

Causal discovery

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IPL

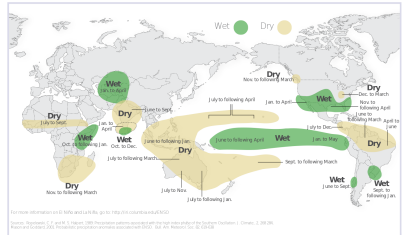
09 May 2023

Causal Discovery

- ▶ Which are the regions most affected by ENSO?

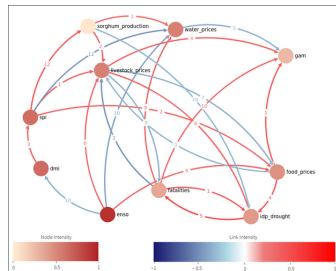
El Niño and Rainfall

El Niño conditions in the tropical Pacific are known to shift rainfall patterns in many different parts of the world. Although they vary somewhat from one El Niño to the next, the strongest shifts remain fairly consistent in the regions and seasons shown on the map below.



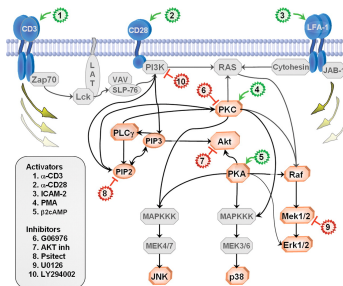
Causal Discovery

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- ▶ Which are the causal drivers and the causal relationships involving food insecurity?



Causal Discovery

- ▶ Which are the regions most affected by ENSO?
- ▶ Which are the causal drivers and the causal relationships involving food insecurity?
- ▶ Retrieve the reaction network between genes and proteins from single-cell data



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- ▶ it always require assumptions
- ▶ can use only observational data, or even interventions
- ▶ usually the output is not a complete description of the causal relationships (depends on the assumptions, the type of data etc..)

Causal discovery methods

- ▶ Constrained Based, Score based, Asymmetry based
- ▶ Methods for i.i.d. data or for time-series
- ▶ Bivariate vs multivariate
- ▶ Observational and/or Interventional data

In this session

- ▶ Causal discovery for BN and SCM
- ▶ Causal discovery taxonomy
- ▶ Some methods
- ▶ Examples

We will see only methods that employ observational data . . . thus we will need assumptions

Structural learning for BN

Estimate the structure of a BN from observational data. That is, recovering of G from (i.i.d.) observations sampled from a probability P such that (G, P) is a BN

- ▶ it is a model selection problem
- ▶ no causality involved (yet)
- ▶ Problem: a probability P can be *compatible* with multiple BN!!

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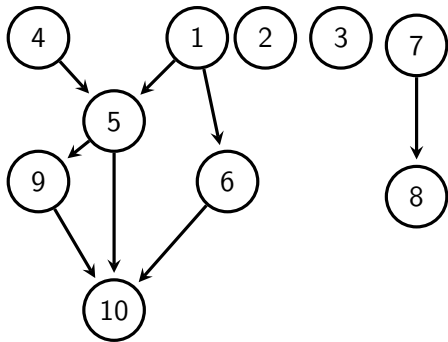
- ▶ $\mathcal{M}(G) = \{P \mid P \text{ is Markov w.r.t. } G\}$
- ▶ If $\mathcal{M}(G_1) = \mathcal{M}(G_2)$, then G_1 and G_2 are Markov equivalent. They share the same set of d-separations and conditional independences.
- ▶ Using observational data alone, Can we hope to learn something more than the Markov equivalence class?
- ▶ A **Markov equivalence class** contains all graph which are Markov equivalent

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we can represent the Markov equivalence class with a partial directed acyclic graph (PDAG)

Taxonomy of methods for BN

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- ▶ Score based or score+search: GES, tabu search, hill-climbing
- ▶ hybrid: max-min-hill-climbing (mmhc)

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- ▶ obtain a PDAG (partial directed acyclic graph) representing the Markov equivalence class

The PC algorithm starts from a fully connected undirected graph and consists of three phases:

1. The *skeleton phase* uses statistical (conditional) independence tests to infer the adjacencies of the underlying causal graph. If two variables X and Y are found to be independent conditional on a (possibly empty) set of variables \mathbf{Z} , then the edge between X and Y is removed.
2. The *collider orientation phase* then orients all *collider motifs*, that is, motifs of the form $X \rightarrow Y \leftarrow Z$ where X and Z are non-adjacent. These orientations can be inferred because collider motifs impose a particular pattern of (conditional) (in-)dependencies.
3. The *orientation phase* finally uses graphical rules [Meek, 1995] to infer the orientation of as many remaining unoriented edges as possible using the acyclicity assumption and the fact that all colliders have been found in the previous step.

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- ▶ GES (greedy equivalent search) in the space of CPDAG (the space of Markov equivalence classes) [under some assumptions it is proven to recover the true Markov equivalence class]

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- ▶ example, Linear non-Gaussian acyclic model (LiNGAM) [Shimizu et al., 2006]

Time series

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- ▶ The *arrow of time* helps in orienting some edges
- ▶ Granger causality, convergent cross-mapping (CCM), PC-based methods (PCMCI), score-based methods, (VAR)LinGAM, TiMINO, ...

Granger causality

$A(t)$ is linearly Granger-cause of $B(t)$ with respect to a fixed time-lag m if the null hypothesis $\{\alpha_\ell = 0 \text{ for } \ell = 1, \dots, m\}$ is rejected for the linear AR model

$$B(t) = \sum_{\ell=1}^m \beta_\ell B(t - \ell) + \sum_{\ell=1}^m \alpha_\ell A(t - \ell) + \beta_0 + \epsilon.$$

- David Maxwell Chickering. Optimal structure identification with greedy search. *Journal of machine learning research*, 3(Nov): 507–554, 2002.
- Clark Glymour, Kun Zhang, and Peter Spirtes. Review of causal discovery methods based on graphical models. *Frontiers in genetics*, 10:524, 2019.
- Christopher Meek. Causal Inference and Causal Explanation with Background Knowledge. In *Proceedings of the Eleventh Conference on Uncertainty in Artificial Intelligence*, Uai'95, page 403–410, San Francisco, CA, USA, 1995. Morgan Kaufmann Publishers Inc. ISBN 1558603859.
- Shohei Shimizu, Patrik O Hoyer, Aapo Hyvärinen, Antti Kerminen, and Michael Jordan. A linear non-gaussian acyclic model for causal discovery. *Journal of Machine Learning Research*, 7(10), 2006.
- Peter Spirtes, Clark N Glymour, Richard Scheines, and David Heckerman. *Causation, prediction, and search*. MIT press, 2000.

T. Verma and J. Pearl. Equivalence and synthesis of causal models. In *Proceedings of the 6th Annual Conference on Uncertainty in Artificial Intelligence (UAI)*, pages 255–270, 1991.