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# AVERAGING OF DECOMPOSABLE GRAPHS BY DYNAMIC PROGRAMMING AND SAMPLING

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We present algorithms for Bayesian learning of decomposable models from data. Priors of a certain form admit exact averaging in $O(3^n n^3)$ time and sampling $T$ graphs from the posterior in $O(4^n + nT)$ time. To target a broader class of priors we associate each sample with an importance weight. Empirically, we compare averaging to optimization and demonstrate the accuracy of our importance sampling estimates.

## PROBLEM

### DECOMPOSABLE MODEL

- Undirected graph $\mathcal{G}$ on $V = \{1, \ldots, n\}$ with a *junction tree*.
- A joint distribution $p(x_1, \ldots, x_n)$ that factorizes as

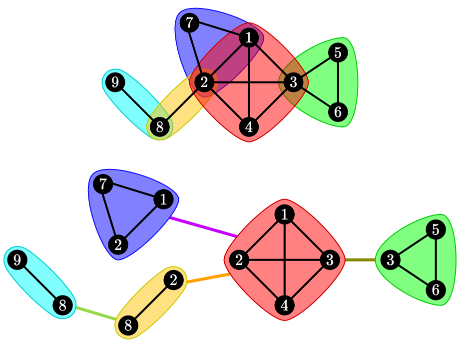
$$p(x_V) = \frac{\prod_{C \in \mathcal{C}} p(x_C)}{\prod_{S \in \mathcal{S}} p(x_S)},$$

where

$\mathcal{C}$ is the set of *cliques* of $\mathcal{G}$,

$\mathcal{S}$ is the multiset of *separators*,

$x_C = (x_v : v \in C)$.



$$\frac{\varphi_c(2,8)\varphi_c(1,2,7)\varphi_c(8,9)\varphi_c(1,2,3,4)\varphi_c(3,5,6)}{\varphi_s(8)\varphi_s(1,2)\varphi_s(2)\varphi_s(3)}$$

### BAYESIAN LEARNING

**Problem:** Compute the *marginal*

$$Z_\varphi = \sum_{\mathcal{G}} \varphi(\mathcal{G}),$$

where $\varphi$ is a *decomposable function*, i.e.,

$$\varphi(\mathcal{G}) = \frac{\prod_{C \in \mathcal{C}} \varphi_c(C)}{\prod_{S \in \mathcal{S}} \varphi_s(S)}, \quad \varphi_c, \varphi_s : 2^V \to \mathbb{R}.$$

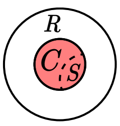
**Example (feature posterior probability):** The posterior probability of a feature $\psi(\mathcal{G})$ is the expectation $\mathrm{E}(\psi(\mathcal{G}) \mid \text{data}) = Z_{\pi\psi}$ where $\pi(\mathcal{G}) \propto \Pr(\text{data} \mid \mathcal{G}) \Pr(\mathcal{G})$.

## EXACT AVERAGING

Computing $Z_\varphi$ for a decomposable $\varphi$ is doable up to $n \simeq 8$. It is more efficient to compute

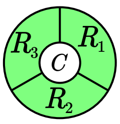
$$Z_{\varphi\tau} = \sum_{\mathcal{G}} \varphi(\mathcal{G}) \tau(\mathcal{G}),$$

where $\tau(\mathcal{G})$ denotes the number of rooted junction trees of $\mathcal{G}$. We get $Z_{\varphi\tau} = f(\emptyset, V)$, where $f$ is obtained by adapting a recent dynamic programming algorithm [1]:



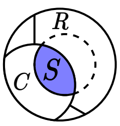

1. Given sets $S$ and $R$, choose a clique $C$ within $R$ that contains $S$ completely:

$$f(S,R) = \sum_{S \subset C \subseteq S \cup R} \varphi_c(C)\, g(C, R \setminus C)$$




2. Partition the remaining vertices into $R_1, \ldots, R_k$:

$$g(C,U) = \sum_{\min U \in R \subseteq U} h(C,R)\, g(C, U \setminus R)$$




3. For each part $R$ choose a separator $S$ contained in $C$. Recurse back to step 1:

$$h(C,R) = \sum_{S \subset C} f(S,R) / \varphi_s(S)$$

The algorithm runs in $O(4^n)$ time and $O(3^n)$ space. By using variants of fast zeta transform and fast subset convolution, we can bring the running time to $O(3^n n^3)$.

## MONTE CARLO AVERAGING

To estimate the posterior expectation $Z_{\pi\psi}$:

1. Run the exact algorithm for a $\varphi \propto \pi$.
2. Backtrack into the recurrences to draw samples $\mathcal{G}_1, \ldots, \mathcal{G}_T$ from $\pi' \propto \pi\tau$.
   (a) *Fixed bucketing*: tunable time/space tradeoff between $O(2^n)/O(3^n)$ and $O(n)/O(4^n)$; or
   (b) *Adaptive caching*: good if $\pi$ is skewed.
3. Obtain the self-normalized importance sampling estimate

$$\tilde{Z}_{\pi\psi} = \frac{\sum_{i=1}^T w_i \psi(\mathcal{G}_i)}{\sum_{i=1}^T w_i}, \quad w_i = \frac{1}{\tau(\mathcal{G}_i)}.$$

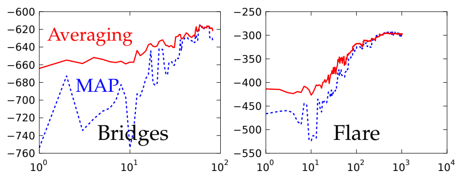
Computing $\tau(\mathcal{G}_i)$ takes $O(n^2)$ time [2].

### EXPERIMENTS

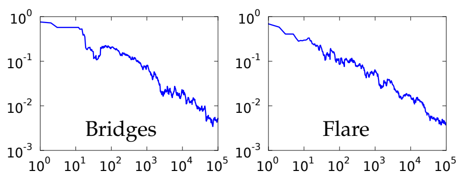
We ran our implementation [3] on datasets of a varying number of variables ($n$) and records ($m$). The table shows the seconds spent in the exact algorithm (E) and sampling $10^7$ graphs (S).

| Dataset | $n$ | $m$ | E | S |
|---|---|---|---|---|
| Asia | 8 | 10000 | 0.018 | 33 |
| Bridges | 12 | 108 | 5.6 | 54 |
| Flare | 13 | 1066 | 24 | 77 |
| Votes | 17 | 435 | 7497 | 167 |

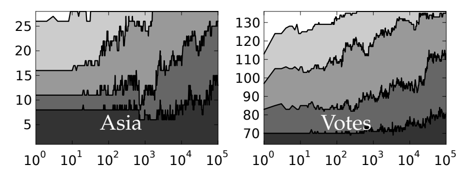
**Prediction accuracy – averaging vs. MAP:** The log probability (y-axis) of a test set for a varying amount of training data (x-axis).




**Edge posterior probabilities:** The largest estimation error over all edges (y-axis) for a varying number of samples (x-axis).




The number of edges (y-axis) with an error at most $10^{-1}$, $10^{-2}$, $10^{-3}$, and $10^{-4}$, for a varying number of samples (x-axis).




[1] K. Kangas, M. Koivisto, and T. Niinimäki. *Learning chordal Markov networks by dynamic programming*. NIPS, 2014.
[2] A. Thomas and P. J. Green. *Enumerating the junction trees of a decomposable graph*. J. Comp. Graph. Stat., 2009.
[3] *Junctor/Adjunct*. Available at www.cs.helsinki.fi/u/jwkangas/junctor.

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