Causal Inference and Machine Learning
Session 8: Causal discovery from observational and experimental data using GIES

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Greedy Equivalence Search from observational data

Causal discovery in one slide

- Suppose we observe a (n, p) data matrix of observations $\boldsymbol{X}$, containing i.i.d. samples of a random vector $X := (X_1, \ldots, X_p)$;
- If X is generated from a Markovian Structural Causal Model with causal structure represented by $\mathcal{D}$, then a set of DAG-specific conditional independencies $\mathcal{I}(\mathcal{D})$ holds in the distribution of X, so that its pdf factorises as

$$p(x_1, \ldots, x_p) = \prod_{j=1}^{p} p(x_j \mid x_{\mathrm{pa}_{\mathcal{D}}(j)});$$

- If **faithfulness** is assumed, then one can try to learn the DAG from data by "testing" for these conditional independencies;
- Two main categories of causal discovery methods: constraint-based (PC algorithm) and score-based (Hill climbing);

Score-based methods: Introduction

- Score-based methods assign a score to each DAG and then select the DAG that maximises that score;
- Assuming a parametric distribution for X with parameter $\Theta_{\mathcal{D}}$, a popular choice for the score is the BIC:

$$\text{BIC}(\mathcal{D}, \boldsymbol{X}) = \log p(\boldsymbol{X}; \hat{\Theta}_{\mathcal{D}}) - \frac{\dim(\Theta_{\mathcal{D}})}{2} \log(n),$$

where

- $\hat{\Theta}_{\mathcal{D}}$ is the maximum likelihood estimate of $\Theta_{\mathcal{D}}$;
- $\log p(\boldsymbol{X}; \hat{\Theta}_{\mathcal{D}})$ is the likelihood of the data $\boldsymbol{X}$;
- $\dim(\Theta_{\mathcal{D}})$ is the number of free parameters in the distribution induced by the DAG $\mathcal{D}$;

Score-based methods: BIC

- Different scores may lead to different results!
- However, the BIC enjoys many useful properties:
  - It is **decomposable**: it can be written as

$$\text{BIC}(\mathcal{D}, \boldsymbol{X}) = \sum_{j=1}^{p} \log p(\boldsymbol{X}_{\cdot j} \mid \boldsymbol{X}_{\cdot \text{pa}_{\mathcal{D}}(j)}; \hat{\Theta}_{\mathcal{D}}^{(j)}) - \frac{d_j}{2} \log(n)$$

    where $\Theta_{\mathcal{D}}^{(j)}$ are the parameters associated with the j-th conditional density of the factorization and $d_j = \dim(\Theta_{\mathcal{D}}^{(j)})$
  - It is **consistent**: as $n \to \infty$, it is highest for the true DAG;
  - It guarantees **score equivalence**: two unidentifiable (Markov equivalent) DAGs $\mathcal{D}_1, \mathcal{D}_2$ are assigned the same score;

Score-based methods: fundamental problem

- We are interested in

$$\hat{\mathcal{D}} = \text{argmax}_{\mathcal{D} \in \mathcal{S}_p} \text{BIC}(\mathcal{D}, \boldsymbol{X});$$

- You can guess what's the problem...

Score-based methods: fundamental problem

- We are interested in

$$\hat{\mathcal{D}} = \text{argmax}_{\mathcal{D} \in \mathcal{S}_p} \text{BIC}(\mathcal{D}, \boldsymbol{X});$$

- You can guess what's the problem...

p	$\lvert\mathcal{S}_p\rvert$ (No. of DAGs)
1	1
3	3
5	543
7	3781503
9	783702329343
11	4175098976430598143
13	521939651343829405020504063
15	143942814104439833494179071983953510 3

- We can't enumerate all the DAGs, we need **greedy algorithms**!

Score-based methods: Hill Climbing

- The easiest example of **greedy algorithm** for causal discovery is the **hill climbing algorithm**;
- It starts from an initial DAG $\mathcal{D}^{(0)}$ (often the empty DAG) and, at each iteration $s > 1$:
  - It constructs the set neigh_s of neighboring DAGs that can be obtained by **adding**, **deleting**, or **reversing** a single edge;
  - For each $\tilde{\mathcal{D}} \in \text{neigh}_s$, computes $\text{score}(\tilde{\mathcal{D}}, \boldsymbol{X})$;
  - Sets $\mathcal{D}^{(s)} = \text{argmax}_{\tilde{\mathcal{D}} \in \text{neigh}_s} \text{score}(\mathcal{D}, \boldsymbol{X})$;

  these steps are repeated until the score can't be improved

Score-based methods: Comments Hill Climbing

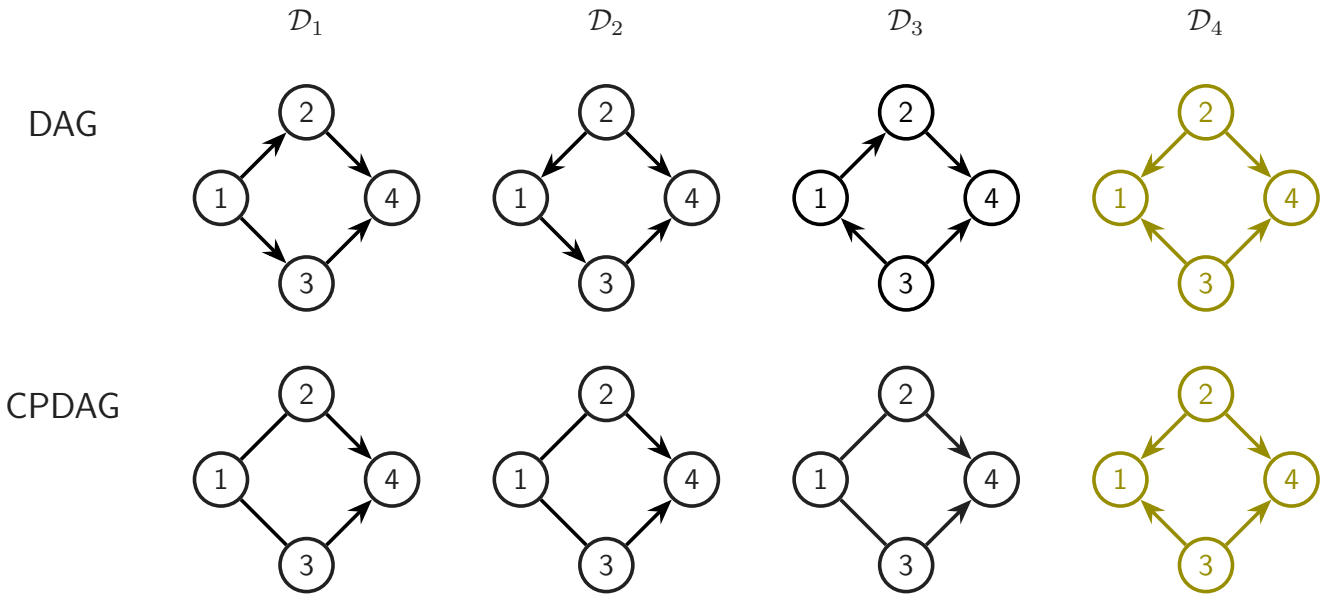
- The combination of local moves considered by the algorithm and decomposable scores leads to significant computational savings;
- However, even if the score is consistent, the algorithm is not: it may remain stuck in local modes, without reaching the local optimum $\hat{\mathcal{D}}$;
- Morover, if the score satisfies score equivalence, there is no unique global optimum, but as many as the DAGs in a Markov Equivalence class;
- **Solution:** Greedy algorithm defined on the space of Markov equivalence classes: **Greedy Equivalence Search** (GES);

Markov Equivalence classes and CPDAGs

- A DAG $\mathcal{D}_1$ implies a set of conditional independencies $\mathcal{I}(\mathcal{D}_1)$ that can be read-off from the graph using d-separation and is reflected in the factorization of the pdf;
- It may happen that, for two DAGs $\mathcal{D}_1$ and $\mathcal{D}_2$, $\mathcal{I}(\mathcal{D}_1) = \mathcal{I}(D_2)$. When this happens, we say that $\mathcal{D}_1$ and $\mathcal{D}_2$ are **Markov Equivalent**;
- Two Markov equivalent DAGs share the same **skeleton** and the same set of **v-structures**: they differ only for the reversal of **some** edges;
- One can use a graph with undirected and directed edges to represent a Markov Equivalence class of DAGs. This is called **Essential graph** or **Completed Partially Directed Acyclic Graph** (CPDAG);

CPDAGs: Example

- For instance, here are four DAGs and their CPDAGs:



- $\mathcal{D}_1, \mathcal{D}_2, \mathcal{D}_3$ are Markov equivalent and share the same CPDAG!

GES: Introduction

- Greedy Equivalence Search is a greedy causal discovery algorithm that works directly on the space of CPDAGs $\mathcal{G}$;
- As such, it requires (i) a **score** associated with each CPDAG and (ii) a set of **local moves** to explore the space of possible CPDAGs;
- Moreover, GES is composed of two distinct phases.
  - **Forward phase**: starting from a CPDAG $\mathcal{G}^{(0)}$ with no edges, undirected and directed edges are greedily inserted until the score can't be improved. It returns a CPDAG $\mathcal{G}^{(fp)}$;
  - **Backward phase**: starting from $\mathcal{G}^{(fp)}$, edges are greedily removed. It returns the candidate CPDAG $\hat{\mathcal{G}}$;

GES: Score

- Different possibilities for the score. We will focus again on the BIC:

$$\mathrm{BIC}(\mathcal{G}, \boldsymbol{X}) = \log p(\boldsymbol{X}; \hat{\Theta}_{\mathcal{G}}) - \frac{\dim(\Theta_{\mathcal{G}})}{2} \log(n),$$

- For any two DAGs $\mathcal{D}_1$ and $\mathcal{D}_2$ belonging to the same Markov equivalence class represented by $\mathcal{G}$, we have that

$$\mathrm{BIC}(\mathcal{D}_1, \boldsymbol{X}) = \mathrm{BIC}(\mathcal{D}_2, \boldsymbol{X}) = \mathrm{BIC}(\mathcal{G}, \boldsymbol{X}).$$

  Because of score equivalence, the score of the CPDAG is the same of any of the DAGs it represents

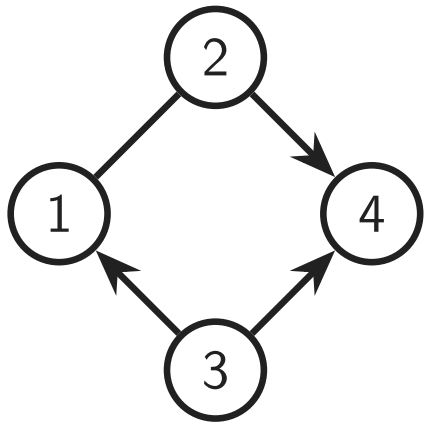
- The BIC inherits all the nice properties it has in the DAG setting (it is *consistent* and *decomposable*)

GES: Local moves

- For two nodes i and j in $\mathcal{G}$, we say that i, j are *adjacent* if they are connected by a directed or undirected edge in $\mathcal{G}$ and that i, j are *neighbors* if they are connected by an undirected edge;
- Chickering (2002) proposed the following two operations, each corresponding to one of the two phases:
  - **Insert**$(i, j, \boldsymbol{T})$: For non-adjacent nodes i and j in $\mathcal{G}$, and for any subset $\boldsymbol{T}$ of the neighbors of j that are not adjacent to i, insert $i \to j$ and, for each $k \in \boldsymbol{T}$, direct $k - j$ as $k \to j$;
  - **Delete**$(i, j, \boldsymbol{H})$: For adjacent nodes i and j in $\mathcal{G}$, and for any subset $\boldsymbol{H}$ of the neighbors of j that are adjacent to i, delete the edge between i and j, and for each $k \in \boldsymbol{H}$, direct the $j - k$ as $j \to k$ and direct any previously undirected edge between i and k as $i \to k$.

GES: Invalid local moves

- The local moves by Chickering can still lead to **invalid** CPDAGs, i.e. graphs with undirected and directed edges that do not represent any Markov equivalence class;
- Consider for instance the following graph:



  It is not a CPDAG, as directing in any way the undirected edge $1 - 2$ leads to DAGs which are in two different Markov Equivalence classes!
- The validity of CPDAG must be manually checked. Chickering (2002) also provides a relatively quick way to do that;

GES: Summary

- In the **forward** (**backward**) phase, GES starts from the empty CPDAG $\mathcal{G}^{(0)}$ (the CPDAG $\mathcal{G}^{(fs)}$) and, at each iteration $s > 1$:
  - It constructs the set neigh_s of neighboring CPDAGs that can be obtained by one **Insert** (**Delete**) operation;
  - For each $\tilde{\mathcal{G}} \in \text{neigh}_s$, computes $\text{score}(\tilde{\mathcal{G}}, \boldsymbol{X})$;
  - Sets $\mathcal{G}^{(s)} = \text{argmax}_{\tilde{\mathcal{G}} \in \text{neigh}_s} \text{score}(\mathcal{G}, \boldsymbol{X})$;

  these steps are repeated until the score can't be improved. Then a CPDAG $\mathcal{G}^{(\text{fs})}$ ($\hat{\mathcal{G}}$) is returned;

GES: Final comments

- If used with a consistent score, **GES is consistent**: It identifies the CPDAG corresponding to the true DAG as $n \to \infty$;
- Working directly on the space of Markov equivalence classes, it also provides better results in finite samples;
- However, the local moves are more difficult to define and their validity more difficult to check than for Hill-Climbing. It may be more computational demanding;
- It is still much more efficient than constraint-based methods, and recent developments are making it even faster using heuristics (Ramsey et al., 2017)

GES: Software

- An implementation of GES is available via the constructor `new()` and the function `ges()` of the `R` package `pcalg`
- Inputs of `new()` are
  - `Score` : which score must be used;
  - `data`: the data matrix $\boldsymbol{X}$
- Input of `ges()` is only the score produced by `new()`
- Let's see how it works in `R`!

Beyond Markov equivalence: Making use of experimental data

Experimental data: definition

- When only **observational data** are available, even assuming that X is generated by a Markovian SCM only leads us as far as the Markov equivalence class of the true causal structure;
- We define **experimental data** as any data observed after an external intervention to the system. In particular, we consider only **hard interventions**, fixing the value of a **target** variable to a constant;
- Intuitively, using experimental data should help up uncovering more of the causal structure, but how exactly?

Experimental data: how

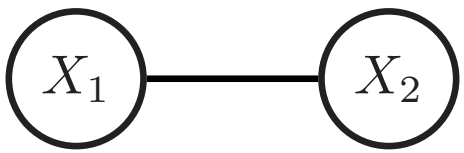
- Key assumptions of SCMs: each mechanism is stable and autonomous

$\Longrightarrow$ an external intervention *only* affects the mechanisms of the target variables, destroying the dependence with their parents (i.e. its causes) in the DAG!

$\Longrightarrow$ If we are undecided on the direction of an edge $i - j$, we can intervene on one of the two nodes and see whether the dependence represented by $i - j$ is destroyed.
If **yes**, the intervened node is the effect.
If **no**, the intervened node is the cause!

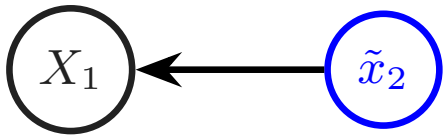
Using experimental data: example - 1

- Let's consider a very simple case in which we have a $(n_1, 2)$ data matrix $\boldsymbol{X}^{(1)}$ with i.i.d. measurements of (X_1, X_2);
- Suppose there are no condtional independencies in the data, so that any causal discovery algorithm returns the following CPDAG:



Using experimental data: example - 2

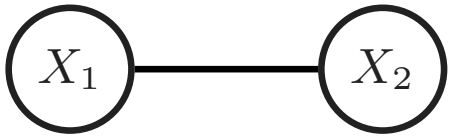
- Suppose now we have access to measurements of $(X_1, X_2) \,|\, \text{do}(X_2)$, stored in the $(n_2, 2)$ matrix $\boldsymbol{X}^{(2)}$.
- The intervention on X_2 only modifies its mechanism, meaning that
  - if $X_2 \to X_1$ the post-intervention DAG will be



  - If $X_1 \to X_2$, the post-intervention DAG will be

Using experimental data: example - 3

- Suppose we now use a causal discovery algorithm on $\boldsymbol{X}^{(2)}$;
  - If its output is



    then $X_2 \to X_1$ is the true causal structure!
  - Otherwise, if its output is

    then $X_1 \to X_2$ is the true causal structure!
- By using experimental data, we are going beyond Markov equivalence!

Using experimental data: comments

- As the **invariances**/**differences** between observational and experimental data are DAG-specific, we can use them to learn the causal structure!
- But **how far** can these invariances bring us?

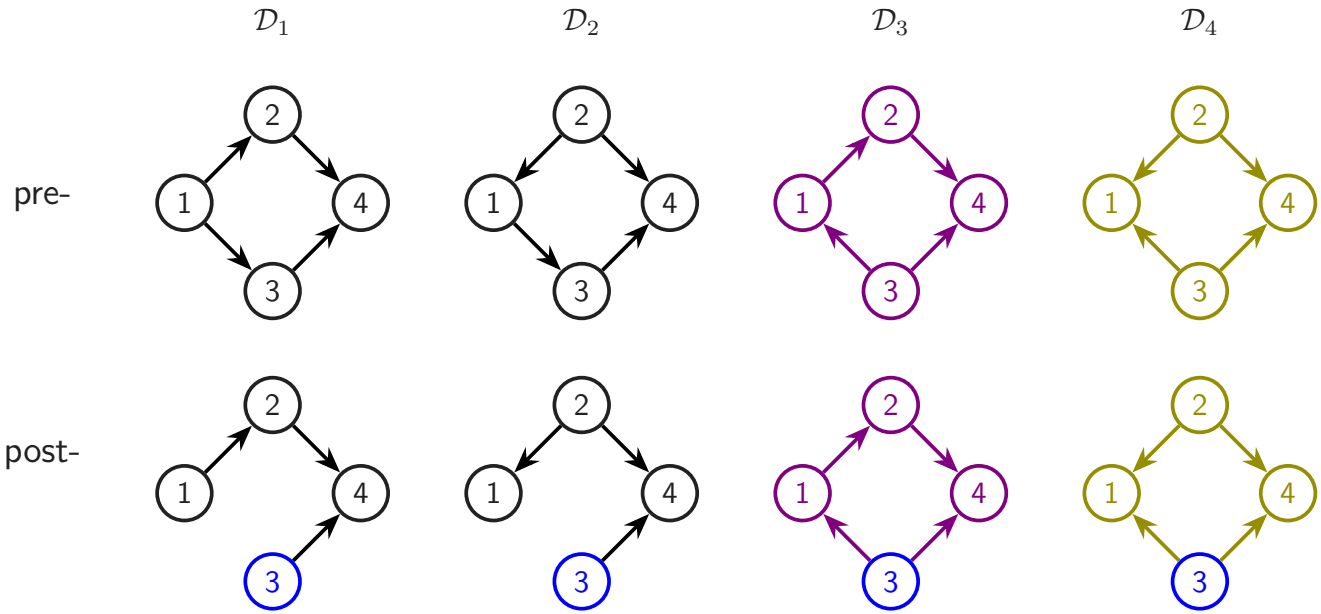
Using experimental data: setting

- **Setting:** we observe a set of K data matrices $\{\boldsymbol{X}^{(k)}\}_{k=1}^{K}$, where
  - $\boldsymbol{X}^{(1)}$ contains i.i.d. samples from the observational distribution of X;
  - $\boldsymbol{X}^{(2)}, \dots, \boldsymbol{X}^{(K)}$ contain samples from the post-intervention distributions of X given a hard intervention on the target nodes $\boldsymbol{T}^{(k)}$.

  We also denote with $\mathcal{T} = \{\boldsymbol{T}^{(k)}\}_{k=1}^{K}$ the multi-set of intervention targets and $\{p_k(x)\}_{k=1}^{K}$ the corresponding post-intervention distributions;
- **Goal:** Design a causal discovery algorithm that takes as input $\{\boldsymbol{X}^{(k)}\}_{k=1}^{K}$ and $\mathcal{T} = \{\boldsymbol{T}^{(k)}\}_{k=1}^{K}$ and returns an estimate of the causal structure $\mathcal{D}$
- **Preliminary question**: Can we actually identify the DAG?

I-Markov equivalence

- Consider the following four DAGs and the corresponding post-intervention DAGs produced by an intervention on X_3:



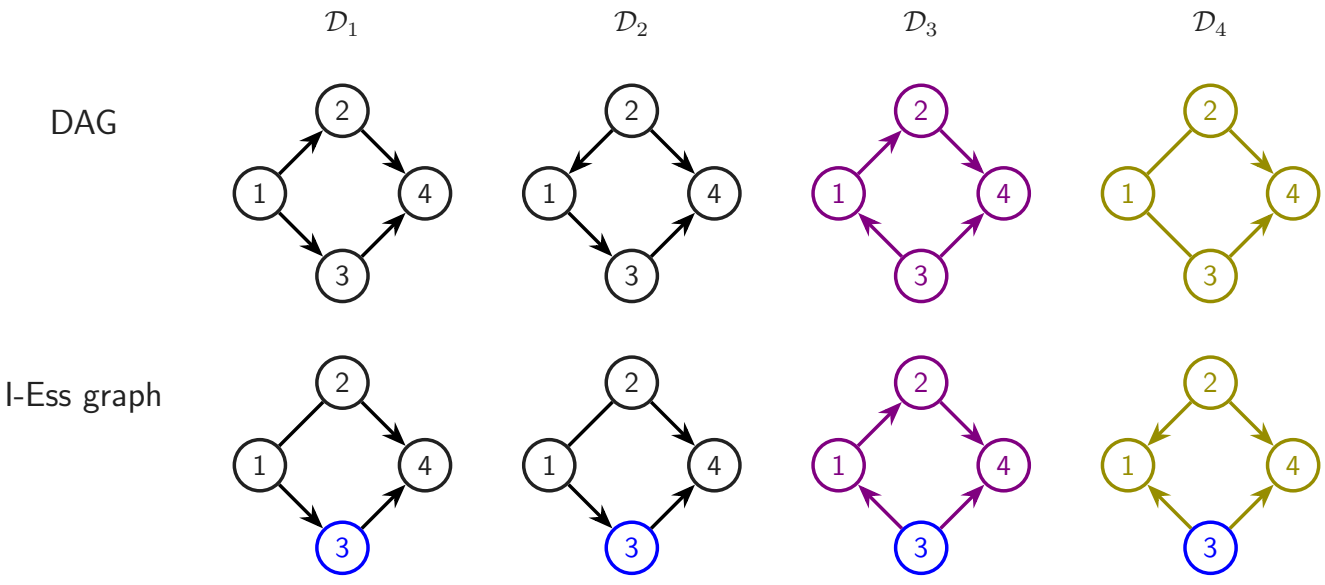
- $\mathcal{D}_1, \mathcal{D}_2$ imply the same set of conditional independencies and invariances: they're **I-Markov equivalent** given an intervention on X_3;

I-Markov equivalence and I-Essential graphs

- I-Markov equivalence classes are the identifiability limit when also experimental data are available;
- Hauser & Bühlmann (2012) provide two **graphical characterizations** of I-Markov equivalence:
  - All I-Markov equivalent DAGs have the same *skeleton* and the same set of *v-structures* in all pre- and post-intervention DAGs;
  - Two DAGs are I-Markov equivalent if they have the same **I-Essential graph**;
- As for the observational case, the **I-Essential Graph** is a graph with undirected edges in correspondence of the edges that can be directed in both ways without going out of the I-Markov equivalence class;

I-Essential graph: Example

- Let's consider the same four DAGs as before, with $\mathcal{T} = \{\emptyset, \{3\}\}$:



GIES:

- We want to design algorithms that use **both** the *conditional independencies* within each dataset and the *invariances* across datasets to learn the causal structure
- In what follows, we will consider an extension of GES called Greedy Interventional Equivalence Search (Hauser & Buhlmann, 2012);

GIES: Introduction

- Greedy Interventional Equivalence Search is a **greedy**, **score-based** causal discovery algorithm that works directly on the space of I-Essential graphs $\mathcal{E}$;
- As usual, it requires (i) a **score** associated with each I-Essential graph and (ii) a set of **local moves** to explore the space of possible I-Essential graphs;
- GIES is composed of three distinct phases.
  - **Forward phase**: starting from a CPDAG $\mathcal{E}^{(0)}$ with no edges, directed and undirected edges are greedily inserted until the score can't be improved. It returns an I-Essential graph $\mathcal{E}^{(\text{fp})}$;
  - **Backward phase**: starting from $\mathcal{E}^{(\text{fp})}$, edges are greedily removed. It returns an I-Essential graph $\mathcal{E}^{(\text{bp})}$;
  - **Turning phase**: starting from $\mathcal{E}^{(\text{bp})}$, edges are greedily turned. It returns the candidate I-Essential graph $\hat{\mathcal{E}}$

GIES: Score

- As for any score-based method, there are different possibilities for the score. Usually, consistent and score-equivalent ones are preferred
- We will use again the BIC that, in this setting becomes:

$$\text{BIC}(\mathcal{E}, \{\boldsymbol{X}\}_{k=1}^{K}) = \sum_{k=1}^{K} \log p(\boldsymbol{X}^{(k)}; \hat{\Theta}_{\mathcal{E}}) - \frac{\dim(\Theta_{\mathcal{E}})}{2} \log(n),$$

- BIC is still decomposable, as it can be written as

$$\text{BIC}(\mathcal{E}, \{\boldsymbol{X}\}_{k=1}^{K}) = \sum_{j=1}^{p} \log p(\boldsymbol{X}_{.j}^{A(j)} \,|\, p(\boldsymbol{X}_{.\text{pa}_{\tilde{\mathcal{D}}}(j)}^{A(j)}; \hat{\Theta}_{\mathcal{E}}^{(j)}) - \frac{\dim(\Theta_{\mathcal{E}}^{(j)})}{2} \log(n)$$

  where $A(j) := \{k \in [K] : j \notin \boldsymbol{T}^{(k)}\}$ and $\tilde{\mathcal{D}}$ a DAG represented by $\mathcal{E}$
- The BIC is **consistent** in the Gaussian setting (Hauser & Buhlmann, 2015);

GIES: Local moves

- We will not go into the details of the local moves used by GIES in each phase, as they require some preliminary work to be understood and can be quite complicated;

Input : $G = ([p], E)$: $\mathcal{I}$-essential graph; $(\mathcal{T}, \mathbf{X})$: interventional data for $\mathcal{I}$
Output: $G' \in \mathcal{E}^+_{\mathcal{I}}(G)$, or G
$\Delta S_{\max} \leftarrow 0$;
foreach $v \in [p]$ **do**
  foreach $u \in [p] \setminus \mathrm{ad}_G(v)$ **do**
    $N \leftarrow \mathrm{ne}_G(v) \cap \mathrm{ad}_G(u)$;
    foreach *clique* $C \subset \mathrm{ne}_G(v)$ *with* $N \subset C$ **do** `// Proposition 25(i) and (ii)`
      if $\nexists$ *path from* v *to* u *in* $G[[p] \setminus C]$ **then** `// Proposition 25(iii)`
        $\Delta S \leftarrow s(v, \mathrm{pa}_G(v) \cup C \cup \{u\}; \mathcal{T}, \mathbf{X}) - s(v, \mathrm{pa}_G(v) \cup C; \mathcal{T}, \mathbf{X})$;
        if $\Delta S > \Delta S_{\max}$ **then**
          $\Delta S_{\max} \leftarrow \Delta S$;
          $(u_{\max}, v_{\max}, C_{\max}) \leftarrow (u, v, C)$;
if $\Delta S_{\max} > 0$ **then**
  $\sigma \leftarrow \textsc{LexBFS}((C_{\max}, v_{\max}, \ldots), E[T_G(v_{\max})])$;
  Orient edges of $G[T_G(v_{\max})]$ according to σ;
  Insert edge $(u_{\max}, v_{\max})$ into G;
  return $\textsc{ReplaceUnprotected}(\mathcal{I}, G)$; `// See Algorithm 1`
else return G;

Algorithm 3: $\textsc{ForwardStep}(G; \mathcal{T}, \mathbf{X})$. One step of the forward phase of GIES.

GIES: Final comments

- GIES uses both observational and experimental data to learn the causal structure generating the data;
- Its output is an I-Essential graph representing an I-Markov equivalence class of indistinguishable DAGs;
- I-Markov equivalence classes contain strictly fewer DAGs than Markov equivalence classes $\implies$ we are learning more of the causal structure!
- **However**, unline GES, **GIES** is **not consistent**, even when a consistent score such as the BIC is used;
- We will see in the following lectures other methods that overcome this problem;

GIES: Software

- An implementation of GIES is available via the constructor `new()` and the function `gies()` of the `R` package `pcalg`
- Inputs of `new()` are:
  - `Score` : which score must be used;
  - `data` : data matrix $\boldsymbol{X}$ obtained by stacking $\{\boldsymbol{X}^{(k)}\}_{k=1}^{K}$ vertically;
  - `targets` : list of targets $\mathcal{T}$;
  - `target.index` : vector of length n indicating which observation belongs to which experimental setting;
- Inputs of `gies()` is only the score produced by `new()`:
- Let's see how it works in `R`!

Thank you!

References:

- Chickering, D. M. (2002). *Optimal structure identification with greedy search*. Journal of machine learning research, 3(11), 507-554.
- Hauser, A., & Bühlmann, P. (2012). *Characterization and greedy learning of interventional Markov equivalence classes of directed acyclic graphs*. The Journal of Machine Learning Research, 13(1), 2409-2464.
- Hauser, A., & Bühlmann, P. (2015). *Jointly interventional and observational data: estimation of interventional Markov equivalence classes of directed acyclic graphs*. Journal of the Royal Statistical Society Series B: Statistical Methodology, 77(1), 291-318.
- Ramsey, J., Glymour, M., Sanchez-Romero, R., & Glymour, C. (2017). *A million variables and more: the fast greedy equivalence search algorithm for learning high-dimensional graphical causal models, with an application to functional magnetic resonance images*. International journal of data science and analytics, 3, 121-129.