Unconditional Equivalence in Causal Discovery

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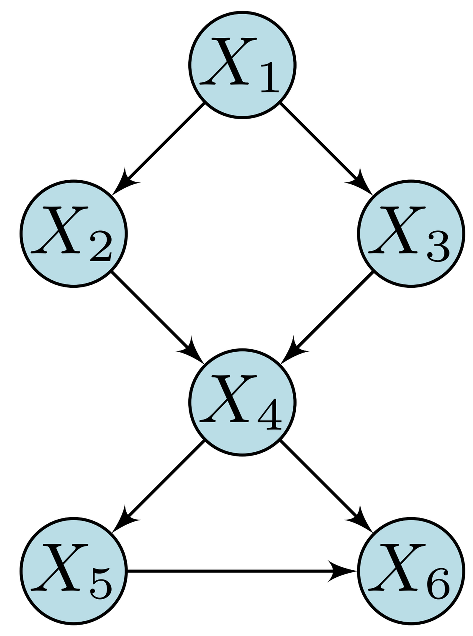
Setup

Directed acyclic graphs (DAGs) or bayesian networks are directed simple graphs without cycles.

- A DAG is used to model a **causal system**, i.e., a distribution $\mathbb{P}$ of $X_1, \ldots, X_n$ that encodes conditional independence statements.
- **Conditional independence (CI)** statements $X_A \perp\!\!\!\perp X_B \mid X_C$ in $\mathbb{P}$ can be expressed in the DAG $\mathcal{G}$ through connectivity rules.

Assumption: The distribution $\mathbb{P}$ is **Markov** to its underlying causal system: a DAG $\mathcal{G}$ that encodes exactly the CI statements that hold in the distribution.

Challenge: Given observed data from $\mathbb{P}$, can we recover $\mathcal{G}$?



MECs and UECs

Markov Equivalence:

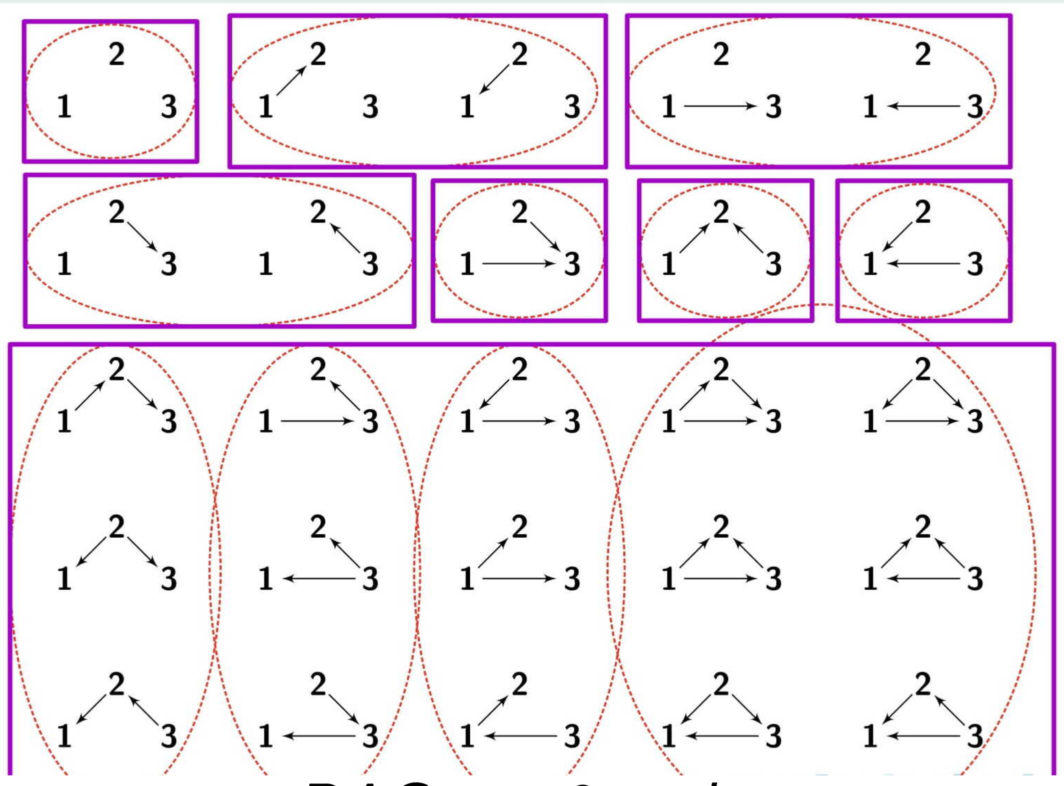
- We partition the space of DAGs into **Markov Equivalence Classes (MECs)** based on their CI relations.

Problem: Given data from $\mathbb{P}$, find the MEC of $\mathcal{G}$.

Unconditional Equivalence:

- The MEC partition is a refinement of the UEC partition:

Two DAGs are in the same **Unconditional Equivalence Class (UEC)** if they encode the same unconditional independence statements $(X_A \perp\!\!\!\perp X_B \mid \emptyset)$.

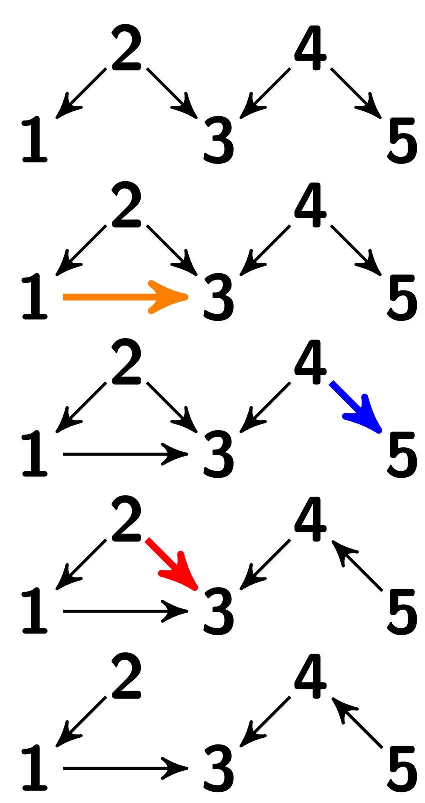


DAGs on 3 nodes

The structure of a UEC

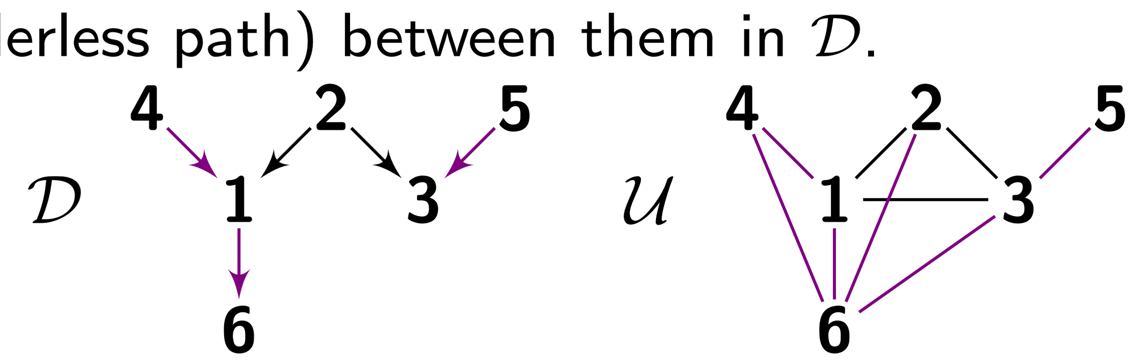
Transformational Characterization [1]:
Let $\mathcal{D}, \mathcal{D}'$ be DAGs in the same UEC. There is a sequence of edge insertions, reversals and deletions that transforms $\mathcal{D}$ into $\mathcal{D}'$ such that:

- Each edge inserted or deleted in is partially weakly covered or implied by transitivity.
- Each edge reversed in $\mathcal{D}$ is weakly covered.
- After each operation, the resulting DAG is in the same UEC as $\mathcal{D}$.



Structural Characterization:
The **unconditional dependence graph** $\mathcal{U}$ of a DAG $\mathcal{D}$ has the same nodes as $\mathcal{D}$ and an edge between v, w if there is a trek (colliderless path) between them in $\mathcal{D}$.

Example:



References

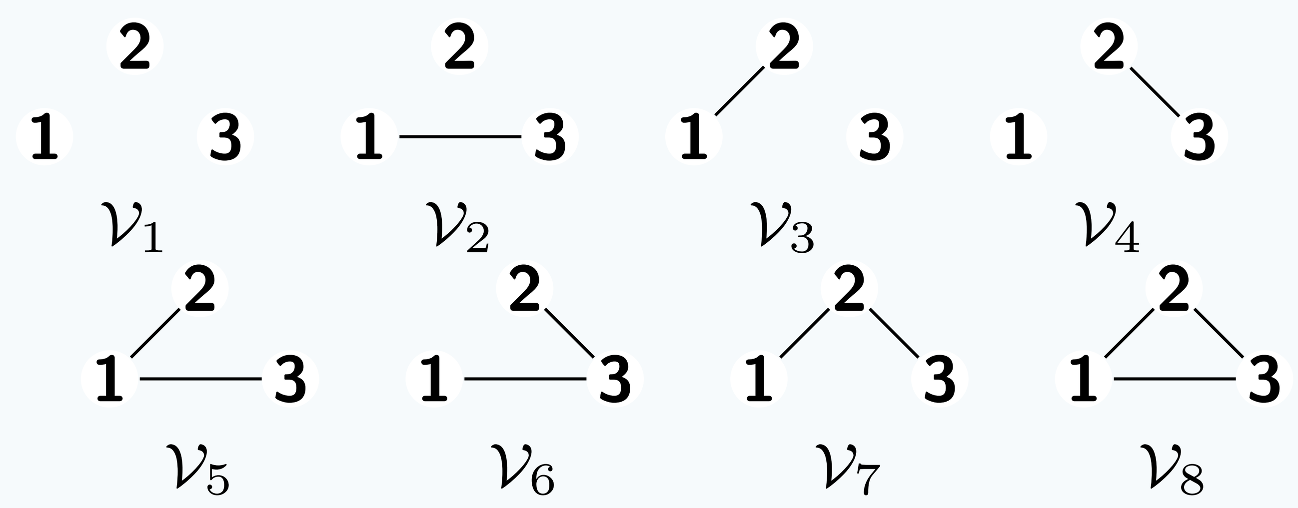
[1] *Transformational Characterization of Unconditionally Equivalent Bayesian Networks*, A. Markham, D. Deligeorgaki, P. Misra and L. Solus, 11th International Conference on Probabilistic Graphical Models (PGM), 2022.

[2] *Combinatorial and algebraic perspectives on the marginal independence structure of Bayesian networks*, D. Deligeorgaki, A. Markham, P. Misra and L. Solus, arXiv:2210.00822v1, 2022.

Traversing the space of UECs

In [2] we give a **Transformational and Structural Characterization** of the graphs representing a UEC of DAGs, using algebraic geometry (e.g., Gröbner bases) and combinatorics.

List of graphs representing a UEC on 3 nodes:

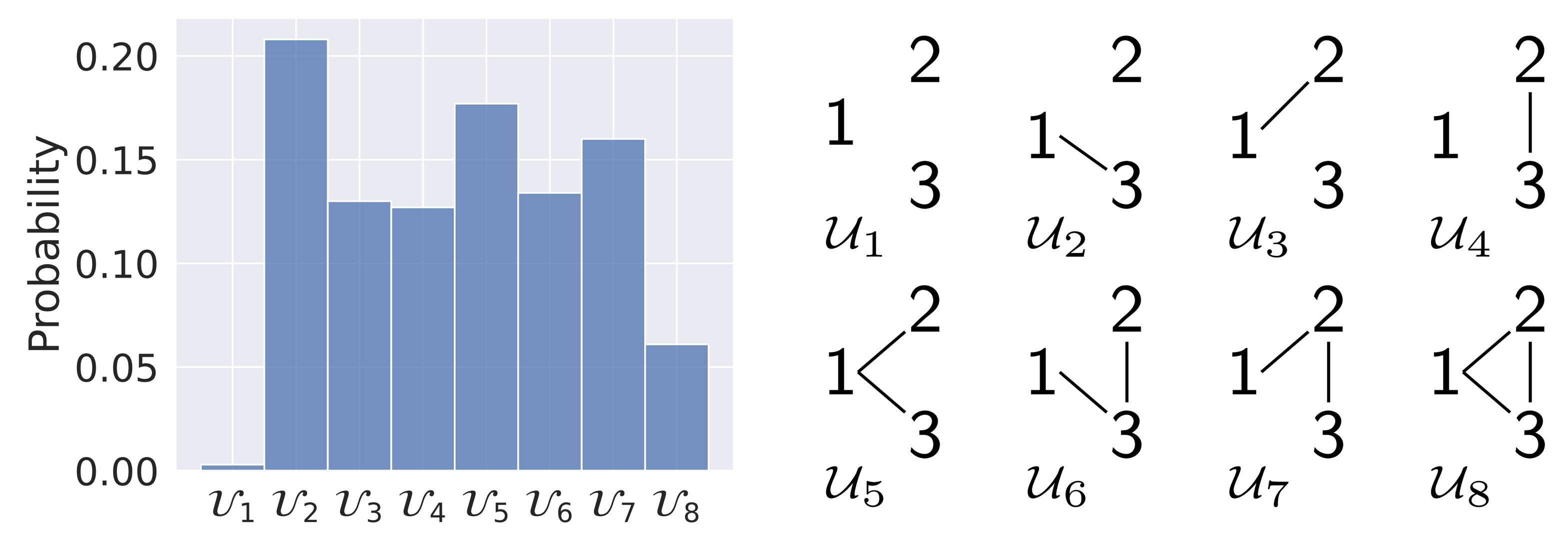


Number of UECs on 1,2,3,... nodes: 1,2,8,49,462,6424,...

Applications

Using the transformational characterization, we implemented an MCMC method for estimating the UEC of $\mathcal{G}$, **GrUES** (Gröbner-based Unconditional Equivalence Search).

A) We simulated a data set (1000 samples) over 3 nodes using the Gaussian linear model (with randomly generated weights) $X_1 = \epsilon_1, \quad X_2 = \epsilon_2, \quad X_3 = -0.9247 X_1 + \epsilon_3$.



▶ Histogram of the Markov chain indicates a MAP estimate $\pi(\mathcal{U}_2 | X) = 0.208$ (i.e., $\mathcal{U}_2$ has the highest frequency).

B) 100 linear Gaussian DAG models on 5 nodes for edge probability $p \in \{0.1, 0.2, \ldots, 0.9\}$ and random edge weights