Efficient Stepwise Selection in Decomposable Models

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Decomposable Models

- Undirected graphical models (Markov Networks)
  - Applications: Image processing, translation models, word-sense disambiguation, multi-dimensional histograms
- Decomposable Models :
  - Subclass with underlying graphical structure equivalent to chordal (triangulated) graphs
- Advantages :
  - MLE can be computed analytically
  - Closed form expressions for test statistics
  - Can be represented by means of both directed and undirected graphs
- Mixtures of Decomposable Models can be used for more representational power

Searching for Optimal Decomposable Model

- Intractable in general
- Heuristic Search Techniques
  - Need to make sure we stay in the space of Decomposable Models
  - Backward Selection: Remove edges from the model incrementally
    - Theorem [Wermuth 76]: An edge can be removed from a decomposable model iff it belongs to exactly one maximal clique of the graph.
  - Forward Selection: Add edges to a model incrementally
    - Naive Algorithm : $O(n^4)$ per step
- We will focus on Forward Selection in this talk

Forward Selection Problem Definition

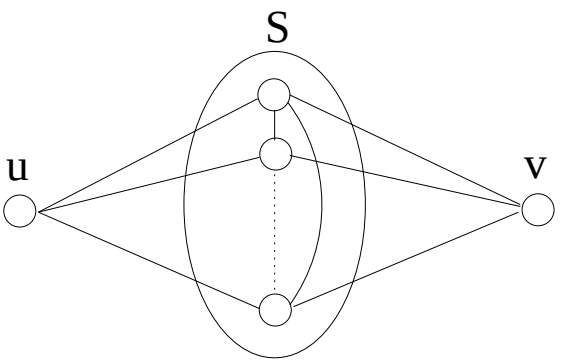
- Add an edge to a given decomposable model to get the decomposable model that has the highest $score$ amongst possible such models.
  - Step 1: Identify the edges that can be added without violating chordality of the graph.
  - Step 2: Choose the best edge given a score function and add that edge to the model.
- Example of a Score Function
  - Kullback-Leibler Divergence

Overview of the Talk

- ☞ Characterization of edges eligible for Forward Selection
- ☞ Auxiliary structures required
- ☞ Updating the auxiliary structures
- ☞ Complexity of the complete forward selection procedure
- ☞ Extensions

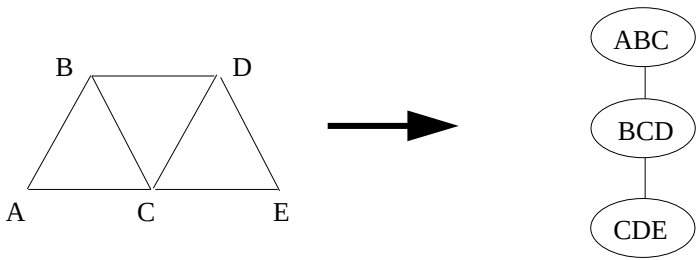
Characterization

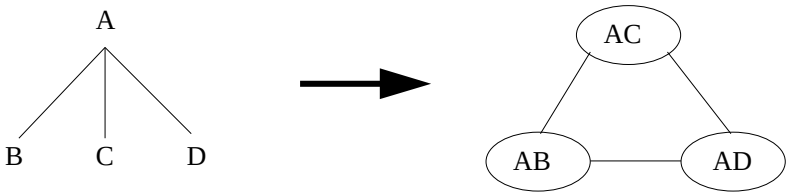
- An edge (u, v) can be added to a chordal graph (V, E) while maintaining its chordality iff :
  - $\exists\ S \subseteq V - \{u, v\}$ s.t. $(u, x), (x, v) \in E \quad \forall x \in S$
  - S is the *minimal separator* for v and v



Clique Graph CG_G of a Chordal Graph G

- $CG_G = (V_{CG}, E_{CG})$ where :
  - V_{CG} = maximal cliques of G
  - $(C_1, C_2) \in E_{CG}$ iff $S = C_1 \cap C_2$ separates $C_1 - S$ and $C_2 - S$





Properties of Clique Graph

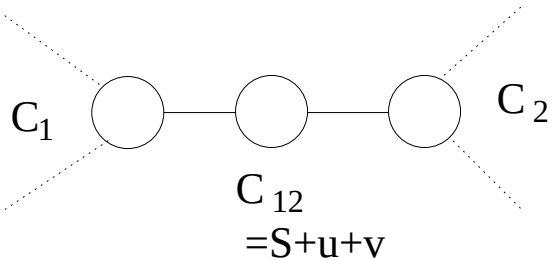
- A maximum spanning tree of CG_G is a junction tree of G
- CG_G is union of all junction trees of G
- Equivalent to Almond Trees in representational power
- Can be used for inference as well
- Two nodes u and v in G satisfy the forward selection criterion iff $\exists\ (C_1, C_2) \in E_{CG}$ s.t. $u \in C_1$ and $v \in C_2$
  - Can be used to enumerate edges eligible for forward selection
  - $O(n^4)$ worst case

Auxiliary Structures

- $n \times n$ matrix, $\mathcal{E}_G$
  - Indexed by the nodes of G
  - $\mathcal{E}_G(u, v) =$ true iff (u, v) eligible for forward selection
  - Used to enumerate eligible edges in $O(n^2)$ time
- Clique graph CG_G of the model graph
  - Required to update $\mathcal{E}_G$ in time $O(n^2)$ after adding an edge
- Time complexity of enumeration : $O(n^2)$

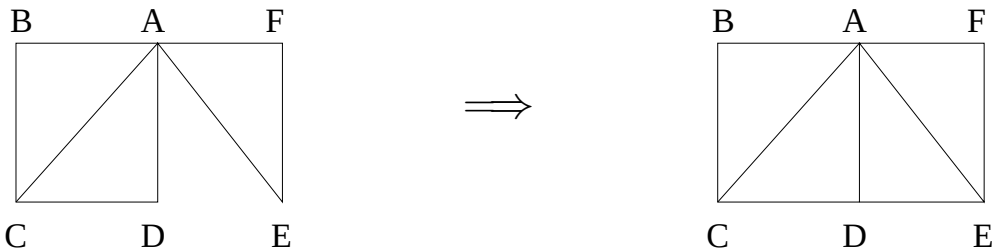
Updating the Clique Graph

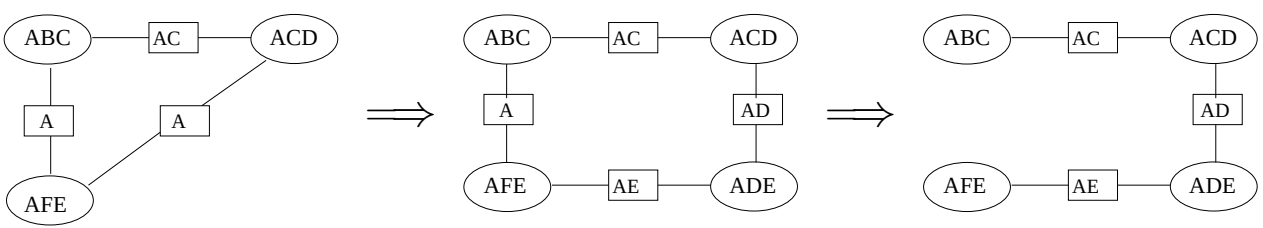
- Step 1 : Add the newly generated maximal clique



- Step 2 : Remove existing edges if required
  - Theorem: An edge (C_i, C_j) may have to be removed only if :
    - $C_i \cap C_j = S$.
    - u is connected to C_i and v to C_j in $G - S$.
- Step 3 : Add edges involving C_{12}

Updating the Clique Graph : Example





Updating $\mathcal{E}_G$

- Since some edges have been deleted from the clique graph, previously eligible node pairs may not be eligible any more.
- New node pairs of the form (u, x) or (v, x) may become eligible for forward selection.

	A	**B**	**C**	**D**	**E**	**F**
A	F	F	F	F	F	F
B	F	F	F	T	T	T
C	F	F	F	F	T	T
D	F	T	F	F	T	T
E	F	T	T	T	F	F
F	F	T	T	T	F	F

$\Longrightarrow$

	A	**B**	**C**	**D**	**E**	**F**
A	F	F	F	F	F	F
B	F	F	F	T	**F**	**F**
C	F	F	F	F	T	**F**
D	F	T	F	F	**F**	T
E	F	**F**	T	**F**	F	F
F	F	**F**	**F**	T	F	F

Step 2 of Forward Selection Procedure

- KL Divergence from the saturated model (completely connected graph)
  - Equivalent to minimizing entropy of the model
    - $H(\mathcal{M}) = \Sigma_{C \in \mathcal{C}} H(C) - \Sigma_{S \in \mathcal{S}} H(S)$
      where $H(A_1, A_2, \ldots, A_k) = \Sigma_a \frac{f(a)}{N} \log \frac{f(a)}{N}$
  - Only require the list of maximal cliques ($\mathcal{C}$) and separators ($\mathcal{S}$) in a junction tree
  - Theorem: If $\mathcal{M}'$ is obtained from $\mathcal{M}$ by adding edge (u, v), then

$$H(\mathcal{M}) - H(\mathcal{M}') = H(S + u) + H(S + v) - H(S + u + v) - H(S)$$

  - Precompute all the entropies required for the next step
  - Theorem: Number of new entropies that need to computed after adding an edge is at most $4n$.

Overall Complexity of Update

- $O(n^2 + nE)$, where E is average time required to compute an entropy
  - Enumerating eligible edges and selecting the $best$ edge, $O(n^2)$
  - Updating the auxiliary structures, $O(n^2)$
  - Precomputing entropies required for next step, $O(nE)$
- Naive computation of entropies using sorting
  - $E = O(m \log m)$, where m is the number of data points
  - Time to compute the entropies can be reduced significantly by simultaneous computation

Extensions

- Backward Selection
  - Similar time complexity
  - Number of entropies required to be computed at each step at most n
- Strong Decomposability
  - $E.g.$, Mixed Graphs, Decision Graphs
  - Mixed Graphs :
    - Theorem (Lauritzen, 1996): Given a strongly decomposable mixed graph $G = (V, E)$, with $V = V_d \cup V_c$, the graph $G' = (V + *, E + E_*)$, with $E_* = \{(*, v) \forall v \in V_d\}$, is chordal.

Conclusions

- ☞ Proposed a characterization for edges eligible for forward selection
- ☞ Presented an algorithm to do stepwise selection efficiently
- ☞ $O(n^2)$ time complexity per step as opposed to $O(n^4)$ of the naive algorithm

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