ETH zürich

Marginalization in Bayesian Networks: Integrating Exact and Approximate Inference

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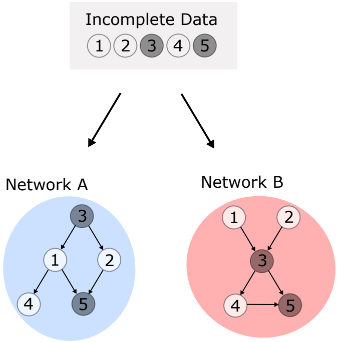
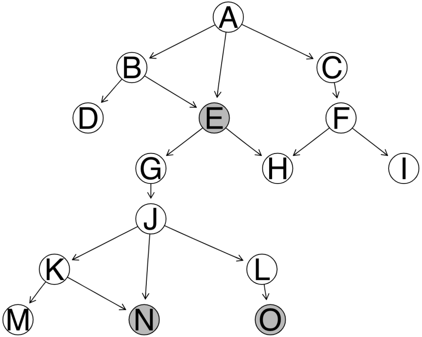
Example Classification of Cancer Subgroups

- Assume data is clustered into groups, e.g. cancer subgroups
- Classification of data against the clusters



Introduction to Bayesian Networks
(Categorical Case)

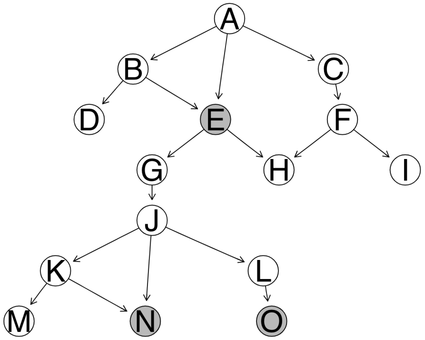
- Most popular causal model
- Allows graphical interpretation
- Challenges
  - Learning the graph structure (NP-hard)
  - Marginalization (NP-hard)
- Missing data requires marginalization



Introduction to Bayesian Networks

- DAG $\mathcal{G} = (V, E)$ with nodes V and edges E
- Nodes V are associated with variables X_V with probability distribution $P(X_V)$
- Factorization (Markov conditions)

$$P(X_V) = \prod_{i \in V} P\big(X_i \mid X_{pa(i)}\big)$$



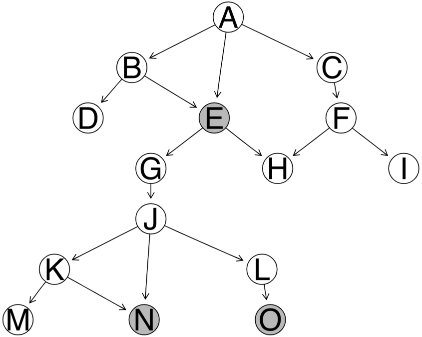
Marginalization in Bayesian Networks
(Categorical Case)

- Let $e \subseteq V$ be evidence nodes, e.g. observed variables
- Marginal probability distribution

$$P(X_e) = \sum_{X_{V'}} P(X_{V'}, X_e)$$

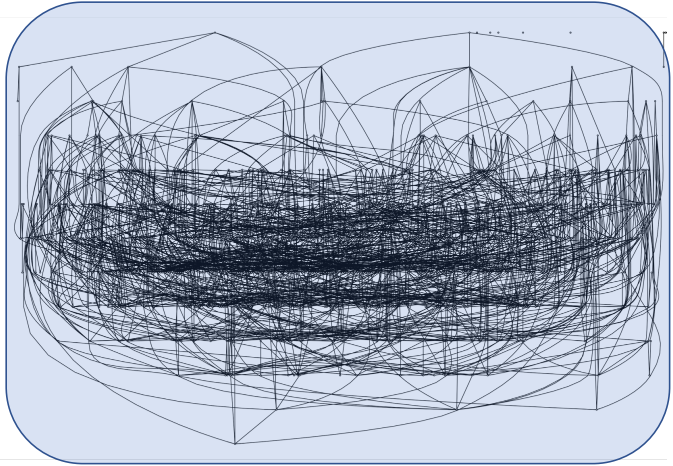
by summing over $V' = V \setminus e$

$\Rightarrow$ Problem is NP-hard



Example of Highdimensional Bayesian Network

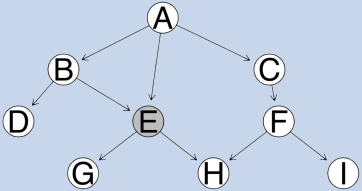
Approximate inference in blue



Reduction of Sampled Variables

Definition (Irrelevant Node)

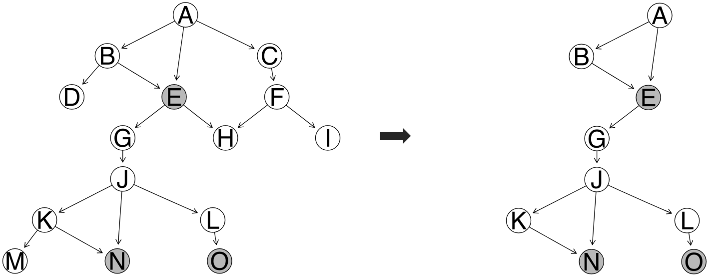
A node $i \in V$ in a DAG $\mathcal{G} = (V, E)$ over X_V is irrelevant w.r.t. a set of nodes e if $\Big(\{i\} \cup de(i)\Big) \cap e = \emptyset$.



Reduction of Sampled Variables

Definition (Relevant Subgraph)

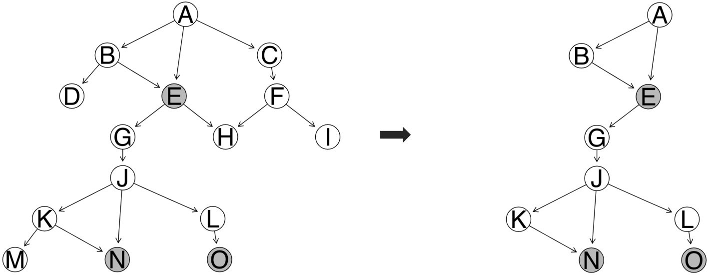
The relevant subgraph $\mathcal{G}'$ of a DAG $\mathcal{G}$ w.r.t. a set of nodes e is the remaining graph after removal of all irrelevant nodes and their edges.



Reduction of Sampled Variables

Proposition (Marginalization over Relevant Subnetwork)

Let $\mathcal{G}'$ be the relevant subnetwork of a DAG $\mathcal{G}$ w.r.t. a set of variables x_e and let $p_{\mathcal{G}'}$ and $p_{\mathcal{G}}$ be the respective probability distributions that satisfy the Markov properties. Then $p_{\mathcal{G}'}(x_e) = p_{\mathcal{G}}(x_e)$.

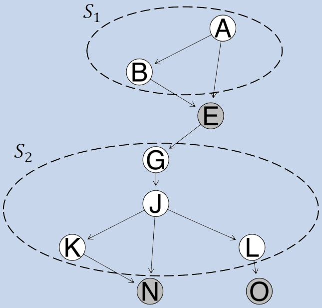


Marginalization in Bayesian Networks

Definition (Conditionally Independent Subset)

Let $U \subset V$. A set of variables $X = \{X_u : u \in U\}$ is a conditionally independent subset w.r.t. a set of variables x_e, if

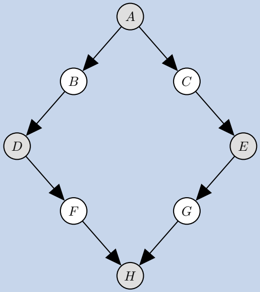
- *all variables in the subset are d-connected, i.e. X_i is d-connected to X_j w.r.t. $e \, \forall i, j \in U$, and*
- *all variables in the subset are d-separated from the remaining variables, i.e. X_i is d-separated from X_j w.r.t. $e \, \forall i \in U, j \in V \setminus \{U \cup e\}$.*



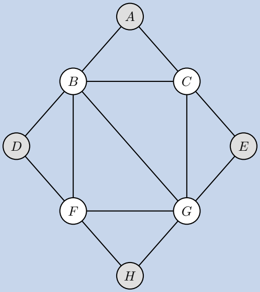
Example for Complexity Reduction
In Junction-Tree Algorithm

Get Moral Graph of a DAG: 1. Moralization, 2. Triangulation

Original DAG

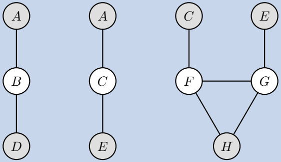


Moral Graph



→ Five additional edges

Moral Graph with SGS



→ One additional edge

Subgroup Separation

Proposition (Marginalization in Subsets)

Let $\mathcal{G}'$ be the relevant subnetwork of a DAG $\mathcal{G}$ w.r.t. a set of nodes e. Let $S = \{S_1, ..., S_n\}$ be the conditionally independent subsets of the relevant subnetwork. Then

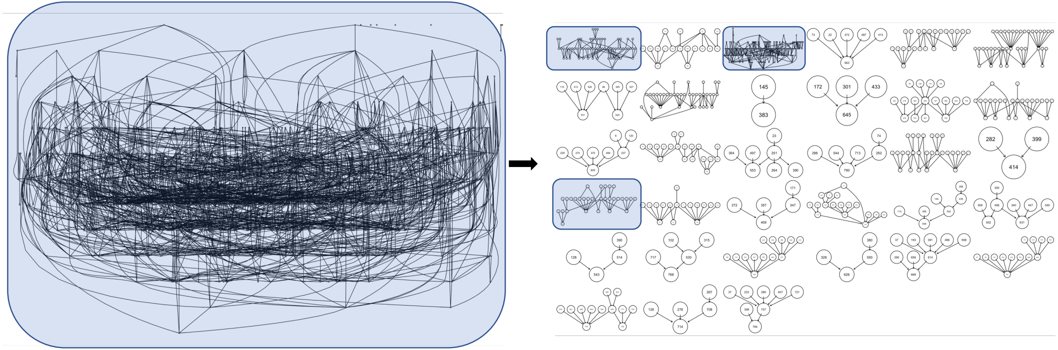
$$P(X_e) = P\left(X_{e'}\right) \underbrace{\prod_{S_i \in S_{\text{exact}}} \sum_{X_{S_i}} P\left(X_{S_i}, X_{e_i^{ch}} \mid X_{e_i^{mb} \setminus e_i^{ch}}\right)}_{\text{exact inference}} \underbrace{\prod_{S_j \in S_{\text{approx}}} \mathbb{E}_{Q\left(X_{S_j}\right)} \left[\frac{P\left(X_{S_j} \mid X_{e_j^{mb}}\right) P\left(X_{e_j^{ch}} \mid X_{S_j}\right)}{Q\left(X_{S_j}\right)} \right]}_{\text{approximate inference}}$$

where $e_i^{mb} = e \cap \{mb(u) : u \in S_i\}$, $e_i^{ch} = e \cap \{ch(u) : u \in S_i\}$ and $e' = e \setminus \{e_i^{ch} \, \forall i\}$.

Example of Highdimensional Bayesian Network

Subgroup Separation

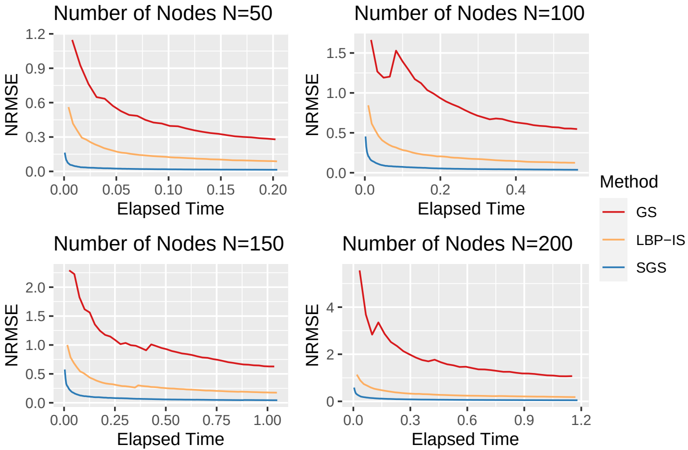
Approximate inference in blue



Benchmark Results
Over Varying Dimensions

- Simulated DAGs
  (100 DAGs, 10 iterations)
- Evidence at random

$$NRMSE =$$
$$\sqrt{\frac{\sum_{i=1}^{n}(P(X_e) - \mathbb{E}_i[P(X_e)])^2}{n}} \cdot P(X_e)^{-1}$$



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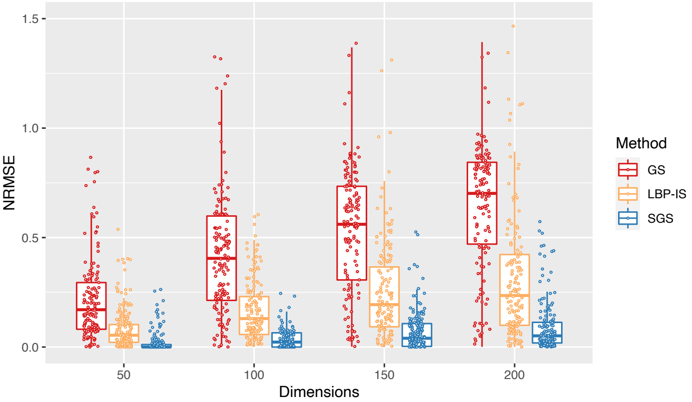
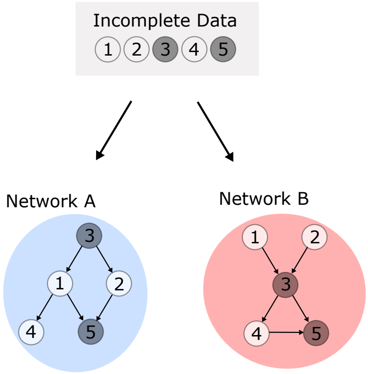


Application
Classification of Cancer Subtypes

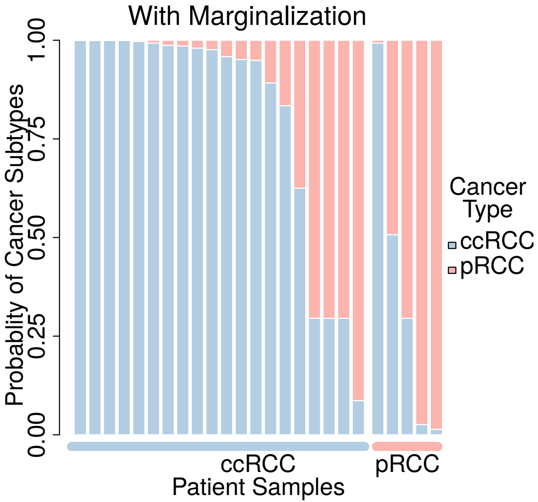
- Determine the cancer subtype of kidney cancer samples
- Patient samples from Korean population study
- Diagnosed with renal cell carcinoma (RCC)
  - Clear cell RCC (ccRCC)
  - Papillary RCC (pRCC)



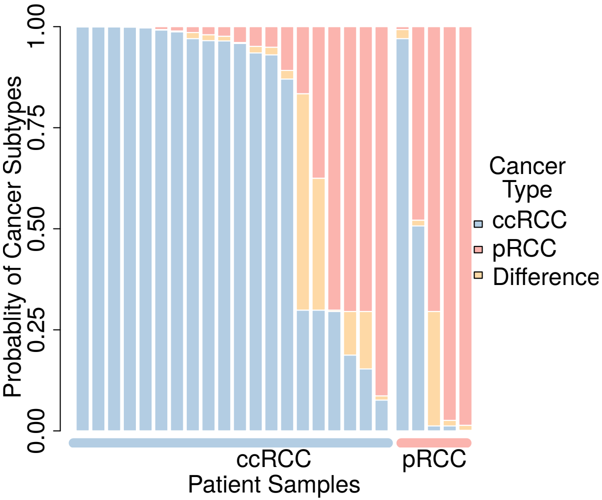
Application Results
Classification of Cancer Subtypes

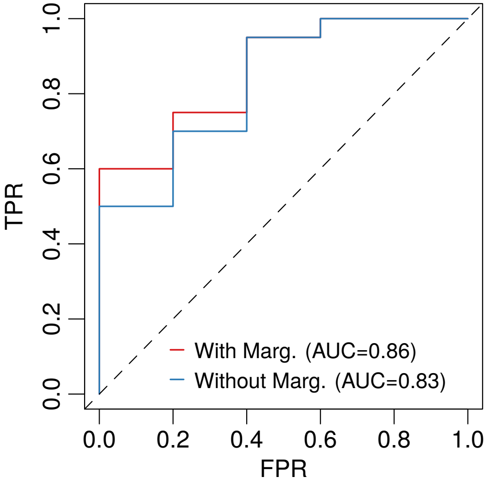
Ratios of correctly assigned cancer type

- 68 % without marginalization
  (cluster 26 genes, classify 26 genes)
- 76 % with marginalization
  (cluster 70 genes, classify 26 genes)
- 83 % with complete data from TCGA
  (cluster 70 genes, classify 70 genes)



Application
Classification of Cancer Subtypes



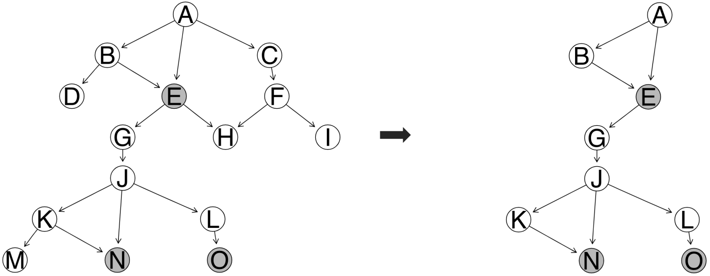


Standard Inference Methods

Standard approximate inference problem
Find probability of a single variable $P(X_i \vert X_e)$

Marginal probability distribution
Find probability of multiple variables $P(X_1, ..., X_n \vert X_e)$ (or $P(X_e)$)

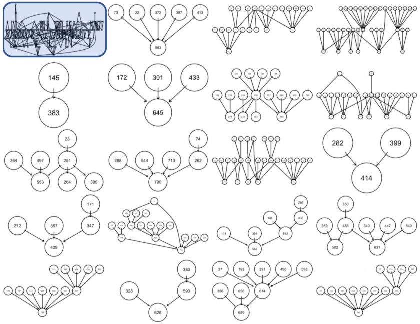
Not easy to unify because $P(X_1, ..., X_n|X_e) \neq \prod_i P(X_i|X_e, X_{pa(i)})$



Conclusion

- Marginalization in Bayesian networks
  - Present efficient method
  - Allows to handle missing data
  - R package **SubGroupSeparation**

- Separation to subgroups can be generalized to other approximate inference schemes



Thank you for your attention!

Preprint: https://arxiv.org/pdf/2112.09217.pdf
Code: https://github.com/cbg-ethz/SubGroupSeparation

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