Bounded Tree-Width Markov Networks

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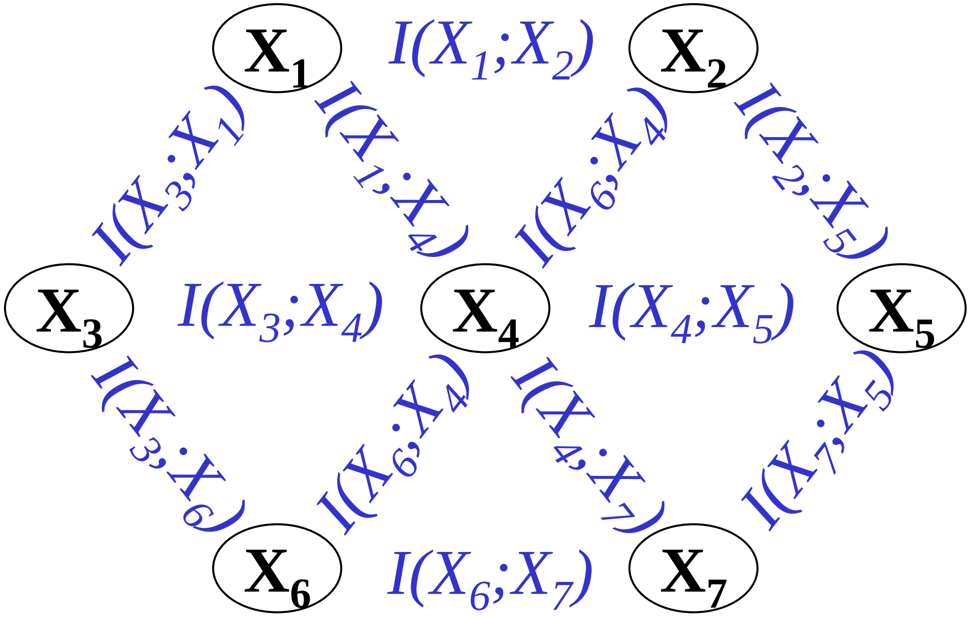
Density Estimation

- T observations of n variables $X_1..X_n$.
- Estimate distribution from which they were sampled.
- Use for inference and other calculations.

Density Estimation, not model selection.

Chow & Liu (1968): Maximum likelihood tree

Weight of an edge = mutual information between endpoints.



(not all weights shown)

Chow & Liu (1968): Maximum likelihood tree

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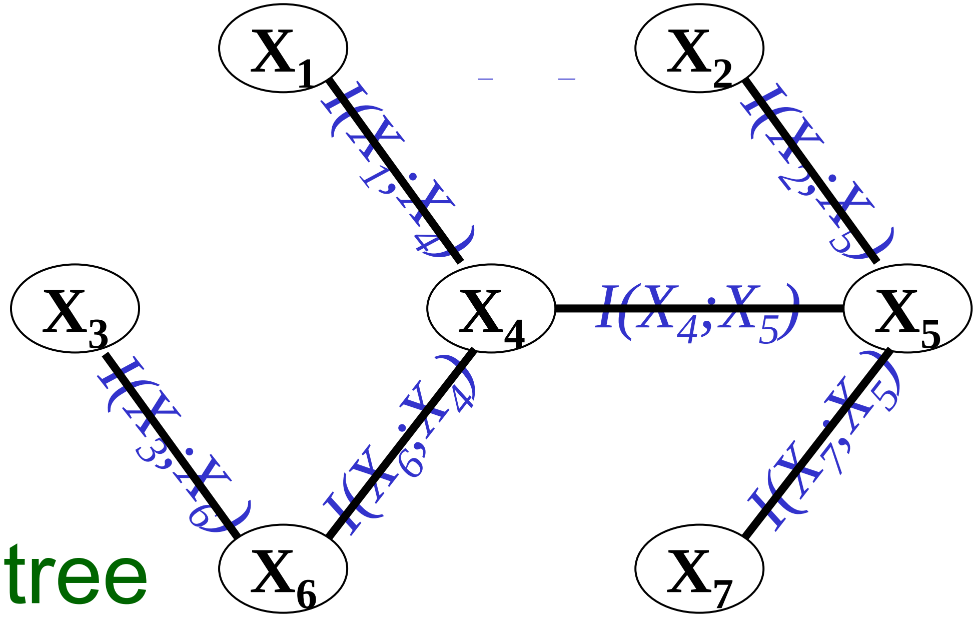

ML tree is max-weight tree

Chow & Liu (1968): Maximum likelihood tree

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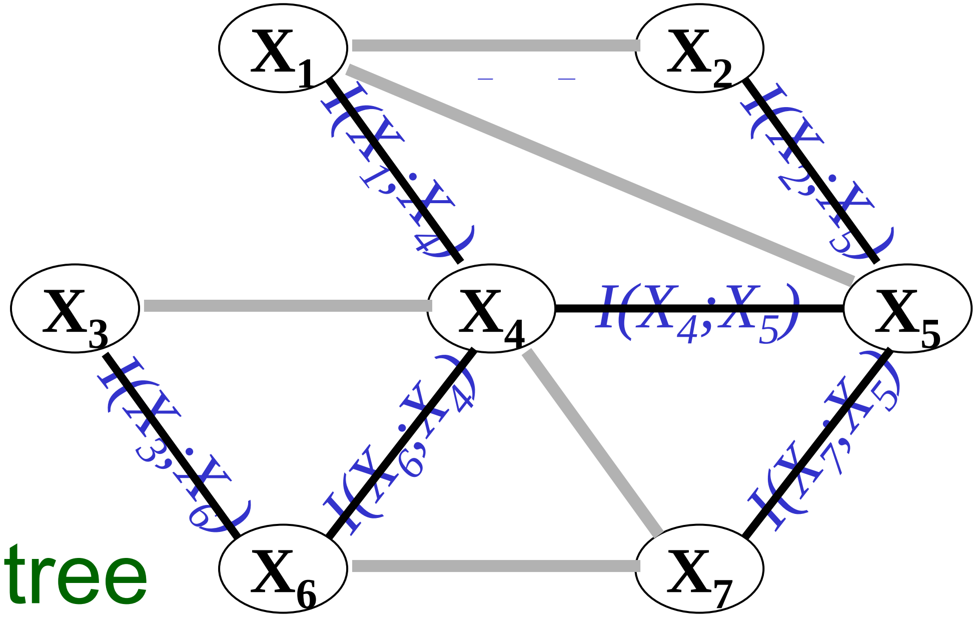


ML tree is max-weight tree

Maximum likelihood Markov network:

Empirical distribution

(Markov-net over complete graph)

Bounding the Complexity

- Small clique size.
- Even with small clicks: non-tractable.
- Tree-width of a graph: minimum over all triangulations, of the maximum clique size of the triangulation, minus one.

Problem Statement: ML Narrow Markov Networks

- For a specified k, maximum likelihood Markov network of tree-width at most k.

- Equivalently, over a triangulated graph with cliques of size at most $k+1$.

ML Narrow Markov Networks

- $k=1$: Trees (Chow and Liu)
- $k\geq 2$: Local search heuristics (eg Malvestuto, 1991)

Cast as combinatorial optimization problem:

- –Hardness
- –Provable “global” optimization algorithms
- –Understand structure

- $k=1$ (trees): ML decomposes to sum of edge weights.

- $k>1$: Would like similar decomposition
  - identify the contribution of "*local structures*"

- Edges are not enough:

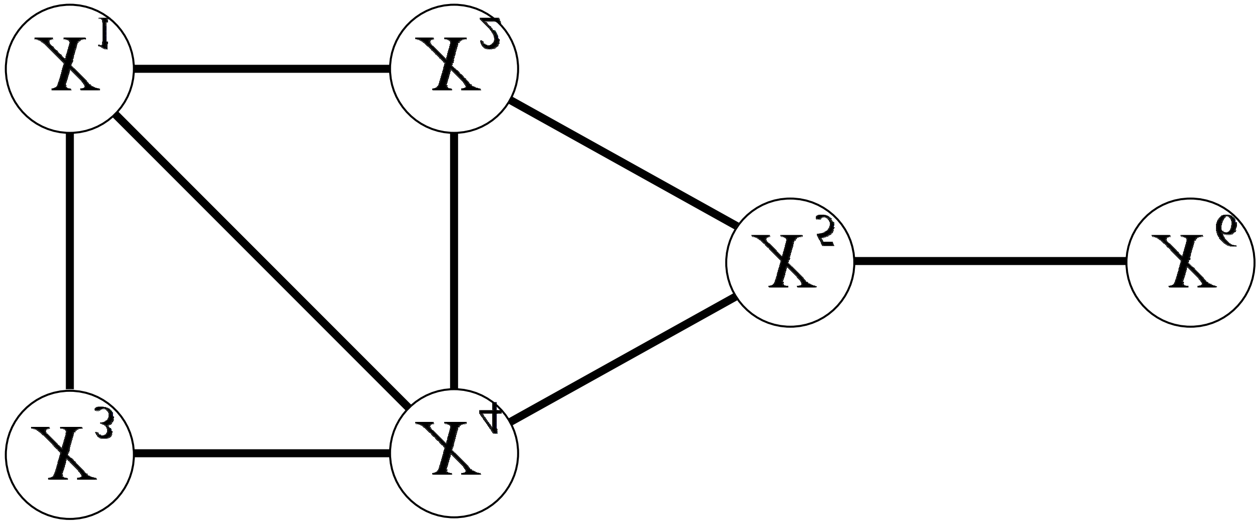
  need to consider larger cliques.

Factorization Over a Triangulated Graph G

$$P_X(x) = \prod_{h \in \mathrm{Cliques}(G)} \varphi_h(x_h)$$

$$\varphi_h(x_h) = \frac{P(x_h)}{\prod_{h' \subset h} \varphi_{h'}(x_{h'})}$$

Product over *all* complete subgraphs, not only over maximal cliques



[illegible]

[illegible]

[illegible] (X_5, X_6)

[illegible]

Factorization Over a Triangulated Graph G

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Product over *all* complete subgraphs, not only over maximal cliques

- Why not subsume smaller cliques in maximal cliques ?

- Very strong locality:
  A clique’s factor depends *only* on the marginal distribution inside the clique. It does *not* depend on the graph structure.

$$\varphi_h(x_h) = \frac{P(x_h)}{\prod_{h' \subset h} \varphi_{h'}(x_{h'})}$$

(unique factorization having this property)

ML distribution over a Triangulated Graph G

$$P_X(x) = \prod_{h \in \text{Cliques}(G)} \hat{\varphi}_h(x_h)$$

$$\hat{\varphi}_h(x_h) = \frac{\hat{P}(x_h)}{\prod_{h' \subset h} \hat{\varphi}_{h'}(x_{h'})}$$

Product over *all* complete subgraphs, not only over maximal cliques

Decomposition of *ML(G)*

$$\begin{aligned}\log ML(G) &= \log \prod_t \prod_{h \in Clique(G)} \hat{\varphi}_h(x_h^t) \\ &= T \sum_{h \in Clique(G)} \boxed{\mathrm{E}_{\hat{P}}[\log \hat{\varphi}_h(\mathrm{X}_h)]}\end{aligned}$$

Depends only on the empirical distribution inside clique, independent of the graph.

Decomposition of *ML(G)*

$$\log\ ML(G) = \log \prod_{t} \prod_{h \in Clique\ (G)} \hat{\varphi}_h(x_h^t)$$

$$= T \sum_{h \in Clique\ (G)} \mathrm{E}_{\hat{P}}[\log \hat{\varphi}_h(\mathrm{X}_h)]$$

$$= \sum_{h \in Clique\ (G)} w(h)$$

A property of the variables in the clique. Can be precalculated once, and then summed up in all graphs containing the clique

Decomposition of $ML(G)$

$$\log ML(G) = \sum_{h \in \text{Cliques}(G)} w(h)$$

$$= \boxed{\log ML(\phi)} + \sum_{h \in \text{Cliques}(G), |h| > 1} w(h)$$

$$\sum_{v} w(\{v\}) = \sum_{v} H(X_v) = \log \text{ML}$$ of fully independent model

Decomposition of $ML(G)$

$$\log ML(G) = \sum_{h \in \text{Cliques}(G)} w(h)$$

$$= \log ML(\phi) + \sum_{h \in \text{Cliques}(G), |h| > 1} w(h)$$

Combinatorial optimization problem: triangulated graph G, maximizing its clique-weights.

$$\begin{aligned} w(h) &= \mathrm{E}_{\hat{P}}[\log \hat{\varphi}_h(\mathrm{X}_h)] \\ &= \mathrm{E}_{\hat{P}}\left[\log \frac{\hat{P}(x_h)}{\prod_{h'\subset h} \hat{\varphi}_{h'}(x_{h'})}\right] \\ &= -H(\hat{P}(h)) - \sum_{h'\subset h} w(h') \end{aligned}$$

$$w(h) = -\sum_{h'\subseteq h} (-1)^{|h|-|h'|} H(\hat{P}(h'))$$

Weight of a doubleton

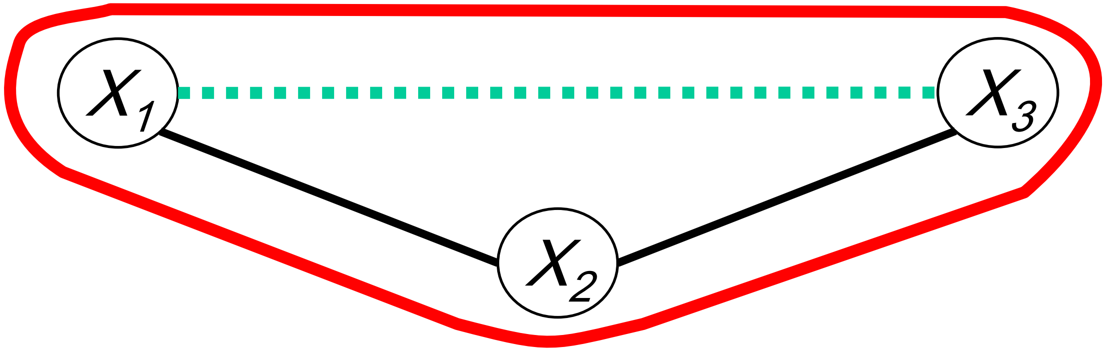
$$
\begin{aligned}
w(\{u,v\}) &= -H(\hat{P}_{\{u,v\}}) - w(u) - w(v) \\
&= -H(\hat{P}_{\{u,v\}}) + H(\hat{P}_{u}) + H(\hat{P}_{v}) \\
&= I_{\hat{P}}(u;v) \geq 0
\end{aligned}
$$

Weight of a triplelton with no pairwise interactions

$I(X_1;X_2)= I(X_1;X_2)= I(X_1;X_2)=0$

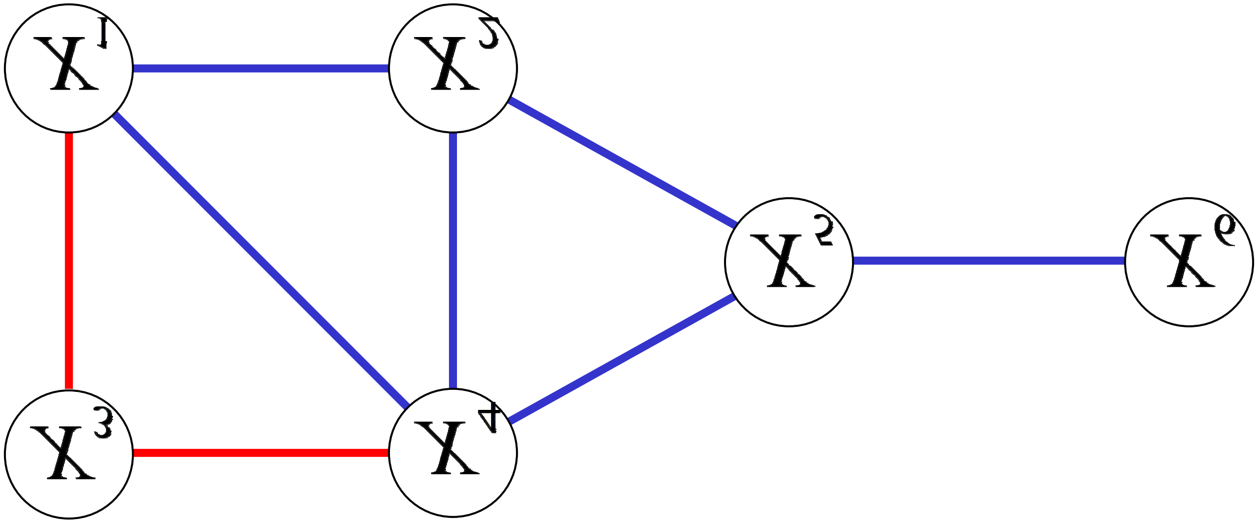
$$\begin{aligned} w(X_1, X_2, X_3) &= H(X_1) + H(X_2) + H(X_3) \\ &\quad - H(X_1, X_2, X_3) \\ &= D(\hat{P}_{\{1,2,3\}} \| \hat{P}_1 \cdot \hat{P}_2 \cdot \hat{P}_3) \geq 0 \end{aligned}$$

Weights in a Markov chain



$$\begin{aligned} w(1,2,3) &= H(1,3) - H(1) - H(3) \\ &\quad + H(1,2) + H(2,3) - H(2) - H(1,2,3) \\ &= -I(1;3) < 0 \end{aligned}$$

Monotone Weights



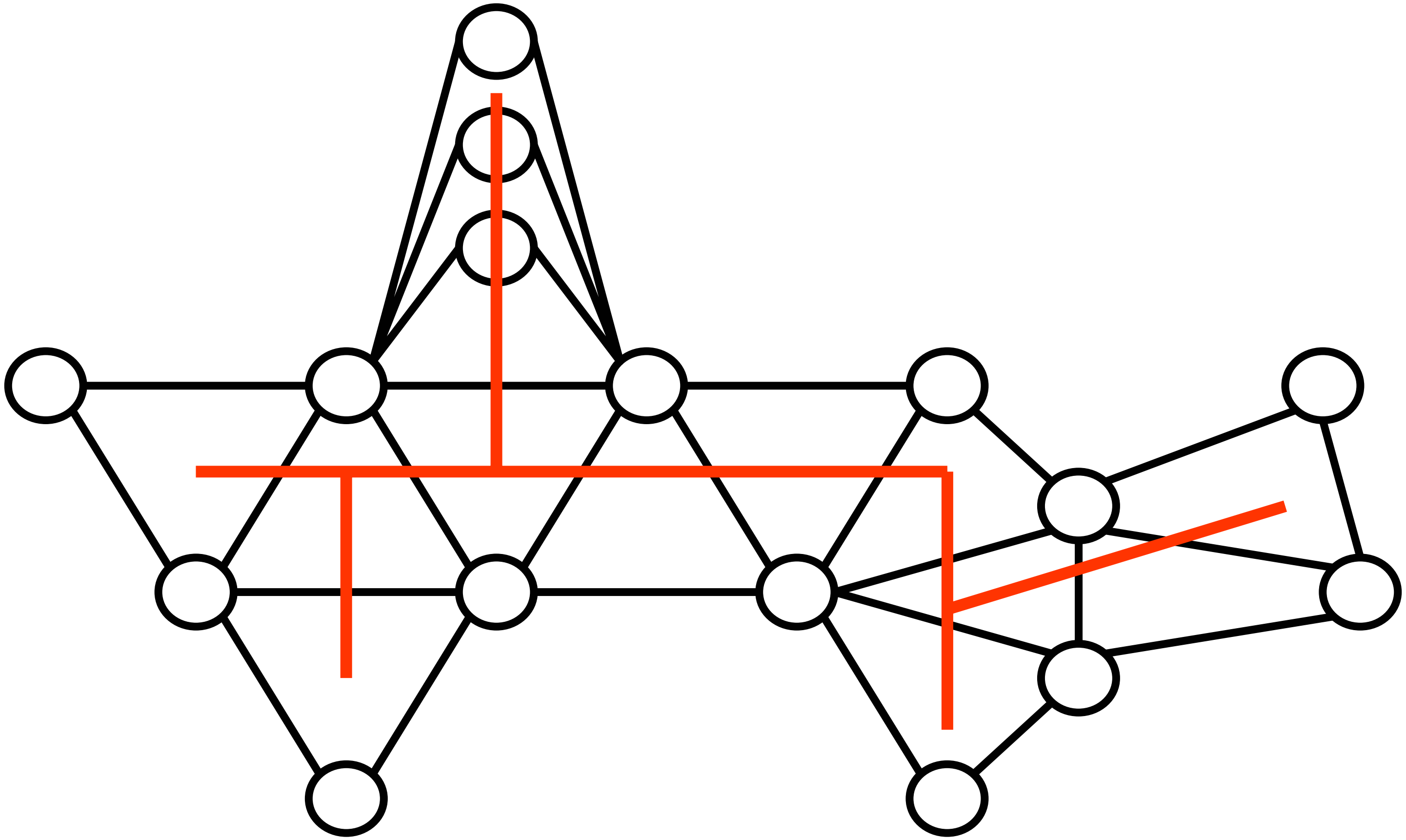
Adding to a graph
cannot decrease its total weight.

The combinatorial optimization problem

- Given:
  - a width k,
  - a monotone weight function on candidate cliques of size at most $k+1$
- Find a triangulated graph with clique size at most $k+1$ that maximizes the sum of weights of its cliques.

The Maximum Weight ***k***-Hypertree Problem

2-Hypertree



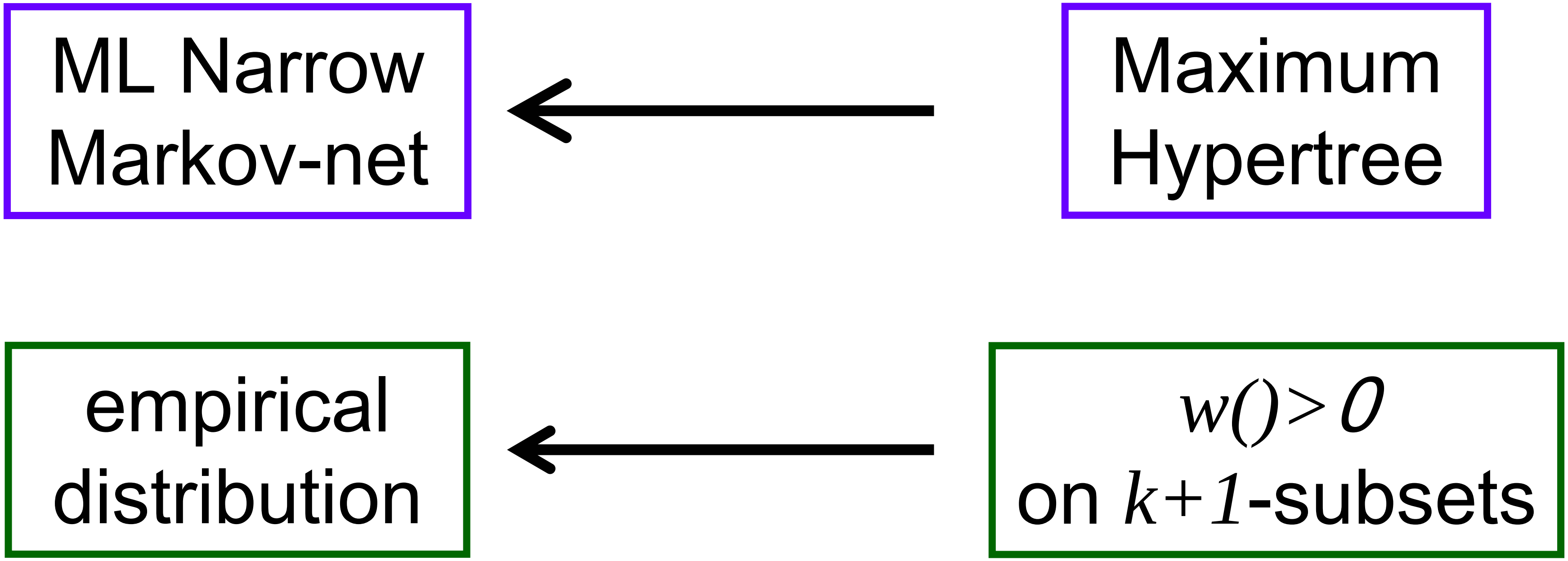
Junction trees are (roughly) hypertrees

Maximum Hypertrees

- For k=1: essentially linear time [Prim, Kruskal]
- For k>1: NP-hard, even for k=2.
  (and even with 0/1 weights, and weights only on 2-cliques)

We're not there yet: does not immediately imply hardness of ML narrow Markov nets…

Hardness



ML Narrow Markov-net

Maximum Hypertree

empirical distribution

$w() > 0$ on $k+1$-subsets

Creating a distribution for *w()*

- Uniform, except biases on parity of *(k+1)*-subsets.

- Mixture of $\binom{n}{k+1}$ components, one for each *(k+1)*-subset.

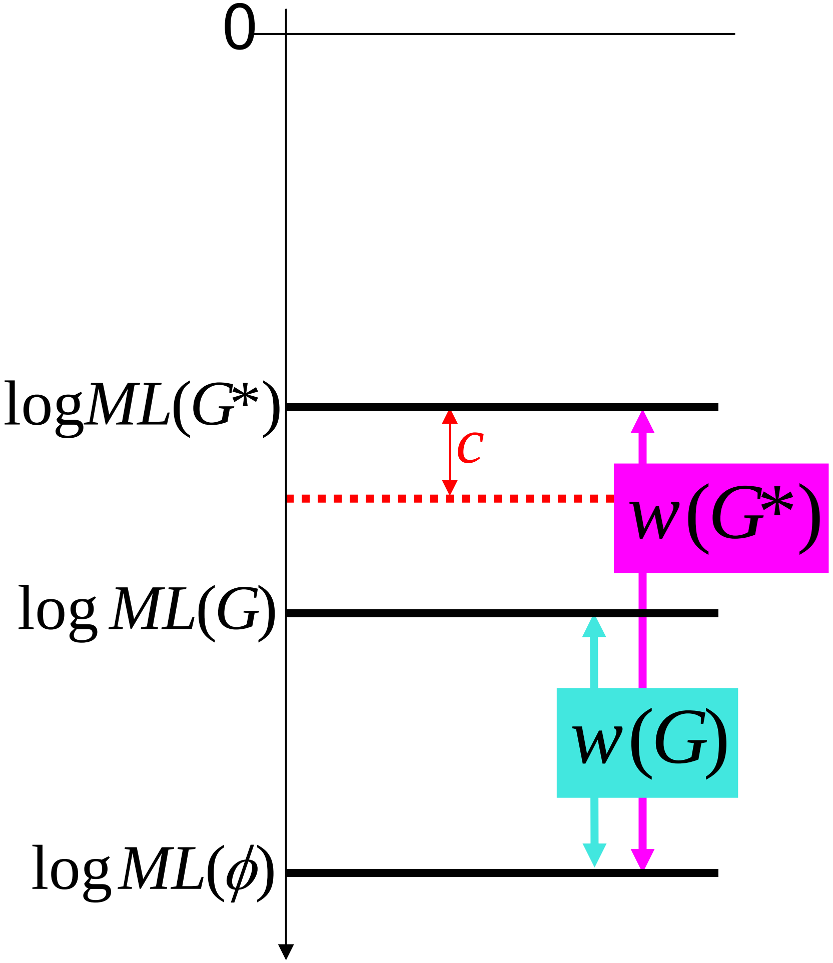
Now construct sample with this distribution…

Hardness of Max-Hypertree translates to hardness of ML Narrow Markov-net:

- NP-hard.
- NP-hard to approximate within an additive offset.

What are we approximating ?

$$\log ML(G) = \log ML(\phi) + \sum_{h \in \text{Cliques}(G), |h|>1} w(h)$$

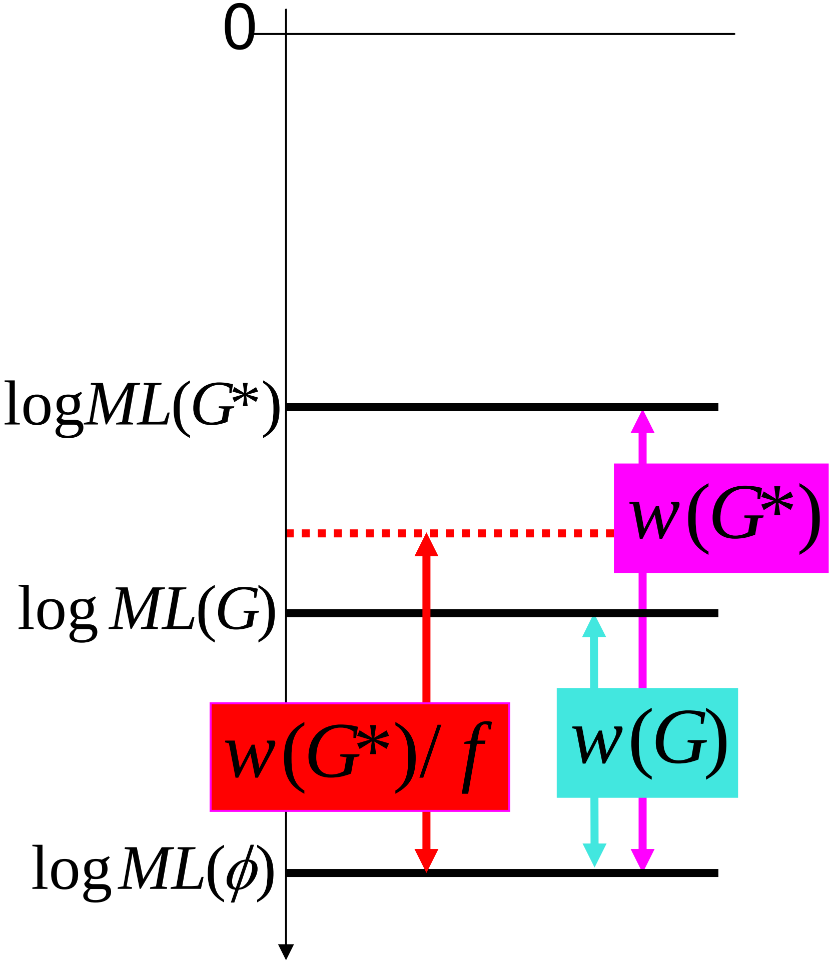


Hard to approximate gain to within additive offset.

Hard to approximate likelihood to within multiplicative factor

What are we approximating ?

$$\log ML(G) = \log ML(\phi) + \sum_{h \in \mathrm{Cliques}(G), |h|>1} w(h)$$



Approximate to within multiplicative factor of gain ?

Approximation Algorithm
[with David Karger, SODA 2001]

- For any constant k:

  Find a triangulated graph G with max clique $k+1$, such that:

$$w(G) \geq \frac{\max_{\text{trig } G^*, \text{width} \leq \text{k}} w(G^*)}{f(k)}$$

$$w(G) \geq \frac{\max_{\text{trig } G^*, \text{width} \leq \text{k}} w(G^*)}{f(k)}$$

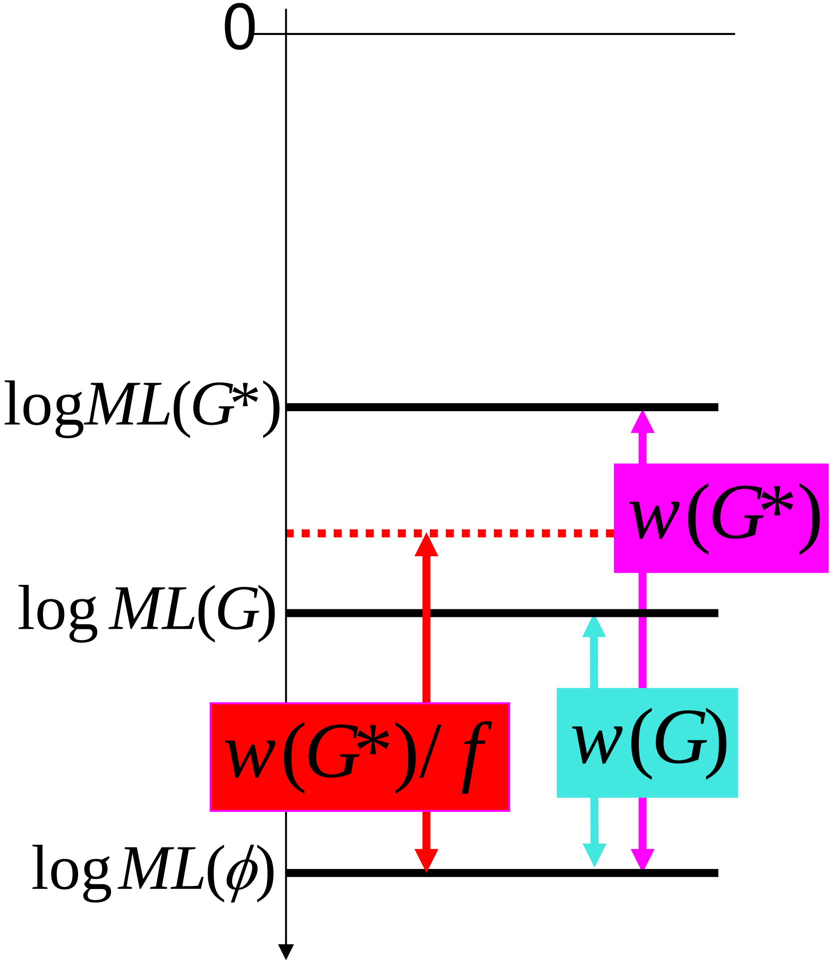
$$f(k) = 8^k k!(k+1)!$$

Running time: polynomial in number of weight, i.e. $n^{O(k)}$

Greedily adding one clique at a time can be arbitrarily bad on certain inputs.

What are we approximating ?

$$\log ML(G) = \log ML(\phi) + \sum_{h \in \mathrm{Cliques}(G), |h|>1} w(h)$$

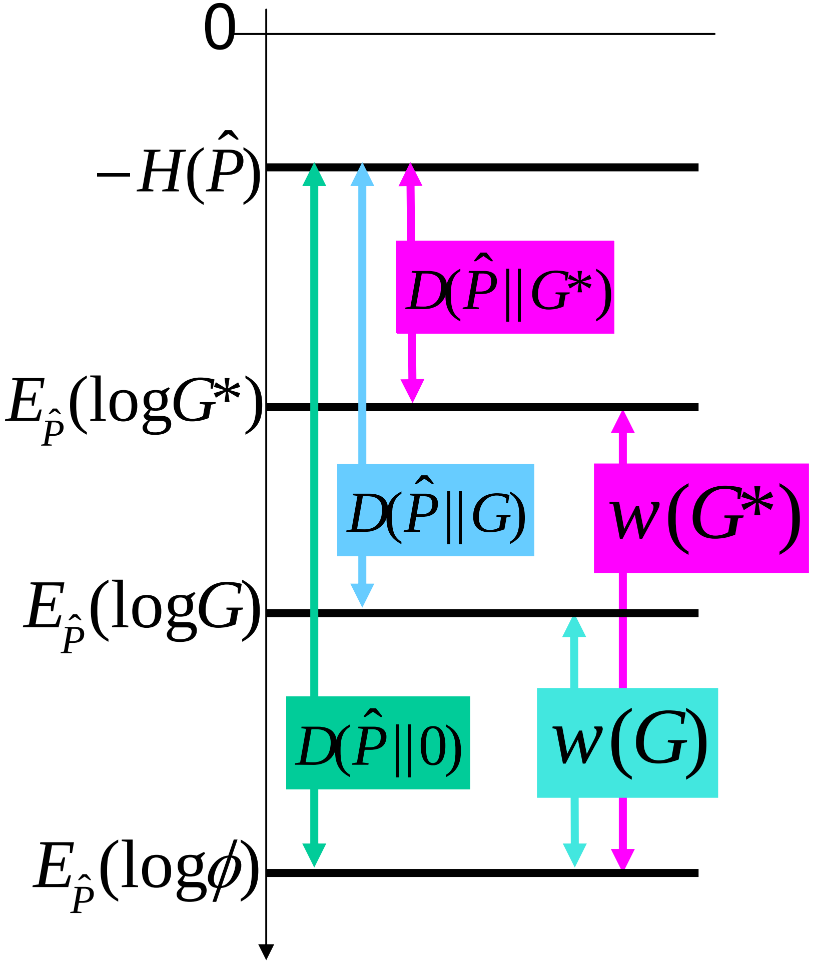


Approximate to within small multiplicative factor ?

-Independent of k ?

-Arbitrarily small ?

What are we approximating ? (the distribution projection view)



Can we get approximation on the relative entropy ?

Be very good when the target (true) distribution is almost a Markov network?

- Is there a distribution yielding any monotone weight function ?

- What is the “right” condition on the weight function ?

Summary

- ML Narrow Markov Network problem as a combinatorial optimization problem:
  - Hardness results
  - Analyzable algorithms of *"global"* nature
  - *"linked"* to Max-Hypertree problem

- Weights: an interesting information decomposition.

http://theory.lcs.mit.edu/~natis/HyperTrees/