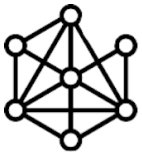
University of Basel



Benchpress

Run and develop structure learning algorithms using Benchpress

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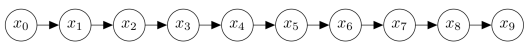
Markov property and graphical models

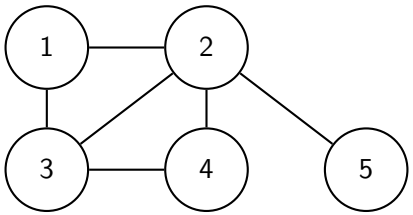
Definition (Markov property)

Let $G = (V, E)$ be a graph where $V = \{1, \ldots, p\}$, $E \subset V \times V$. A probability distribution P for a random vector $Y = (Y_i)_{i=1}^p$ is said to be Markov w.r.t. G if for disjoint subsets $A, B, C \subseteq V$

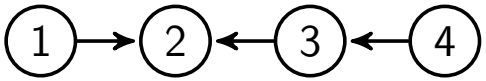
$$A \perp\!\!\!\perp_G B \mid C \implies Y_A \perp\!\!\!\perp_P Y_B \mid Y_C.$$



Markov chain



Undirected graph



Directed acyclic graph (DAG)

Gaussian graphical models

Example of an undirected graphical model

For a multivariate Gaussian distribution with covariance matrix $\mathbf{\Sigma}$, a graph G can be inferred from the non-zero pattern of its inverse (precision matrix), i.e.:

$$(\mathbf{\Sigma}^{-1})_{ij} \neq 0 \iff (i,j) \in G.$$

Structure learning in graphical models

Graph inference given a set of data is called **structure learning** (sometimes causal discovery). An NP-hard problem. Three main strategies:

- **Score-based**: optimizes a score function defined on graphs.
- **Constraint-based**: infers the edges by hypothesis testing.
- **Hybrid**: score based method on a graph space restricted by a constraint based method.

Structure learning in graphical models

Most structure learning algorithms are available open-source.
Comparing algorithms is challenging since:

- Not all are implemented in the same programming language
- Different implementations may have different formats/output
- Large comparisons require parallel computations
- Hard to structure results
- Many different comparison metrics
- Time consuming to implement
- ...

Benchpress

Benchpress is a **Snakemake** workflow which addresses the problems of benchmarking.

- Runs existing open-source software (any language) in containers using **Apptainer**.
- Separate modules for graph/parameters/data sampling, structure learning, and benchmarking.
- Fully parallel algorithm execution (grid, multicore, . . .).
- Reproducible and interpretable results in a unified format.
- Simple JSON-file interface.

Benchpress technology

- **Snakemake** is a rule-based workflow management system for reproducible data analysis, widely used in e.g. bioinformatics. (>7 citations a week)
- **Apptainer** is a secure container system for high-performance computing (HPC).

Todays tutorial

Introduction to Benchpress through the documentation

Introduction to the docs

- Installation
- Introduction to the modules
- Structure of the JSON file
- Example studies
- 15 min break (for questions, installation, and to run *config/config.json*)

Todays tutorial

Get introduced to Benchpress through the documentation

Using Benchpress

- Run *config/config.json* according to the examples in the docs.
- Look into the *results/output* folder.
- Change some parameters in the config file.
- Add the **PC** algorithm (Spirtes P. and Glymour C., 2000) from *gCastle* to the study.

Using Benchpress

Developing using Benchpress

Adding a new algorithm

- Add a new algorithm module for **GRaSP** (Lam, W. Y., Andrews, B., Ramsey, J., 2022) and call it `causallearn_grasp`.
- Try it in *config/config.json* and check the plots (TP, FP, etc.)
- Fill out *docs.rst*, *bibtex.bib*, and *info.json* and update the docs.

Using Benchpress

Developing using Benchpress

Challenge 1 (R or Python)

- Improve the `new_alg` template for estimating an undirected Gaussian graphical model.
- Hint: Estimate the precision matrix.
- Tips: Use the sandbox config and the template commands from the docs.

Challenge 2 (Python)

- Use the `new_alg` template to add the **GES** algorithm (Chickering, D. M. 2022) algorithm from *causal-learn* (and call it `causallearn_ges`).
- Tips 1: The causal-learn package is installed on the Docker image *bpimages/causal-learn:0.1.3.3*.
- Tips 2: See the causal-learn documentation for how to extract the adjacency matrix from the returned objects.

Github and documentation

- `https://github.com/felixleopoldo/benchpress`
- `https://benchpressdocs.readthedocs.io`