

Inferring model structure from data: MCMC for DAGs

Radu Craiu

Department of Statistical Sciences
University of Toronto

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Outline



Morris Greenberg

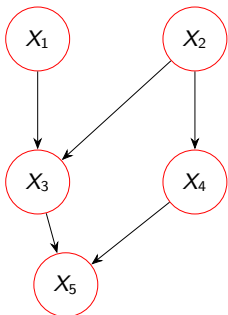


Kieran Campbell

- ▶ Overview
- ▶ MCMC in the space of restricted orders
- ▶ Allow the restricted space to evolve
- ▶ Simulations and data analysis

Inferring a DAG from data

- ▶ Multivariate distributions can be represented through a graph plus parameters; each vertex is a unique variable.
- ▶ When it is represented by an acyclic graph, the joint distribution can be factored by a product of conditionals defined by the edges.



- ▶ DAG-type learning is of interest in fields where the causal direction is desired.
- ▶ For this graph:

$$P(X_1) \cdot P(X_2) \cdot P(X_3 \mid X_1, X_2)$$

$$P(X_4 \mid X_2) \cdot P(X_5 \mid X_3, X_4).$$

Finding model structure via MCMC

- ▶ Goal: given data D on p variables, infer a DAG that characterizes the conditional independences in the distribution of D or sample the DAG posterior $\pi(G \mid D)$.
- ▶ A typical pipeline:
 - ▶ estimate an undirected **skeleton** (PC);
 - ▶ explore the discrete space of DAGs by MCMC, e.g. by scoring graphs (or orders).
- ▶ Direct sampling of DAGs is prohibited by a **super-exponential** search space, score-equivalent plateaus, and acyclicity constraints.

Why direct sampling of DAGs is challenging

- ▶ The number of labelled directed graphs is $2^{p(p-1)}$; the fraction that are DAGs **vanishes** as p grows:

p	5	8	10	20
# graphs	1.0×10^6	7.2×10^{16}	1.2×10^{27}	2.5×10^{114}
# DAGs	2.9×10^4	7.8×10^{11}	4.2×10^{18}	2.3×10^{72}
# DAGs / # graphs	2.8%	1.1×10^{-5}	3.4×10^{-9}	9.5×10^{-43}

- ▶ Finding a highest-scoring DAG is NP-complete even with a bounded parent set ([Chickering, 1996](#)).
- ▶ Structure MCMC (add/delete/reverse one edge) must test acyclicity at every proposal and mixes slowly on this discrete space.
- ▶ Score-equivalent DAGs share the same likelihood, so the chain can wander inside a class for lengthy periods

Graph inference methods

- ▶ Three main methods: *constraint-based (CB)*, *score-based (SB)*, and *hybrid (H)* methods
- ▶ CB infer graph structure by estimating conditional dependencies
 - ▶ Yield consistent estimators of the true DAG under mild assumptions, e.g., faithfulness, maximum degree of the graph. ([Kalisch and Bühlmann 2007](#))
 - ▶ Require a large number of conditional independence tests ([Spirtes et al. 2000](#))
- ▶ SB infer structure via an objective function (*score*) that measures the relative merits of each graph
 - ▶ Score ties the graph directly to model quality
 - ▶ Scalability as sample space is exponential in p (no. of nodes)
- ▶ H combine strategically CB and SB
 - ▶ Use CB to construct a reduced space of graphs
 - ▶ Use SB to explore the space

DAG notation

- ▶ A graph is $G = (V, E_G)$ where V is set of vertices (or nodes) and set of edges is E_G
- ▶ In a directed G , edges are ordered: $i \rightarrow j$ indicates i is a parent of j and $i \leftarrow j$ implies the reverse.
- ▶ We denote the parents of node i as $pa_G(i)$ (or $pa(i)$)
- ▶ No node is both an ancestor and a descendant of another).
- ▶ Every DAG G is compatible with at least one **topological order**, $\prec \in \mathbb{S}^p$, i.e. a permutation of $\{1, \dots, p\}$ that exhibits the ancestry of the vertices.
- ▶ If $\prec_{[i]} < \prec_{[j]}$ for all $i \rightarrow j$ in G , then $G \in \mathcal{G}_\prec$. Additionally, i is a *predecessor* of j in $\prec$, or $i \in pr_\prec(j)$ for short.

Faithfulness

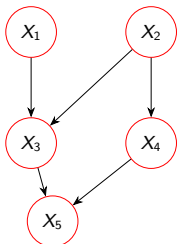
- ▶ Two DAGs are **Markov equivalent** if they share the same skeleton and the same v -structures (Verma and Pearl, 1990).
- ▶ When the true DAG belongs to a nontrivial equivalence class, structure learning from observational data alone becomes unidentifiable.
- ▶ **Faithfulness**: Every (conditional) independence in P is encoded by d -separation in G and vice versa .
- ▶ Faithfulness is needed to identify the Markov equivalence class from the conditional independence relations in the data.

PC skeleton

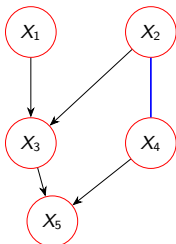
- ▶ The **PC algorithm** (Kalisch and Bühlmann, 2007) starts from the complete undirected graph and deletes $X_i - X_j$ whenever $X_i \perp X_j \mid S$ for some conditioning set $S \Rightarrow$ **skeleton**
- ▶ Faithfulness is fragile: near path-cancellations make tests unstable (Uhler et al., 2013).
- ▶ Hybrid MCMC takes this skeleton as the initial set of allowed edges, then samples orientations/orders/subsets of edges inside it.

Faithfulness and Markov equivalence

DAG

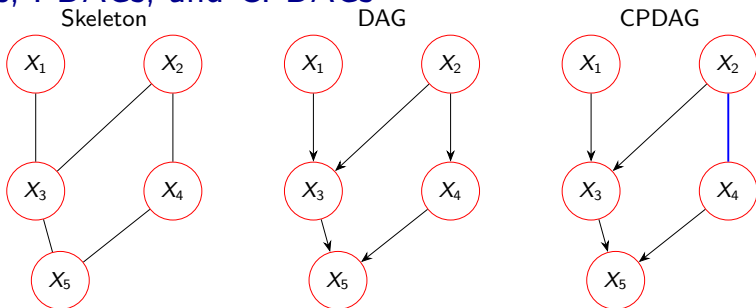


CPDAG of the same class



- ▶ Here $X_2 \rightarrow X_4$ is reversible: the DAG with $X_4 \rightarrow X_2$ is in the same class.
- ▶ The **CPDAG** is the unique completed representative of that class: compelled arrows stay directed; reversible edges (blue) stay undirected.
- ▶ Faithfulness means P is a perfect map of G , so the independences in the data are exactly the d -separations common to every graph in the class.
- ▶ Without faithfulness, extra independencies appear that no DAG in the class encodes, and observational data no longer identify the equivalence class.

DAGs, PDAGs, and CPDAGs



- ▶ **DAG:** every edge oriented.
- ▶ **PDAG:** a mix of directed and undirected edges (directed part acyclic). Intermediate output of orientation rules; not unique.
- ▶ **CPDAG** (completed PDAG / essential graph): the unique representative of a Markov equivalence class — compelled arrows stay directed; reversible edges (blue) stay undirected.
- ▶ Observational data identify a CPDAG, not a single DAG.

Ingredients: Scores

- ▶ A score $Q(G, D)$ measures how well graph G explains the data D .
- ▶ Common choices include:
 - ▶ **Information criteria:** BIC or AIC-type scores, usually based on penalized likelihood.
 - ▶ **Bayesian posterior scores:** unnormalized posterior scores such as

$$Q(G, D) \propto P(D \mid G)\pi(G).$$

- ▶ **Bayesian network scores:** BDe for multinomial data and BGe for Gaussian data.
- ▶ Decomposable scores are especially useful:

$$Q(G, D) = \prod_{i=1}^p S(X_i, \mathbf{Pa}_G(i) \mid D),$$

so local graph updates only require rescoreing affected nodes.

Computing the BGe scores

- ▶ Rely on **closed-form marginal likelihoods** $P(D \mid G)$ under conjugate priors (Heckerman and Geiger, 1995).
- ▶ **BGe** (Gaussian, normal–Wishart). The local score is a ratio of complete-model marginals

$$S_{\text{BGe}}(X_i, \mathbf{Pa}(i) \mid D) = \frac{p(D_{i \cup \mathbf{Pa}})}{p(D_{\mathbf{Pa}})},$$

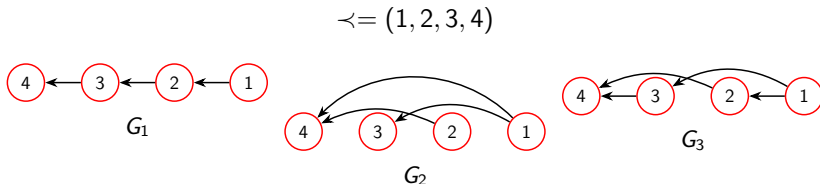
and each $p(D_Y)$ is a product of Gamma terms and a ratio of determinants of prior/posterior scatter matrices R_0, R (Kuipers et al., 2014).

- ▶ Markov equivalent DAGs receive the same value.
- ▶ It is usually assumed that the data are approximately Gaussian, as the BGe score and other Gaussian DAG scores are fast to compute; limited work on non-Gaussian DAG scores.

Ingredients: Orders

- ▶ We move away from MCMC on the space of graphs to the space of orders.
- ▶ Using the order space:
 - ▶ Allows for "larger" moves than using the graph space.
 - ▶ Reduces the computation complexity to $O(p^K)$ (K is the max index)

Multiple DAGs for the same order



- ▶ Each graph has arrows only from earlier to later nodes in $\prec$, that is from right to left in this layout.
- ▶ Hence $G_1, G_2, G_3 \in \mathcal{G}_{\prec}$ even though their edge sets differ.

Ingredients: Restricted spaces

- ▶ Let $\mathcal{H} = (V, E_{\mathcal{H}})$ denote the restricted space, with corresponding adjacency matrix H (where $H_{ji} = 1$ if $j \rightarrow i \in \mathcal{H}$) and $\mathbf{h}^i = \{X_j : H_{ji} = 1\}$.
- ▶ Index (number of parents) is restricted to be less than K
- ▶ The admissible DAGs are $\mathcal{G}_{\mathcal{H}} := \{G : G = (V, E_G) \in \mathbb{G}_p, E_G \subseteq E_{\mathcal{H}}\}$.
- ▶ [Kuipers et al. 2021](#) use a *restricted search space* estimated via constraint-based methods in a hybrid setup. The restricted space is allowed to grow until a stopping rule is met. Samples are collected using the final space.

Hybrid sampler in the order space

- ▶ The posterior for order $\prec$ is proportional to the score $R(\prec | D)$

$$\pi_{Ord}(\prec | D) \propto R(\prec | D)$$

$$\propto \sum_{G \in \mathcal{G}_{\prec}} \pi_{DAG}(G | D) \propto \prod_{i=1}^p \sum_{\mathbf{Pa} \in \mathbf{Pa}_{\prec}(i)} S(X_i, \mathbf{Pa} | D)$$

- ▶ When using a restricted space $\mathcal{H}$ the posterior becomes

$$R_{\mathcal{H}}(\prec | D) \propto \prod_{i=1}^p \sum_{\substack{\mathbf{Pa} \subseteq \mathbf{h}^i \\ \mathbf{Pa} \in \mathbf{Pa}_{\prec}(i)}} S(X_i, \mathbf{Pa} | D)$$

- ▶ Constraining scores to be on the restricted space with graph index at most K **reduces the cost of MCMC steps from $O(p^K)$ to $O(Kp)$** .
- ▶ Caveat: $R_{\mathcal{H}}$ will not be the same target as π_{Ord} .

Why restricting cuts the cost: $O(p^K) \rightarrow O(Kp)$

- ▶ Every order-score step recomputes, for each node i , the local sum over admissible parent sets of size at most K :

$$\sum_{\mathbf{Pa} \in \mathbf{Pa}_{\prec}(i)} S(X_i, \mathbf{Pa} \mid D).$$

- ▶ **Unrestricted:** node i may draw parents from any of its $\leq p - 1$ predecessors, so the number of candidate parent sets is

$$\sum_{k=0}^K \binom{p-1}{k} = O(p^K),$$

and this must be re-evaluated as the order changes.

- ▶ **Restricted space $\mathcal{H}$:** parents of i are confined to the allowed neighborhood $\mathbf{h}^i$ with $|\mathbf{h}^i| \leq K$. These subset-scores are precomputed once; a move only changes which elements of $\mathbf{h}^i$ precede i in $\prec$, an $O(K)$ update per node.
- ▶ Over the p nodes,

$$\underbrace{O(p^K)}_{\text{search over all } p \text{ variables}} \longrightarrow \underbrace{O(Kp)}_{\text{search within } \mathbf{h}^i, |\mathbf{h}^i| \leq K}.$$

Theoretical results

- ▶ Cao et al. (2019): DAG-Wishart priors yield **strong graph-selection consistency** and posterior contraction for the precision matrix, with p allowed to grow, **given a known topological order**.
- ▶ Lee et al. (2019): an empirical sparse Cholesky prior attains **minimax** (or nearly minimax) posterior rates for Cholesky factors, under weaker conditions on dimension, sparsity and signal; model-selection consistency still assumes a known order.
- ▶ Castelletti et al. (2018): score **essential graphs** (CPDAGs) directly with an objective fractional Bayes factor — closed-form marginal likelihood — and explore sparse EG space by MCMC, so the target is the Markov equivalence class rather than a single DAG.
- ▶ Zhou and Chang (2023): random-walk Metropolis–Hastings on **sparse equivalence classes** mixes in time polynomial in n and p , and an empirical Bayes model is strongly consistent. Mixing of order MCMC is largely open.

MCMC Sampling of DAGs via Birth-death processes

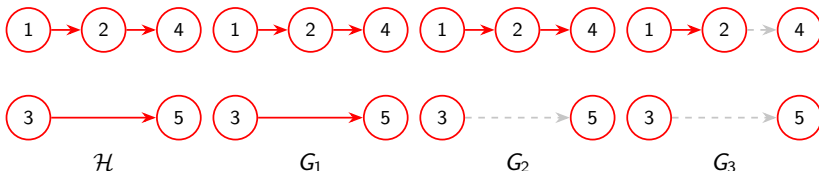
Restricted Over Order Distributions (BROOD)

- ▶ MCMC algorithms for graphs can vary in 3 key ways
- ▶ The score function used
 - ▶ We use decomposable BGe scores
- ▶ The state space used
 - ▶ The state space is restricted ($\mathcal{H}$) but allowed to vary
 - ▶ We work in the order space and the graph space alternating
 - ▶ Sample $\prec \sim \pi_{Ord}(\prec | D, \mathcal{H})$
 - ▶ **Sample $G \sim \pi_{DAG}(G | \prec, D, \mathcal{H})$**
- ▶ The move proposal setup is to alternate between moves in:
 - ▶ the order space given a restricted space
 - ▶ the set of restricted spaces

Compatible graphs for $\mathcal{H}$ and $\prec$

$$\prec = (1, 2, 3, 4, 5), \quad E_{\mathcal{H}} = \{1 \rightarrow 2, 2 \rightarrow 4, 3 \rightarrow 5\}.$$

- Think of $\mathcal{H}$ as a small graph of **allowed** edges.
- A compatible DAG $G \in \mathcal{G}_{\mathcal{H}, \prec}$ keeps a subset of the edges in $E_{\mathcal{H}}$: it may **drop** some allowed edges but never adds new ones.

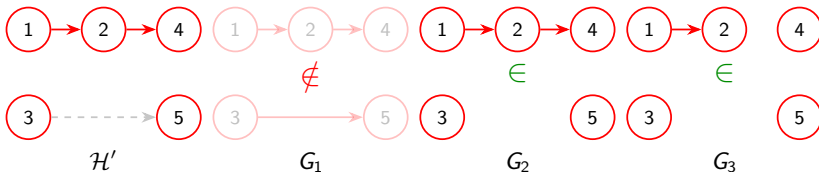


Solid red edges are kept; gray dashed edges are dropped. Each G keeps a subset of the edges of $\mathcal{H}$.

Changing the space: Removing one edge restricts the compatible set

$$E_{\mathcal{H}'} = E_{\mathcal{H}} \setminus \{3 \rightarrow 5\}.$$

- ▶ The edge $3 \rightarrow 5$ is no longer admissible.
- ▶ Every graph that **used** $3 \rightarrow 5$ now drops out of the compatible set; the rest survive.

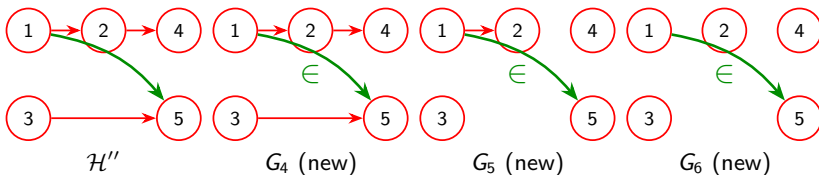


The move $\mathcal{H} \mapsto \mathcal{H}'$ changes the sum from $\sum_{G \in \mathcal{G}_{\mathcal{H}}}$ to a smaller $\sum_{G \in \mathcal{G}_{\mathcal{H}'}}$.

Adding one edge enlarges the compatible set

$$E_{\mathcal{H}''} = E_{\mathcal{H}} \cup \{1 \rightarrow 5\}.$$

- ▶ The new edge $1 \rightarrow 5$ (in green) becomes admissible.
- ▶ Graphs that **use** $1 \rightarrow 5$ were impossible before; they now enter the compatible set.



The move $\mathcal{H} \mapsto \mathcal{H}''$ changes the sum from $\sum_{G \in \mathcal{G}_{\mathcal{H}}}$ to a larger $\sum_{G \in \mathcal{G}_{\mathcal{H}''}}$.

Cost of restricting: Order space

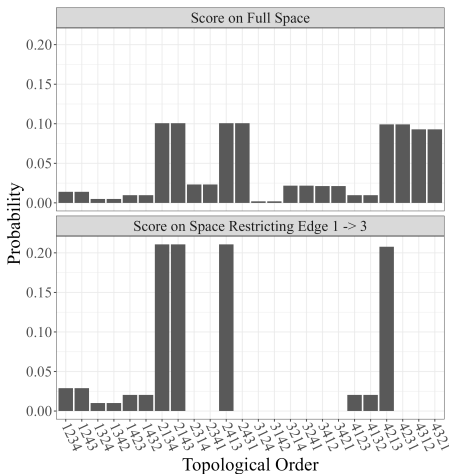


Figure: 4-node example: order posterior for the full search space (top) vs. the restricted space (bottom), where the edge $1 \rightarrow 3$ is excluded.

MCMC on restricted spaces

- **Theorem 1** Let $\mathcal{H} \in \mathbb{D}_p$ be a restricted space with corresponding edge set $E_{\mathcal{H}}$ and admissible DAG set $\mathcal{G}_{\mathcal{H}}$. Let π_{DAG}, π_{Ord} denote the posterior distributions over DAGs and orders, respectively, using the full DAG space $\mathbb{G}_p$, and let $\pi_{Ord}^{(\mathcal{H})}$ be the posterior over orders restricted to $\mathcal{G}_{\mathcal{H}}$. Define $\varepsilon_{\mathcal{H}} := 1 - \pi_{DAG}(\mathcal{H}|D)$ as the posterior mass assigned to DAGs outside of $\mathcal{H}$. Then, for some constant $c \in [0, 1]$,

$$1 - \sqrt{1 - c\varepsilon_{\mathcal{H}}} \leq D_{TV}(\pi_{Ord}^{(\mathcal{H})}, \pi_{Ord}) \leq \min \left(\sqrt{2 - 2\sqrt{1 - c\varepsilon_{\mathcal{H}}}}, 1 \right)$$

where D_{TV} denotes the total variation distance between distributions.

- Shows errors are incurred but is of limited use in algorithmic design.

Challenges

- ▶ We consider moves that grow AND shrink $\mathcal{H}_t$
- ▶ By varying $\mathcal{H}_t$ we aim to reduce the error established in Theorem 1
- ▶ The restricted spaces $\mathcal{H}_t$ are of varying dimension
- ▶ Of interest is the stationary distribution on $(\mathbf{H}, \mathbf{O}) \in \mathbb{D}_p \times \mathbb{S}^p$
- ▶ This requires theoretical validation.

A sampler with varying state spaces

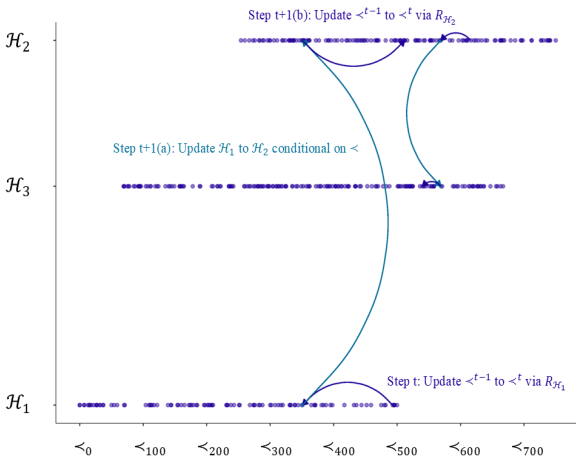


Figure: Illustration of the BROOD Algorithm

Sampling via Restricted MCMC

- ▶ We need to sample:

Step H Challenging: sample the restricted space ($\mathcal{H}$) conditional on the order ($\prec$).

Step O Sample order given the restricted space

Step G Finally, given the restricted space and the order, sample from the set of graphs compatible with both $\mathcal{H}$ and $\prec$.

- ▶ We rely on the framework developed by [Geyer and Møller \(1994\)](#)
- ▶ Consider the MH algorithm sampling on $(\mathcal{H}, \prec) \in \mathbb{D}_p \times \mathbb{S}^p$ that is a mixture of 2 transition kernels:

$$Q_\ell(\mathcal{H}, \prec | \mathcal{H}_t, \prec_t) = (1 - \ell)Q_0(\prec | \mathcal{H}_t, \prec_t) + \ell Q_1(\mathcal{H} | \mathcal{H}_t, \prec_t) \quad 0 \leq \ell \leq 1$$

- ▶ Q_0 is a standard MH procedure concentrated on $\mathcal{H}_t$ for Step 0.
- ▶ Q_1 is concentrated on $H_{m_t-1} \cup H_{m_t} \cup H_{m_t+1}$ where $\mathcal{H}_t \in H_{m_t}$ and the index m_t denotes the number of edges.

The development steps

- ▶ Given the current state $(\mathcal{H}, \prec)$
- ▶ Construct a birth and death process with rates $\beta(\mathcal{H}, \prec)$ and $\delta(\mathcal{H}, \prec)$ that has a stationary distribution.
- ▶ Define a MH algorithm with acceptance probabilities that depend on β and δ
- ▶ Ergodicity follows from the work of [Geyer and Møller \(1994\)](#) (see also [Preston, 1977](#)).

Sampling via Restricted MCMC

Theorem 2: Let $\mathcal{H} \in \mathbb{D}_p$, and $\prec \in \mathbb{S}^p$. Define $B_e(\mathcal{H}, \prec)$ and $D_e(\mathcal{H}, \prec)$ as follows:

$$B_e(\mathcal{H}, \prec) \propto \frac{\frac{1}{|\mathcal{G}_{\mathcal{H}^+e}|} \pi_{DAG}(\mathcal{H}^{+e} | \prec, D)}{\frac{1}{|\mathcal{G}_{\mathcal{H}}|} \pi_{DAG}(\mathcal{H} | \prec, D)} = \frac{1}{2} \frac{\pi_{DAG}(\mathcal{H}^{+e} | \prec, D)}{\pi_{DAG}(\mathcal{H} | \prec, D)}$$

$$D_e(\mathcal{H}, \prec) \propto \frac{\frac{c^*}{|\mathcal{G}_{\mathcal{H}^-e}|} \pi_{DAG}(\mathcal{H}^{-e} | \prec, D)}{\frac{1}{|\mathcal{G}_{\mathcal{H}}|} \pi_{DAG}(\mathcal{H} | \prec, D)} = 2c^* \frac{\pi_{DAG}(\mathcal{H}^{-e} | \prec, D)}{\pi_{DAG}(\mathcal{H} | \prec, D)}$$

where $c^* \in (0, 1]$. Let

$$\beta(\mathcal{H}, \prec) = \sum_{e \notin E_{\mathcal{H}}} B_e(\mathcal{H}, \prec)$$

$$\delta(\mathcal{H}, \prec) = \sum_{e \in E_{\mathcal{H}}} D_e(\mathcal{H}, \prec).$$

Then, a birth-death process defined by the rates β, δ yields a unique solution with a limit that is a tractable probability distribution.

Towards MCMC with varying $\mathcal{H}$

Corollary

Construct a birth-death Markov process $(\mathbf{H}, \mathbf{O}) \in \mathbb{D}_p \times \mathbb{S}^p$ with the birth and death rates specified in Theorem 2. Then, the marginal in $\mathcal{H} \in \mathbb{D}_p$ of the stationary distribution admits the following form:

$$\mu_{Space}^{(c^*)}(\mathcal{H}) \propto (2c^*)^{-|E_{\mathcal{H}}|} \sum_{\prec \in \mathbb{S}^p} \pi_{DAG}(\mathcal{H} | \prec, D), \quad (1)$$

where $\pi_{DAG}(\mathcal{H} | \prec, D) = \sum_{G \in \mathcal{G}_{\mathcal{H}}} \pi_{DAG}(G | \prec, D)$.

Putting it all together

Theorem 3: Let μ be a trans-dimensional probability measure that is compatible with a birth-death process defined by rates β, δ . Then $r(x, \xi)$, the acceptance ratio in the mixture kernel sampler of [Geyer and Møller \(1994\)](#), is defined by :

$$r(x, \xi) = \frac{\frac{1}{\beta(x \cup \xi) + \delta(x \cup \xi)}}{\frac{1}{\beta(x) + \delta(x)}}$$

Time reversibility is ensured with the following acceptance rates:

$$\begin{aligned} \text{death} \rightarrow A_1(x \mid x \cup \xi) &= \begin{cases} \min\{1, 1/r(x, \xi)\} & \text{if } x \cup \xi \in H, \\ 0 & \text{otherwise} \end{cases} \\ \text{birth} \rightarrow A_1(x \cup \xi \mid x) &= \begin{cases} \min\{1, r(x, \xi)\} & \text{if } x \cup \xi \in H, \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

Dealing with the order-induced bias

- ▶ BROOD returns triples $(\mathcal{H}_t, \prec_t, G_t)$: the space comes from the birth-death kernel, and then $\prec_t \sim \pi_{\text{Ord}}(\prec | \mathcal{H}_t, D) \propto R_{\mathcal{H}_t}(\prec | D)$ and $G_t \sim \pi_{\text{DAG}}(G | \prec_t, \mathcal{H}_t, D)$.
- ▶ Each order is drawn **conditionally on the space**, so the sampling law of a triple is

$$q(\mathcal{H}, \prec, G) = \mu_{\text{Space}}^{(c^*)}(\mathcal{H}) \frac{R_{\mathcal{H}}(\prec | D)}{Z_{\mathcal{H}}} \frac{S(G | D) \mathbb{1}\{G \in \mathcal{G}_{\mathcal{H}, \prec}\}}{R_{\mathcal{H}}(\prec | D)}.$$

- ▶ The score $S(G | D) = \prod_{i=1}^p S(X_i, \mathbf{Pa}_G(i) | D) \propto \pi_{\text{DAG}}(G | D)$ carries **no** $\prec$: the order enters only through the admissible set and the normalizers $R_{\mathcal{H}}(\prec | D) = \sum_{G \in \mathcal{G}_{\mathcal{H}, \prec}} S(G | D)$ (which cancels) and $Z_{\mathcal{H}} = \sum_{\prec} R_{\mathcal{H}}(\prec | D)$.

Dealing with the order-induced bias

- ▶ Since $\mathcal{G}_{\mathcal{H}, \prec} = \mathcal{G}_{\mathcal{H}} \cap \mathcal{G}_{\prec}$, the space does not change which orders admit a given G : $\sum_{\prec} \mathbb{1}\{G \in \mathcal{G}_{\mathcal{H}, \prec}\} = n(G)$ for $G \in \mathcal{G}_{\mathcal{H}}$, so

$$q(\mathcal{H}, G) = \mu_{\text{Space}}^{(c^*)}(\mathcal{H}) \frac{n(G) S(G | D)}{Z_{\mathcal{H}}}, \quad n(G) = |\{\prec \in \mathbb{S}^p : G \in \mathcal{G}_{\prec}\}|.$$

- ▶ Both multiplicities favour sparsity: a sparse G has **more** compatible orders and sits in **more** restricted spaces.
- ▶ When using the form of $\mu_{\text{Space}}^{(c^*)}(\mathcal{H})$, each draw is reweighted by

$$w_t = \frac{(2c^*)^{|E_{\mathcal{H}_t}|}}{n(G_t) M(G_t)}, \quad \hat{\mathbb{E}}[f(G)] = \frac{\sum_t w_t f(G_t)}{\sum_t w_t},$$

where $M(G) = |\{\mathcal{H} \in \mathbb{D}_p : E_G \subseteq E_{\mathcal{H}}\}| = \prod_{i=1}^p \sum_{k=d_i}^K \binom{p-1-d_i}{k-d_i}$ counts the spaces admitting G , with $d_i = |\mathbf{Pa}_G(i)|$.

Oil returns and geopolitical risk

- ▶ Daily WTI oil prices and the geopolitical risk (GPR) index of [Caldara and Iacoviello \(2022\)](#), recorded from 1986/01/02 to 2026/04/20.

- ▶ Let $r_n = \log(\text{Oil}_{n+1}) - \log(\text{Oil}_n)$. The object of interest is the transition

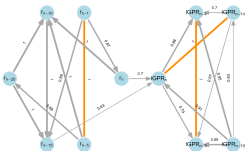
$$p(r_n \mid r_{n-1}, r_{n-5}, r_{n-10}, r_{n-15}, r_{n-20}, \ell\text{GPR}_n, \ell\text{GPR}_{n-4}, \dots, \ell\text{GPR}_{n-19}),$$

with $\ell\text{GPR} = \log(\text{GPR})$.

- ▶ Median graphs contain only those edges $u \rightarrow v$ such that $p_{u \rightarrow v} + p_{v \rightarrow u} \geq 0.5$.
- ▶ If one of those probabilities is greater than 0.6 the edge is directed.

Oil returns and geopolitical risk

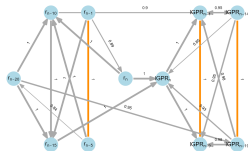
Full Space Sampler



Edge Type $\rightarrow$ Directed ($p > 0.6$) $\rightarrow$ Undirected (Sum $p > 0.5$)

(Note: IGPR denotes $\log(GPR)$)

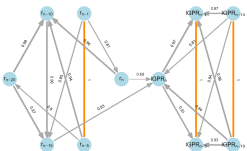
BiDAG Hybrid Sampler



Edge Type $\rightarrow$ Directed ($p > 0.6$) $\rightarrow$ Undirected (Sum $p > 0.5$)

(Note: IGPR denotes $\log(GPR)$)

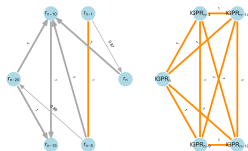
BiDAG with Ad-Hoc Plus-1 Graph Sampling



Edge Type $\rightarrow$ Directed ($p > 0.6$) $\rightarrow$ Undirected (Sum $p > 0.5$)

(Note: IGPR denotes $\log(GPR)$)

BROOD with B-D Kernels



Edge Type $\rightarrow$ Directed ($p > 0.6$) $\rightarrow$ Undirected (Sum $p > 0.5$)

(Note: IGPR denotes $\log(GPR)$)

Improving BROOD

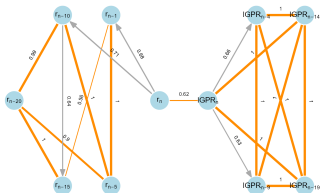
- ▶ We explore a **symmetric** kernel in which birth/death are proposed with prob $1/2$.
- ▶ The acceptance ratio for a proposed birth is

$$\alpha_{\text{sym}}(H \rightarrow H^{+e}) = \min\{1, \beta(H)/\delta(H^{+e})\}.$$

- ▶ We also consider a **symmetric momentum** kernel that acts on (H, v) with $v \in \{+1, -1\}$ and targets $\tilde{\mu}(H, v) = \frac{1}{2}\mu(H)(\mathbf{1}_{\{v=-1\}} + \mathbf{1}_{\{v=1\}})$.
If $v_t = +1$: propose birth only and accept with same probability as above. Accept $\Rightarrow v_{t+1} = +1$; Reject $\Rightarrow v_{t+1} = -1$ and state becomes $(H, -1)$.
- ▶ These yield cleaner median graphs and more decisive edge probabilities.
- ▶ Within-series dependence in the r lags and in the ℓ GPR lags is recovered more sharply; the contemporaneous r_n - ℓ GPR $_n$ link is weaker and often undirected.

Improving BROOD

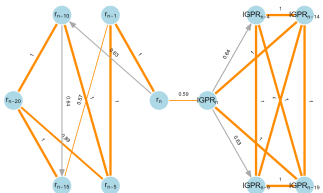
BROOD with Symmetric Kernels



Edge Type → Directed ($p > 0.6$) → Undirected (Sum $p > 0.5$)

Note: IGPR den.

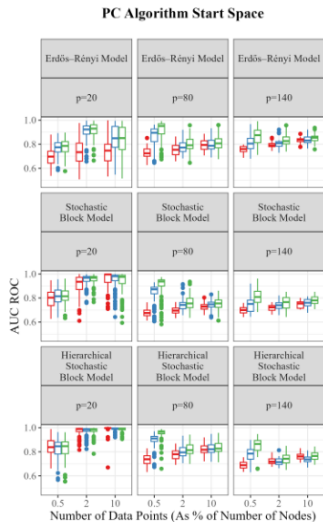
BROOD with Symmetric Momentum Kernels



Edge Type → Directed ($p > 0.6$) → Undirected (Sum $p > 0.5$)

Note: IGPR denotes $\log(GPR)$

Simulation results

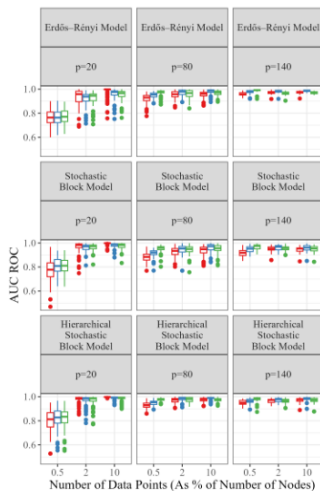


Type

- BiDAG with PC Search Space
- BROOD with PC Start Space
- BROOD+ with PC Start Space

Simulation results - fixed sparsity

Kuipers et al. Expansion Start Space



Type

- BiDAG with MAP Search Space
- BROOD with MAP Start Space
- BROOD+ with MAP Start Space

- ▶ What did we learn?
 - ▶ We lose the intuition given in Euclidian spaces by distances
 - ▶ Space is discrete but enormous and missing "parts" of it can be consequential
 - ▶ Theory for such samplers is challenging, but badly needed.
- ▶ What do we want to know?
 - ▶ In most examples we must impose restrictions on directionality
 - ▶ Incorporate auxiliary information about the nodes and their interrelationships
 - ▶ Design an adaptive version so tuning parameters, say c^* , are optimized?
 - ▶ Integrate everything into downstream data analysis...
- ▶ Paper available here: raducraiu.com/publications/

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