Autocorrelation

Additional assumption:

- Stationary causal structure

CI-based causal discovery for time series

Additional statistical challenges:

- High dimensionality (resolving in time)
- Ill-calibrated statistical tests of independence (autocorrelation)
- Low detection power (autocorrelation)

$\Rightarrow$ standard algorithms often yield bad statistical performance

CI-based causal discovery for time series

Additional statistical challenges:

- High dimensionality (resolving in time)
- Ill-calibrated statistical tests of independence (autocorrelation)
- Low detection power (autocorrelation)

$\Rightarrow$ standard algorithms often yield bad statistical performance

Our contribution:

Statistical problems alleviated by specialized algorithms† developed by the Climate Informatics Group @DLR Jena:

- PCMCI time-lagged links only & no unobserved confounders [Runge et al., 2019]
- PCMCI$^+$ no unobserved confounders [Runge, 2020]
- LPCMCI (Latent-PCMCI) [Gerhardus and Runge, 2020]

†available at: https://github.com/jakobrunge/tigramite

CI-based causal discovery for time series

Additional statistical challenges:

- High dimensionality (resolving in time)
- Ill-calibrated statistical tests of independence (autocorrelation)
- Low detection power (autocorrelation)

$\Rightarrow$ standard algorithms often yield bad statistical performance

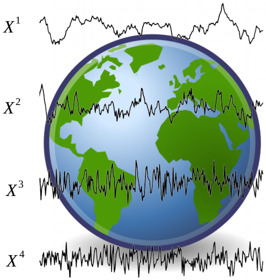
Our contribution:

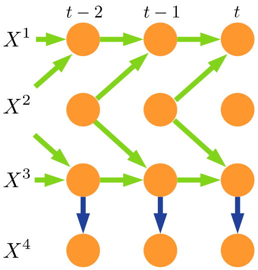
Statistical problems alleviated by specialized algorithms[†] developed by the Climate Informatics Group @DLR Jena:

- PCMCI — time-lagged links only & no unobserved confounders [Runge et al., 2019]
- PCMCI$^+$ — no unobserved confounders [Runge, 2020]
- LPCMCI (Latent-PCMCI) [Gerhardus and Runge, 2020]

[†]available at: https://github.com/jakobrunge/tigramite

LPCMCI: Latent-PCMCI

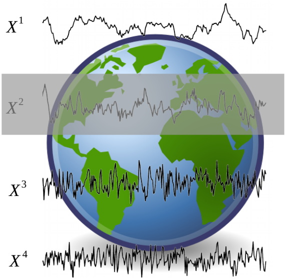


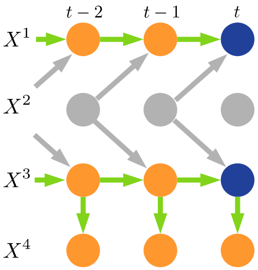


LPCMCI allows for:

- Contemporaneous links (also PCMCI$^+$ does)

LPCMCI: Latent-PCMCI

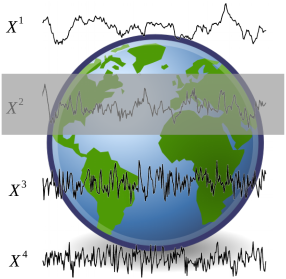


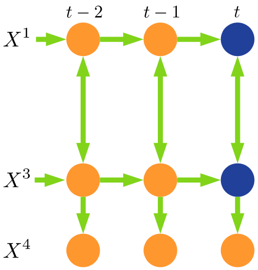


LPCMCI allows for:

- Contemporaneous links (also PCMCI$^+$ does)
- Unobserved confounders

LPCMCI: Latent-PCMCI

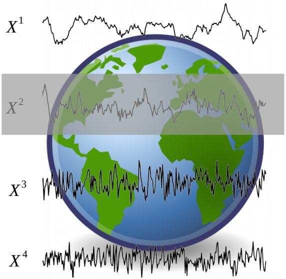


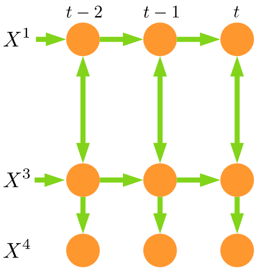


LPCMCI allows for:

- Contemporaneous links (also PCMCI$^+$ does)
- Unobserved confounders

LPCMCI: Latent-PCMCI





LPCMCI allows for:

- Contemporaneous links (also PCMCI$^+$ does)
- Unobserved confounders

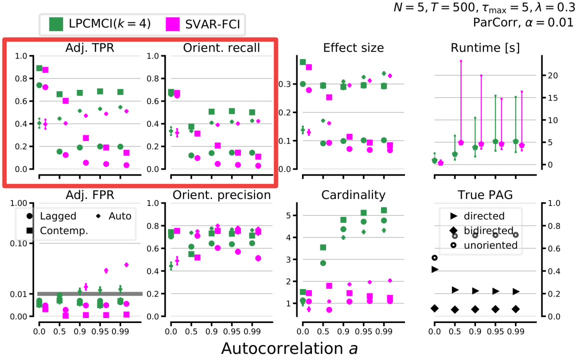
Basic idea:
More powerful CI tests by iterative learning of and subsequent conditioning on direct causes.

LPCMCI achieves strong gains in recall

Results of numerical experiments:

For autocorrelated continuous data LPCMCI shows strong gains in recall as compared to the current state of the art algorithm*

*the SVAR-FCI algorithm by [Malinsky and Spirtes, 2018]



References i

Gerhardus, A. and Runge, J. (2020).
High-recall causal discovery for autocorrelated time series with latent confounders.
In Larochelle, H., Ranzato, M., Hadsell, R., Balcan, M. F., and Lin, H., editors, Advances in Neural Information Processing Systems, volume 33, pages 12615–12625. Curran Associates, Inc.

Malinsky, D. and Spirtes, P. (2018).
Causal Structure Learning from Multivariate Time Series in Settings with Unmeasured Confounding.
In Le, T. D., Zhang, K., Kıcıman, E., Hyvärinen, A., and Liu, L., editors, Proceedings of 2018 ACM SIGKDD Workshop on Causal Disocvery, volume 92 of Proceedings of Machine Learning Research, pages 23–47, London, UK. PMLR.

Pearl, J. (1985).
A Constraint - Propagation Approach to Probabilistic Reasoning.
In Kanal, L. N. and Lemmer, J. F., editors, Proceedings of the First Conference on Uncertainty in Artificial Intelligence, UAI'85, page 31–42, Arlington, Virginia, USA. AUAI Press.

Pearl, J. (1988).
Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference.
Morgan Kaufmann Publishers Inc., San Francisco, CA, USA.

Pearl, J. (2000).
Causality: Models, Reasoning, and Inference.
Cambridge University Press, New York, NY, USA.

References iii

Peters, J., Janzing, D., and Schölkopf, B. (2017).
Elements of Causal Inference - Foundations and Learning Algorithms.
Adaptive Computation and Machine Learning Series. The MIT Press, Cambridge, MA, USA.

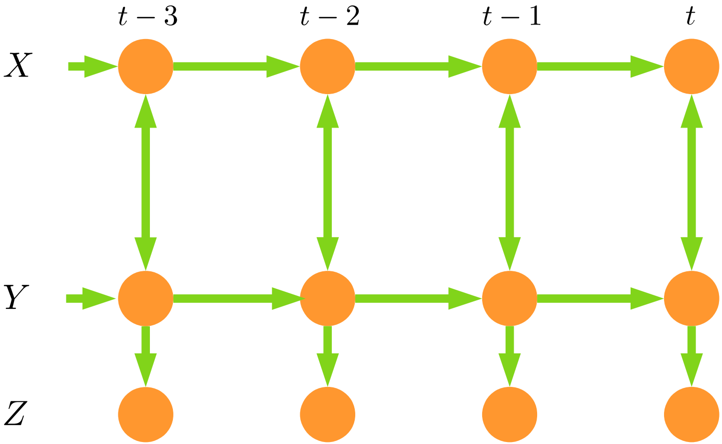
Runge, J. (2020).
Discovering contemporaneous and lagged causal relations in autocorrelated nonlinear time series datasets.
In Adams, R. P. and Gogate, V., editors, Proceedings of the Thirty-Sixth Conference on Uncertainty in Artificial Intelligence, UAI 2020, virtual online, August 3-6, 2020, page 579. AUAI Press.

Runge, J., Nowack, P., Kretschmer, M., Flaxman, S., and Sejdinovic, D. (2019).
Detecting and quantifying causal associations in large nonlinear time series datasets.
Science Advances, 5(11).

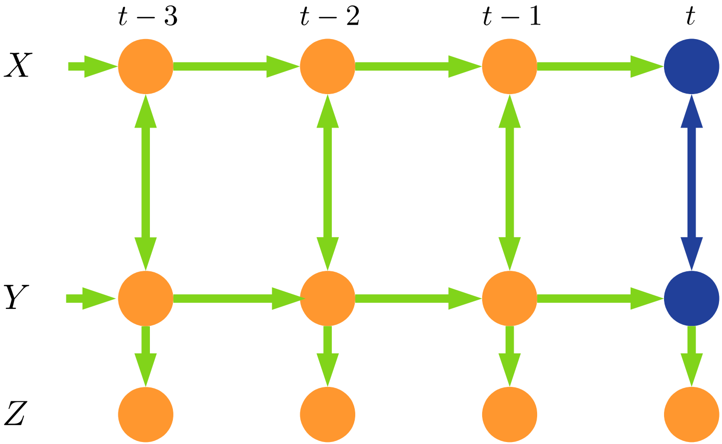
Spirtes, P., Glymour, C., and Scheines, R. (2000).
Causation, Prediction, and Search.
MIT Press, Cambridge, MA, USA.

Backup

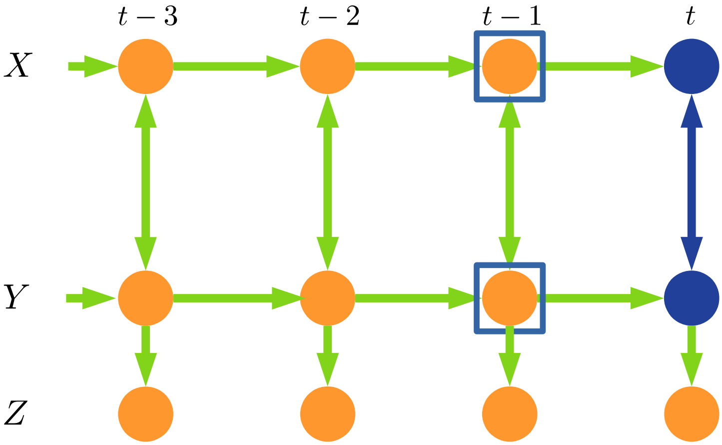
Conditioning sets are extended with known causal parents



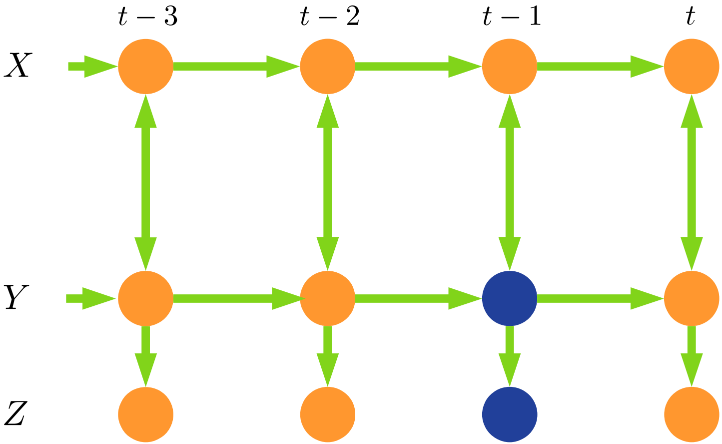
Conditioning sets are extended with known causal parents



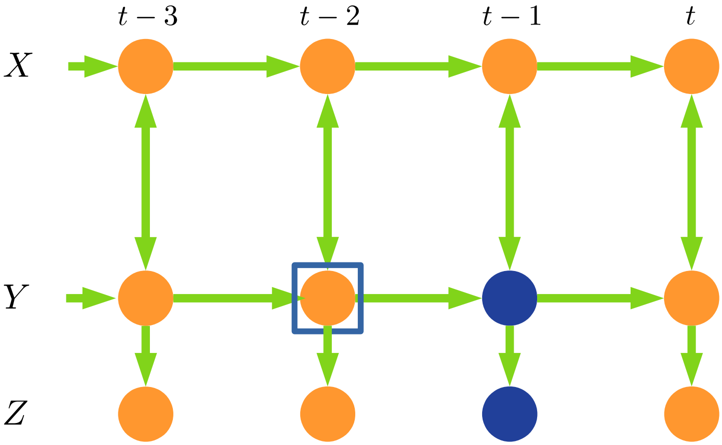
Conditioning sets are extended with known causal parents



Conditioning sets are extended with known causal parents



Conditioning sets are extended with known causal parents



Conditioning sets are extended with known causal parents