COMP9418: Advanced Topics in Statistical Machine Learning

Graphe Decomposition

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Instructor: Gustavo Batista

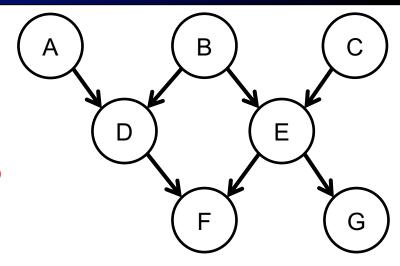
University of New South Wales

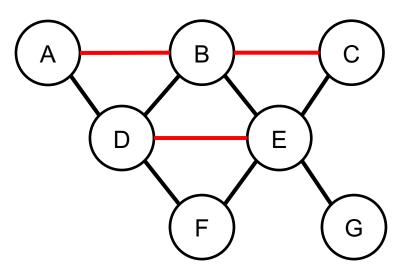
Introduction

- In this lecture, we will study the relationships between Variable Elimination and Jointrees
 - Both can be viewed signer on posing to Every diskin a systematic way
 - VE removes one variable of time
 VE removes one factor at a time
- WeChat: cstutorcs
 We will provide more formal definitions to concepts seen in previous lectures about these topics
- And cover polynomial time algorithms to convert elimination orders to jointrees and vice-versa

Moral Graph

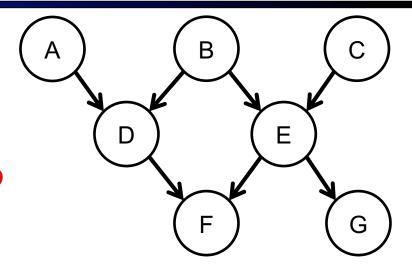
- An interaction graph for factors ϕ_1, \dots, ϕ_n is an undirected graph
 - Nodes correspond to the variables appearing in Help ϕ_1,\ldots,ϕ_n
 - Edges connect variables in the same traces recom
- If the factors are CPTs of G Bayesian network with DAG G, the induced graph can be obtained from G by M by M by M by M and M by M are M by M and M by M are M and M by M are M and M are M and M are M are M are M and M are M ar
 - Add an undirected edge between every pair of nodes that share a common child
 - Convert every directed edge in *G* in an undirected edge

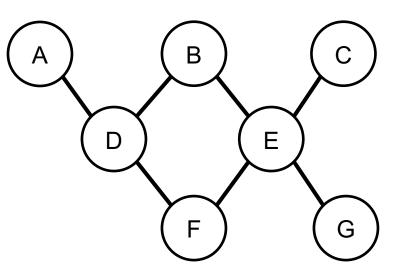




Treewidth

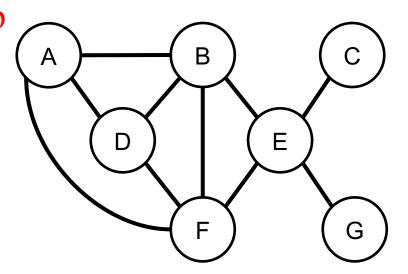
- Treewidth is a central notion to complexity analysis of inference algorithms
 - It is usually defined for undirected graphs Exam Help
 - It can be extended to DAGs through their moral graphs https://tutorcs.com
- The treewidth of a DAG Gwedefined another treewidth of its moral graph
 - We will later define the treewidth for undirected graphs





Other Graph-theoretic Definitions

- We adopt the following definitions for a graph G
 - A neighbor of a node X is a node Y connected to X by an edge in G. We also say X and Y are adjacent Assignment Project Exam Help
 The degree of a node X is the number of neighbors of X
 - The *degree* of a node X is the number of neighbors of X in G https://tutorcs.com
 - A *clique* is a set of nodes in *G* that are pairwise adjacent, i.e., every pair of nodes in the clique are connected by an edge
 - A maximal clique is a clique that is not strictly contained in another clique
 - When we say "graph G" in this lecture, we mean undirected graph. Otherwise, we say "DAG G"



Elimination Order

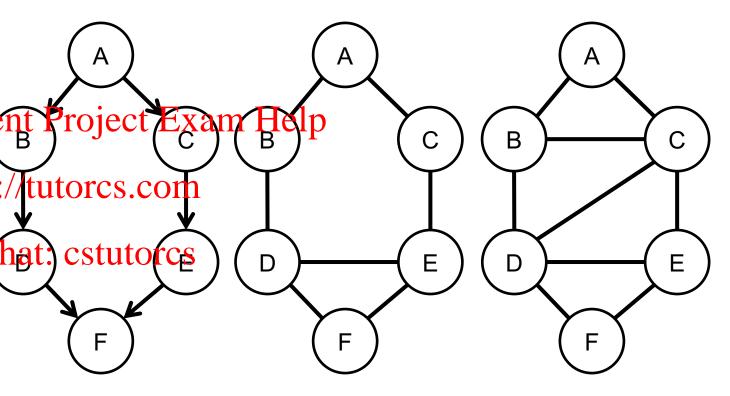
• An elimination order for a graph G is a total ordering π of nodes of G, where $\pi(i)$ is the ith node in the ordering Assignment

The result of eliminating node X tutorcs.com from graph G is another graph
 obtained from G by

We(that) estutore

 Adding an edge between every pair of nonadjacent neighbors of X

- Deleting node X
- The edges added during the elimination process are called fillin edges



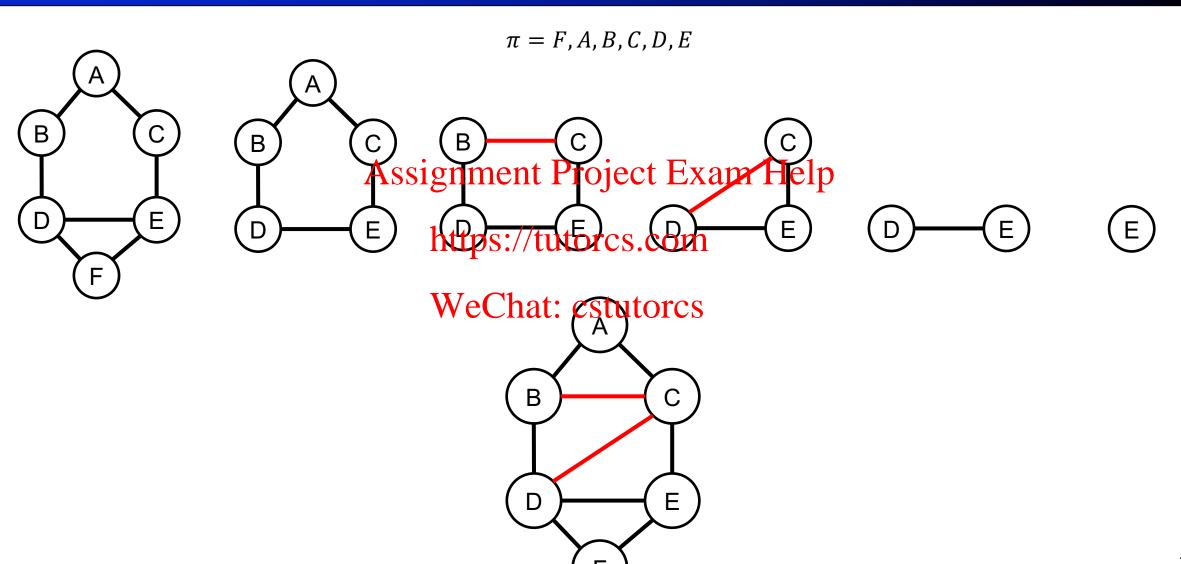
A DAG G

The moral graph G_m

The filled-in graph G_m^{π}

$$\pi = F, A, B, C, D, E$$

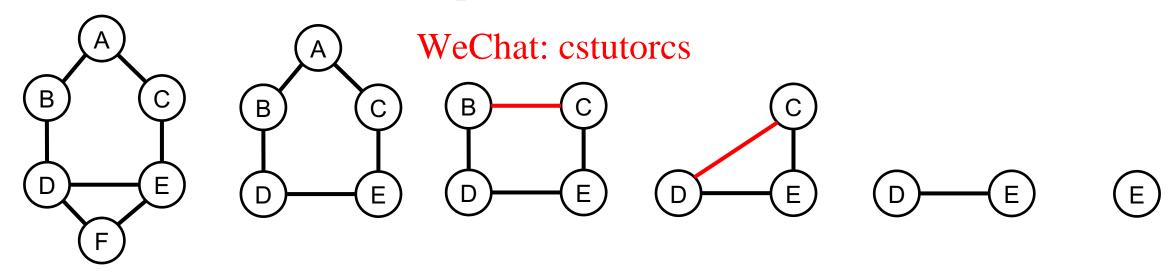
Node Elimination



Graph and Cluster Sequence

- The elimination of nodes from graph G according to order π induces:
 - A graph sequence G_1, \dots, G_n , where $G_1 = G$ a graph G_{i+1} is obtained by eliminating
 - node $\pi(i)$ from graph G_i Assignment Project Exam Help

 A cluster sequence C_1, \dots, C_n , where C_i consists of node $\pi(i)$ and its neighbors in https://tutorcs.com graph G_i



$$C_1 = DEF$$

$$\boldsymbol{C}_2 = ABC$$

$$\boldsymbol{\mathcal{C}}_3 = BCD$$

$$C_4 = CDE$$
 $C_5 = DE$

$$\boldsymbol{C}_5 = DE$$

$$\boldsymbol{C}_6 = \mathbf{E}$$

Elimination Width

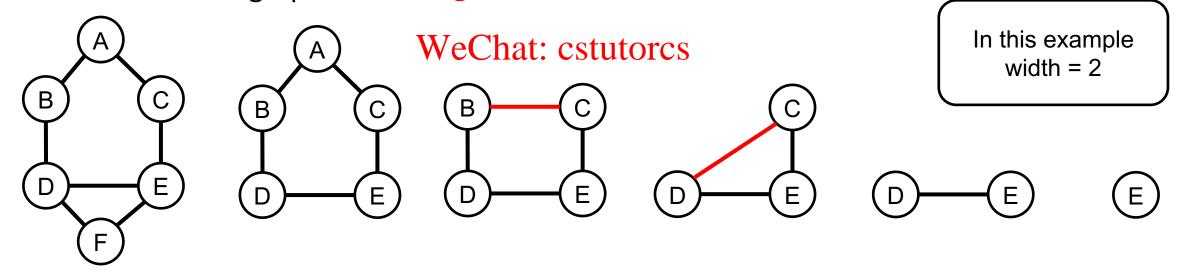
- Let π be an elimination order for a graph G, and C_1, \dots, C_n the induced cluster sequence
 - The width of the elimination order p is width (π,G) He $\max_{i=1}^{n} |C_i| 1$

 $C_3 = BCD$

 $\mathbf{C}_2 = ABC$

 $C_1 = DEF$

• We extend this definition to DAGs: width of π for a DAG is the width of π for the DAG's moral graph https://tutorcs.com



 $C_4 = CDE$

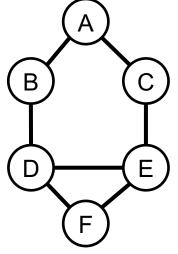
 $C_6 = E$

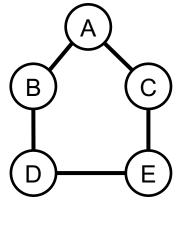
 $C_5 = DE$

Treewidth

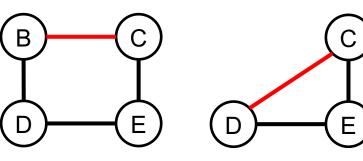
- The width of a graph G is $treewidth(G) \stackrel{\text{def}}{=} \min_{\pi} width(\pi, G)$
 - When the width of an elimination order π equals the treewidth, we say π is optimal
 - When an elimination $\Delta s deg m does Pooleant Example Heripedges, we say <math>\pi$ is a perfect elimination order

Not every graph admits a perfect elimination order

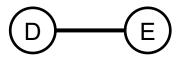




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This elimination order is optimal (why?), but not perfect





$$C_1 = DEF$$

$$\mathbf{C}_2 = ABC$$

$$\boldsymbol{C}_3 = BCD$$

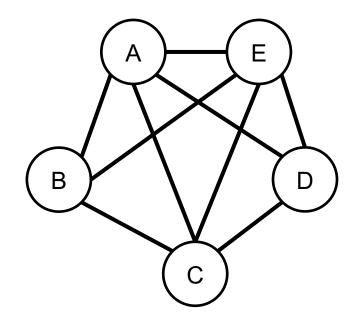
$$C_4 = CDE$$

$$C_5 = DE$$

$$\boldsymbol{C}_6 = \mathbf{E}$$

Elimination Heuristics

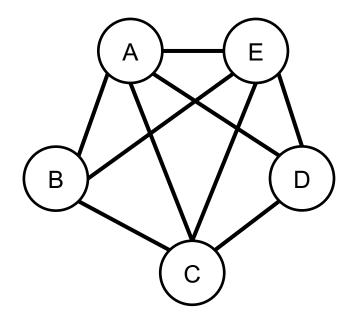
- The computation of an optimal elimination order is NP-hard
 - Several greedy elimination heuristics have been proposed
 - These are ways to eliminate nodes based on local considerations
- The two most common Assignment Project Exam Help
 - Min-degree: eliminate the node having the smallest number of neighbors
 - Min-fill: Eliminate the node that reads adding the smallest number of fill-in edges
- Min-fill typically produces better results
- Min-degree is known to be optimal for graphs with treewidth ≤ 2



Node *C* has degree 4, and min-fill score of 1

Elimination Heuristics

- In practice, it is common to combine heuristics
 - Select nodes with min-fill and break ties with min-degree
 - Select nodes with min-degree and break ties using min-fill
 Assignment Project Exam Help
- Stochastic techniques can be powerful to combine https://tutorcs.com heuristics
 - Same elimination heuristic to elimination heuristic elimination heuristi
 - Different heuristics to eliminate different nodes, where the choice of a heuristic at each node is made stochastically



Node *C* has degree 4, and min-fill score of 1

Optimal Elimination Prefixes

- A *prefix* of elimination order π is a sequence of variables τ that occurs in the beginning of π
 - For example if $\pi = A, B, C, D, E$ then two prefixes are $\tau = A, B, C$ and $\tau = A, B$
- If τ is a prefix of some optimisation brue. Exam Help optimal elimination prefix
 - It can be completed to yield an optimal order https://tutorcs.com
 - The notion of width can be extended to prefixes by considering the cluster sequence of applying the prefix to a graph
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- We can generate optimal prefixes
 - There are preprocessing rules that eliminate a subset of variables
 - While guaranteeing they represent the prefix of some optimal elimination order
 - These rules are not complete, i.e., we cannot always use them to produce a complete elimination order
 - Yet, we can use these rules to eliminate as many nodes as possible before using a heuristic

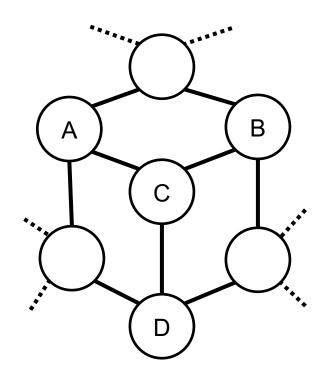
Optimal Elimination Prefixes

- We apply the rules in any order
 - A lower bound (low) is maintained on the treewidth
 - Some rules update this bound
 - While others use it as a constignment Project Exam Help
- If a graph G' is the result of applying any of these rules to G and if low is updated accordingly
 - $Treewidth(G) = max(treewidth(G)) low_stutorcs$
 - Therefore, these rules reduce the computation of treewidth of G into the computation of treewidth of a smaller graph G'
 - Moreover, they are guaranteed to generate only optimal elimination prefixes
- A simplicial node is a node that all its neighbors are pairwise adjacent, forming a clique
 - An almost simplicial node is one that all but one neighbor form a clique

Optimal Elimination Rules

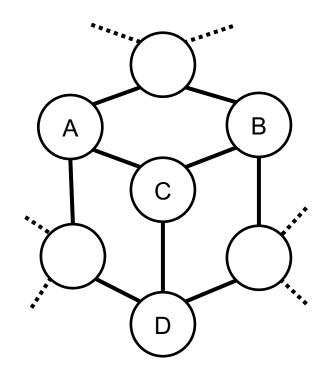
There are four rules

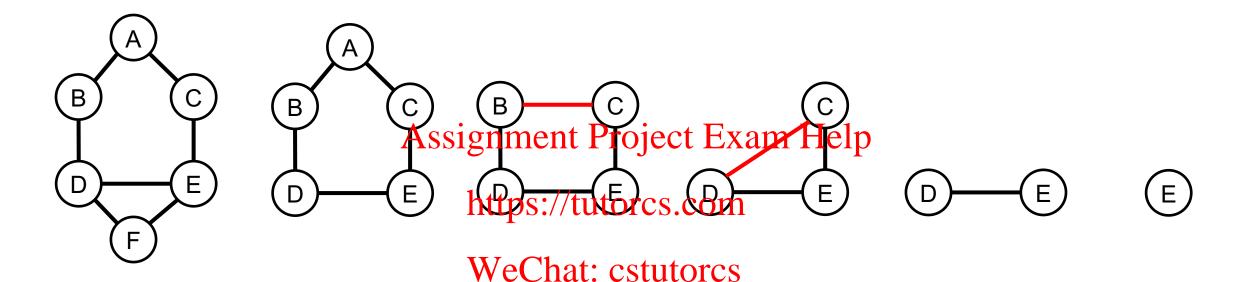
- Simplicial rule: Eliminate any simplicial node with degree d, updating low to $\max(low,d)$
- Almost simplicial rule: Eliansaitg annel nto Risinjolitia Example d as long as $low \ge d$
- Buddy rule: If $low \ge 3$, eliminate psy/pall to prodesign and Y that have degree 3 each and share the same set of neighbors
- Cube rule: If $low \ge 3$, eliminate any set of four Hodes A, B, C, D forming the structure in the figure
- These rules are complete for graphs of treewidth ≤ 3



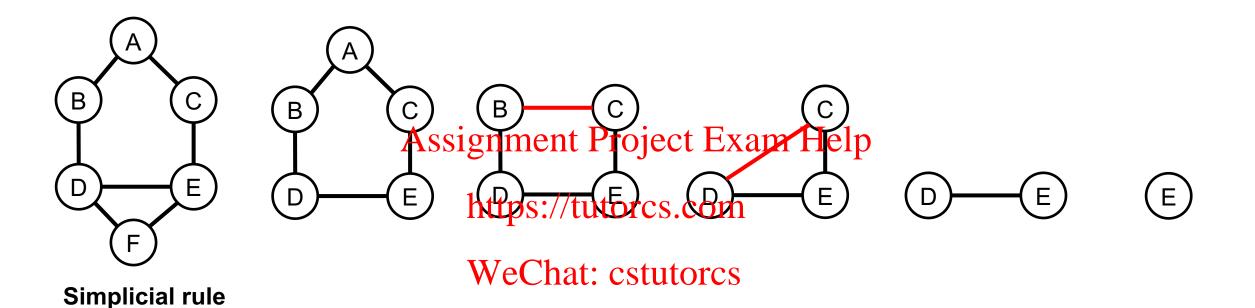
Optimal Elimination Rules

- Special cases for simplicial rule
 - Isler rule: Eliminate nodes with degree 0
 - Twig rule: Eliminate podes with degree 1 Exam Help
- Special cases for almost simplicial rule
 - Series rule: eliminate node with a tegretuzo from ≥ 2
 - Triangle rule: eliminate nodes with degree 3 if $low \ge 3$ and if at least two of the neighbors are connected by an edge



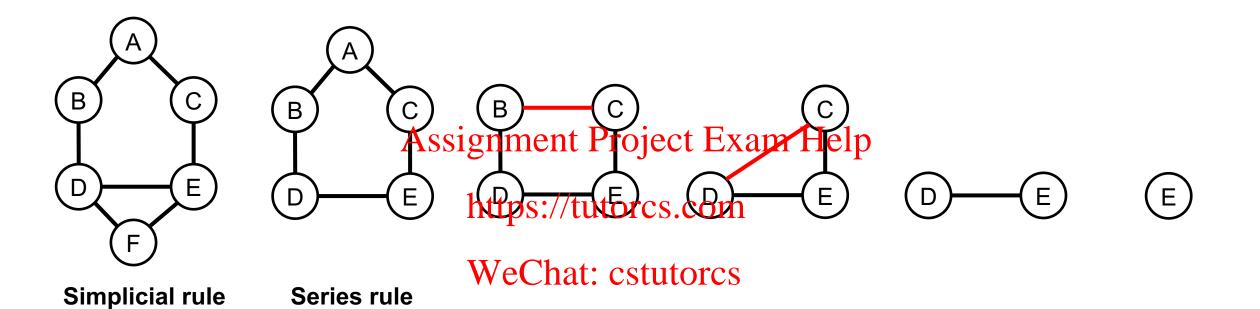


$$\tau = low = 1$$

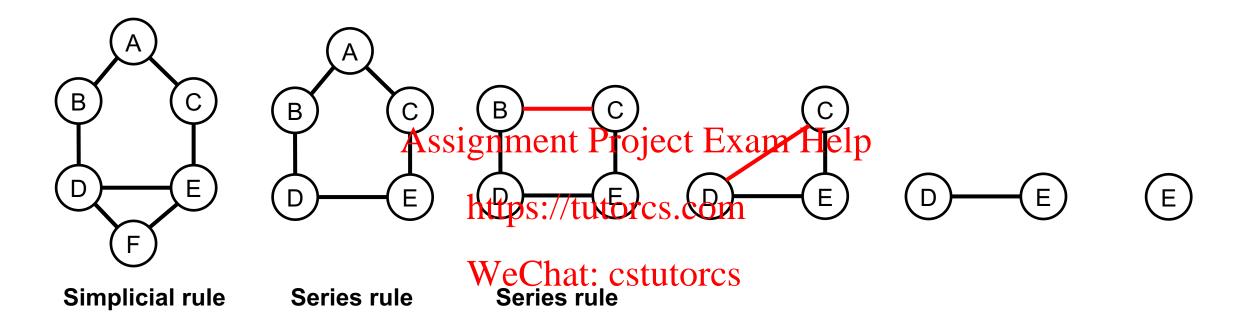


$$\tau = F$$

$$low = 2$$

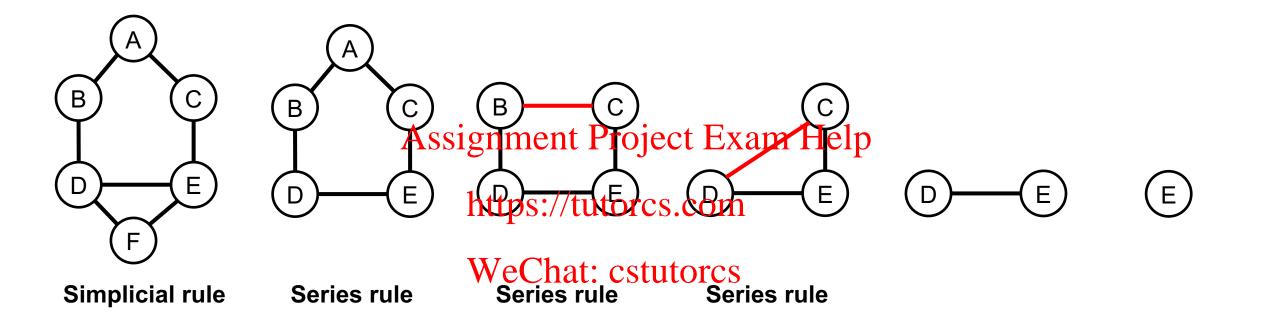


$$\tau = F, A$$
$$low = 2$$

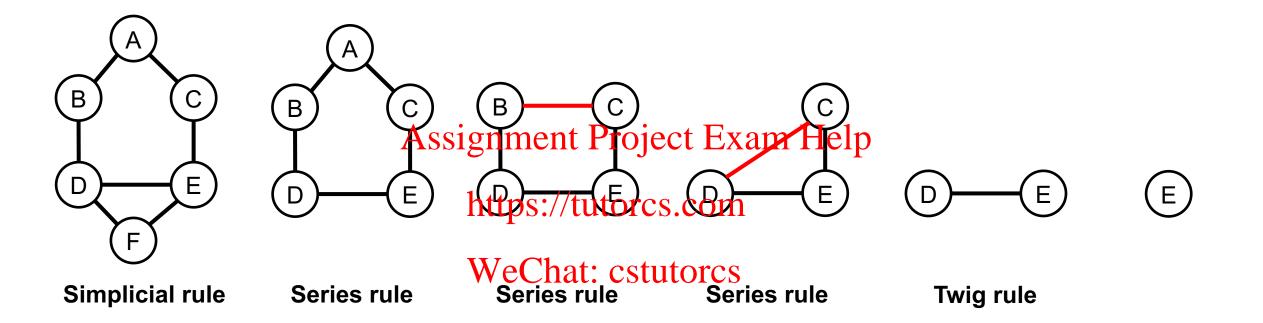


$$\tau = F, A, B$$

$$low = 2$$

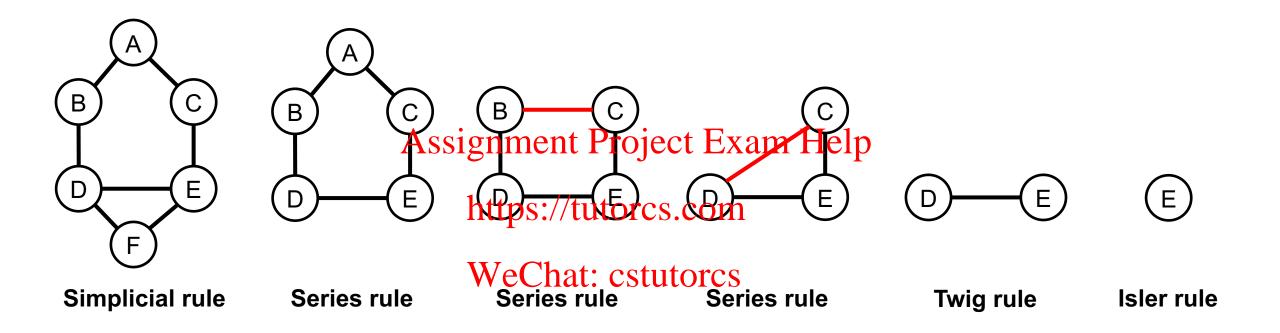


$$\tau = F, A, B, C$$
 $low = 2$



$$\tau = F, A, B, C, D$$

$$low = 2$$

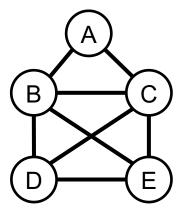


$$\tau = F, A, B, C, D, E$$

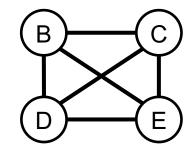
$$low = 2$$

Lower Bounds on Treewidth

- Lower bounds are used to empower the pre-processing rules
 - We can use then to set low to a larger initial value
 - This may allow us to apply more pre-processing elimination rules
- Two well-know, but typically weak ower bounds are Help
 - If a graph G has a clique of size n, then $treewidth(G) \ge n-1$
 - The degree of a graph is a lower bound for treewidth. The degree of a graph is the minimum number of neighbours attained by any of its nodes
- The degeneracy of a graph is the maximum degree attained by any of its subgraphs
 - It is a better bound. It is based on two observations
 - First, the treewidth of any subgraph cannot be larger than the treewidth of the graph containing it
 - Second, the degree of a subgraph may be higher than the degree of the graph containing it



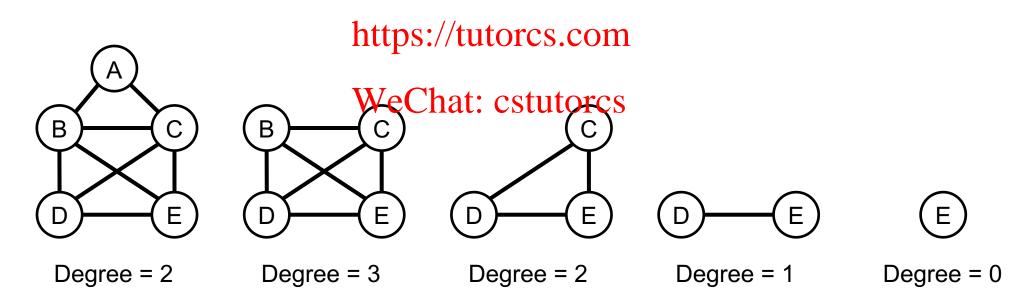
Graph degree is 2



Graph degree is 3

Lower Bounds on Treewidth

- The degeneracy is also known as maximum minimum degree (MMD)
 - MMD is easily computed by generating a sequence of subgraphs
 - Start with the original graph and remove a minimum-degree node
 - The MMD is the maximum segien mented by invertee generated subgraphs



Optimal Elimination Order

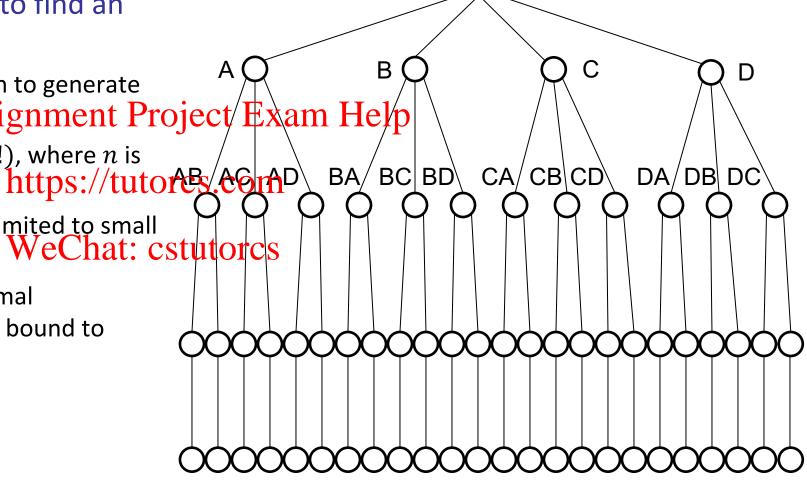
We can use search methods to find an optimal elimination order

For instance, depth-first search to generate all possible elimination or designment Project/Exam Help

The search space has size O(n!), where n is the number of variables

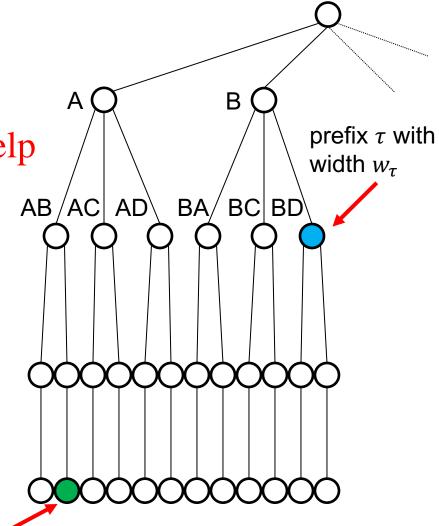
 Therefore, such methods are limited to small WeChat: cstutorcs number of variables

However, we can explore optimal elimination prefixes and lower bound to prune the search space



Optimal Elimination Order: Pruning

- Pruning is essential to improve the efficiency of these search methods
 - If you have a query, use the query pruning techniques of the lecture 7
 Assignment Project Exam Help
 - Use optimal prefix rules to further reduce the graph size and provide an elimination prefix and the provide and the provide and the provide and the provide an elimination prefix and the provide and
- In a depth-first search, each time we reach a leaf node in the search tree, we obtain an elimination explait: cstutorcs
- Suppose we have an elimination order π with width w_{π}
 - We are currently exploring a prefix au with width $w_{ au}$
 - We also have a lower bound b on graph G_{τ}
 - If $\max(w_{\tau}, b) \ge w_{\pi}$, then we cannot improve on order π



Elimination order π with width w_{π} This is our best-so-far width

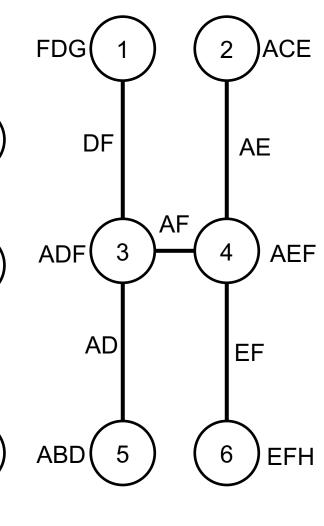
Jointree: Recap

• A *jointree* for a network G is a pair (T, C) where T is a tree and C is a function that maps each node A in the tree A into a label A called cluster. The jointree must satisfy the following properties A tutorcs.com

• The cluster C_i is a set of new extreme C_i is a set of new extreme.

lacktriangle Each factor in G must appear in some cluster $oldsymbol{\mathcal{C}}_i$

If a variable appears in two clusters C_i and C_j , it must appear in every cluster C_k on the path connecting nodes i and j in the jointree. This is known as jointree or running intersection property



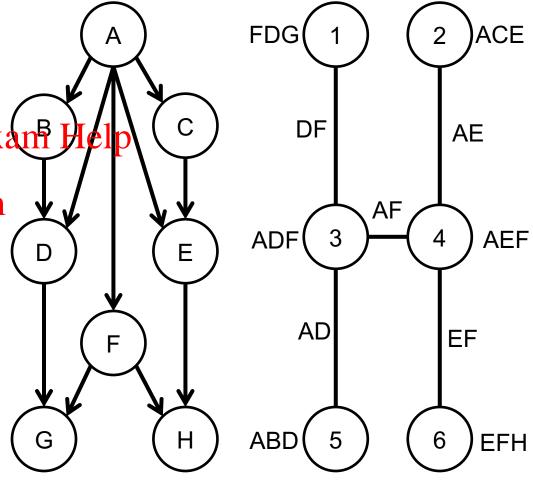
Jointree: Recap

The *separator* of edge i - j in a jointree is a set of variables defined as follows

$$S_{ij} = vars(i,j) \cap vars(j,i)$$
Assignment Project Example

The width of a jointree is defined as the width of a jointree is defin

• A jointree is also called a *junction tree* or a *cluster tree*

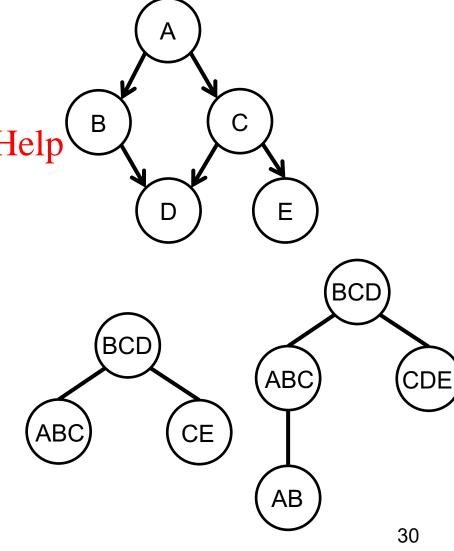


Jointree Operations

 The following transformations preserve all three properties of a jointree

• Add variable: We can add a variable X to a cluster Help C_i if C_i has a neighbour C_j that contains X

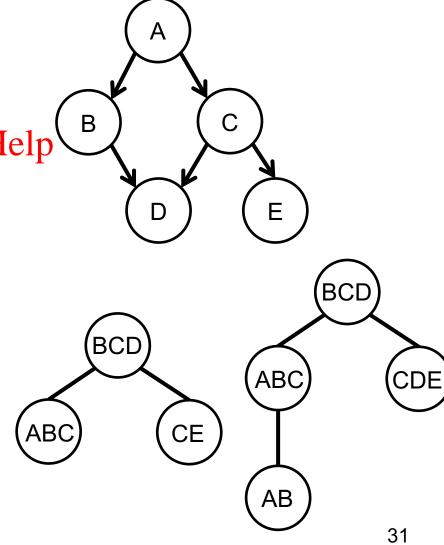
- Merge clusters: We can merge two heighbourng clusters C_i and C_j into a single cluster $C_k = C_i \cup C_j$, where C_k inherits the neighbours of C_i and C_j
- Add cluster: We can add a new cluster C_j and make it a neighbour of an existing cluster C_i if $C_i \subseteq C_i$
- Remove cluster: We can remove cluster C_j if it has a single neighbour C_i and $C_j \subseteq C_i$



Jointree Operations

These transformations have practical applications

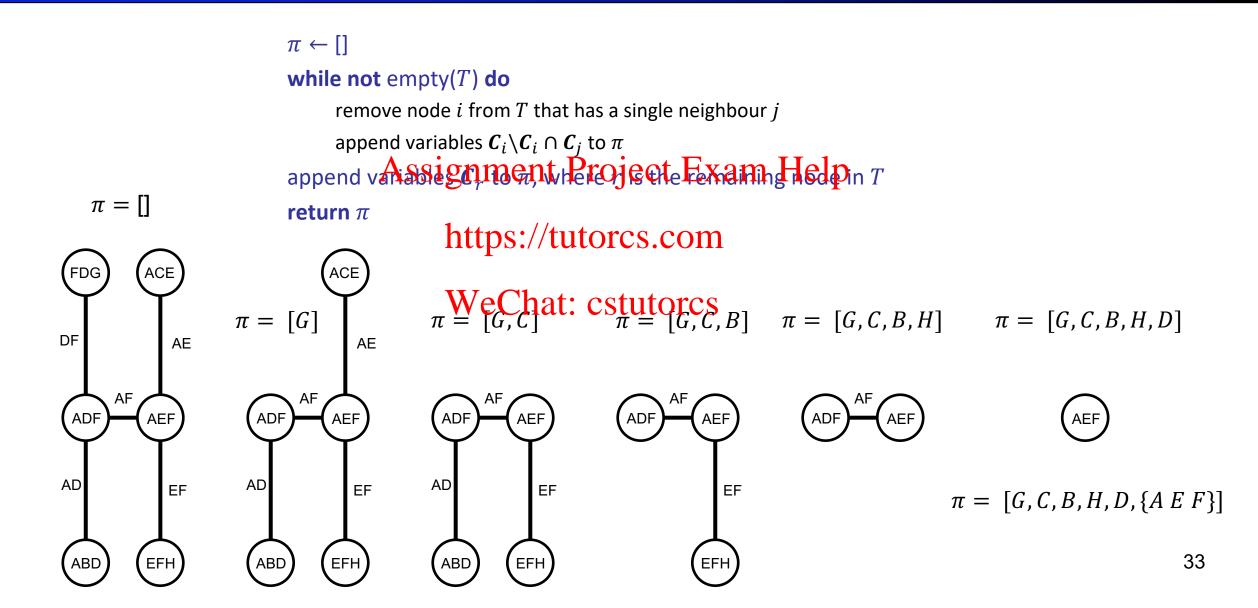
- The addition of variable D allows the jointree to compute marginal over variables CDE
- This marginal will not be Appiged if that algorithm to the left jointree
- Merging two clusters eliminate https://dratorcommedting them
- As the Shenoy-Shafer algorithm created actor to reduce space separator, this transformation can be used to reduce space requirements
- This will also typically increase the running time, as merging clusters can lead to larger clusters and the algorithm is exponential to cluster size
- This transformation can be the basis for time-space trade-offs



Jointree to Elimination Orders

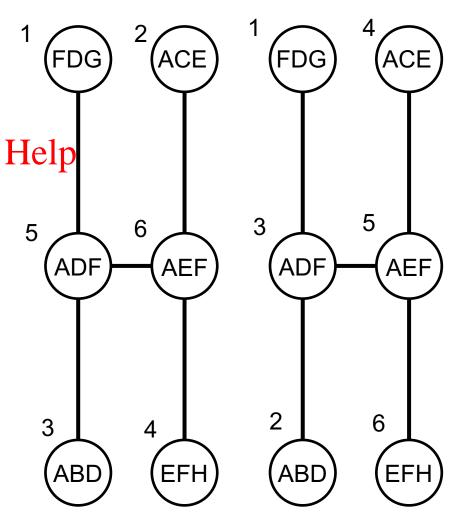
```
\pi \leftarrow []
while not empty(T) do
      remove node i from T that has a single neighbour j
     append variables C_i \backslash C_i \cap C_j to \pi
append vanssignment Projecte Examp Helpin T
return \pi
                  https://tutorcs.com.
                                                                \phi_C(C,A)\phi_E(E,A,C)
                                      \phi_G(G,D,F)
                                                FDG
                        Chat: cstutores
                                                              ΑE
                                         \phi_A(A)\phi_F(F,A)
                                                  ADF
                                                           AEF
                                                 AD
                                                             EF
                                         \phi_B(B,A)
```

Jointree to Elimination Orders



Jointree to Elimination Orders

- This algorithm simulates the process of factor elimination
 - It runs in polynomial time
 - It provides an elimination Argientaler Wiest that am Help the jointree width
- The algorithm leaves a few choices undetermined
 - Choosing the node i to remove wext-from the jointrees
 - Choosing the order in which variables $C_i \setminus C_i \cap C_j$ are appended to π
- None of these choices matter to the guarantees provided by the algorithm



Elimination Orders to Jointrees

- We present a polynomial time, width-preserving algorithm for generating a jointree from an elimination order
 Assignment Project Exam Help
- The algorithm consists of two parts
 - Constructing the clusters WeChat: cstutorcs
 - Assembling the jointree

Elimination Orders to Jointrees: Clusters

 We show how to generate clusters with the following properties

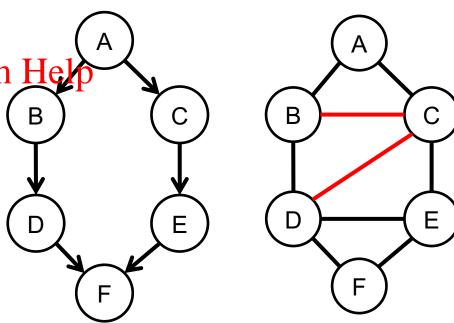
■ The size of every cluster is $\leq width(\pi, G) + 1$

The clusters satisfy conditions ignment lergojacte Exam Helphonition

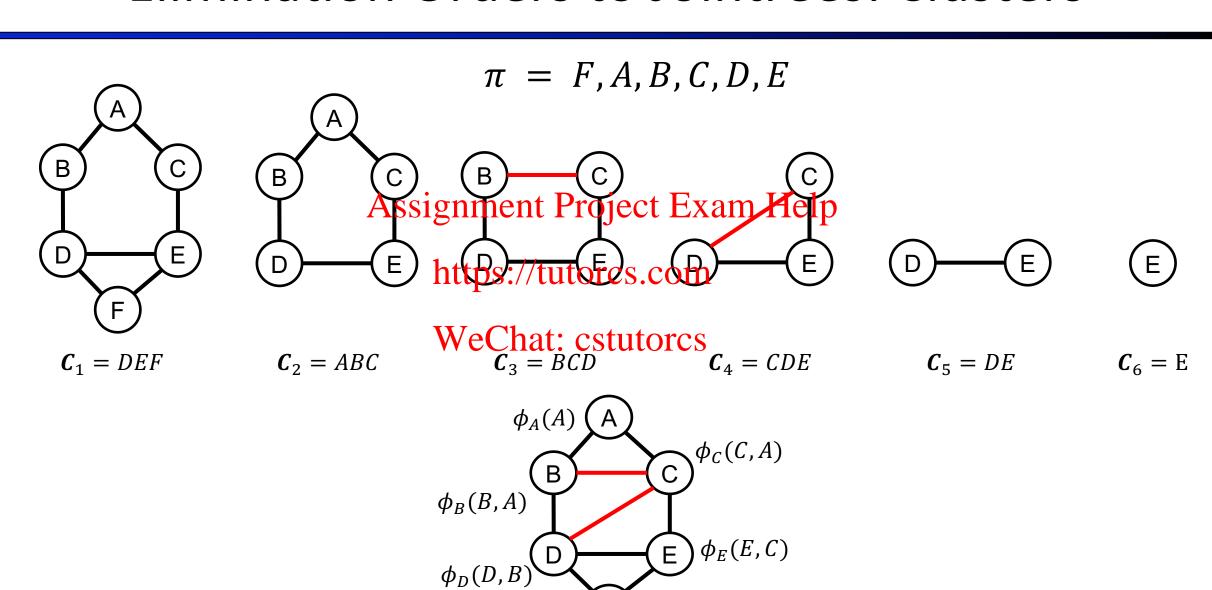
https://tutorcs.com

• Let C_i ,..., C_n be the cluster sequence that results from applying the elimination order π to the undirected graph (or moral graph of a DAG) G. Every family of G is contained in some cluster in the sequence

- C_i ,..., C_n satisfy the first two conditions of the jointree
- The size of each cluster is $\leq width(\pi, G) + 1$

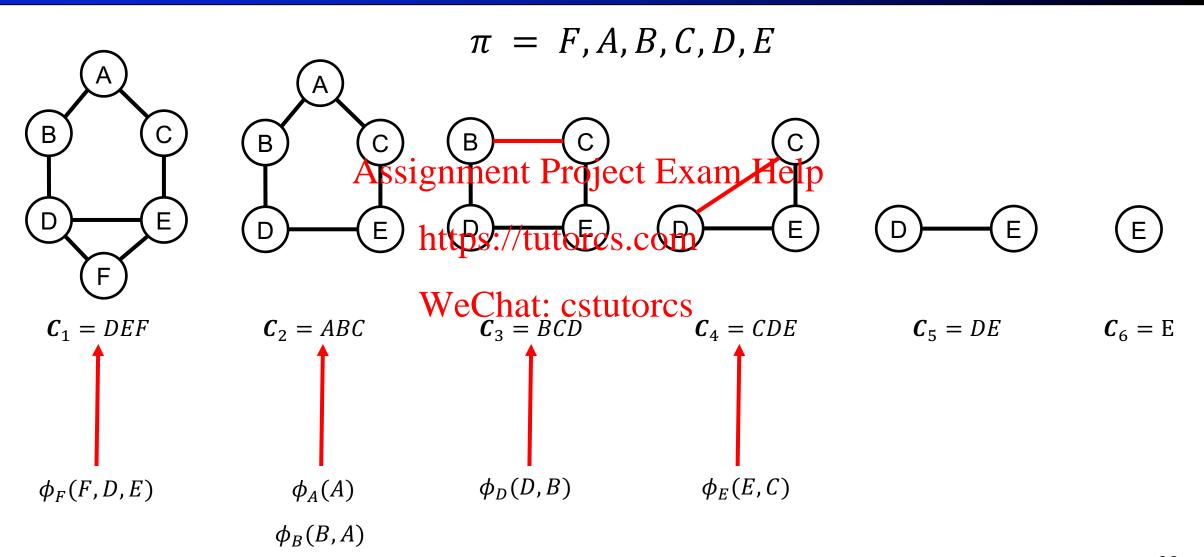


Elimination Orders to Jointrees: Clusters



 $\phi_F(F,D,E)$

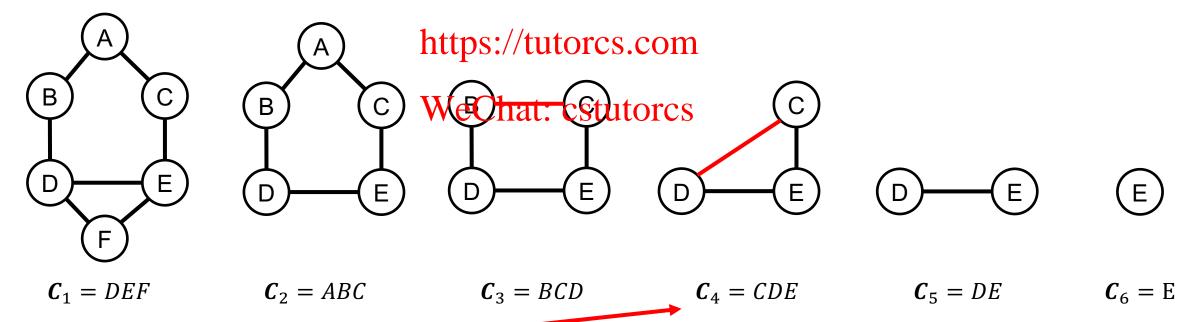
Elimination Orders to Jointrees: Clusters



 $\phi_{\mathcal{C}}(\mathcal{C},A)$

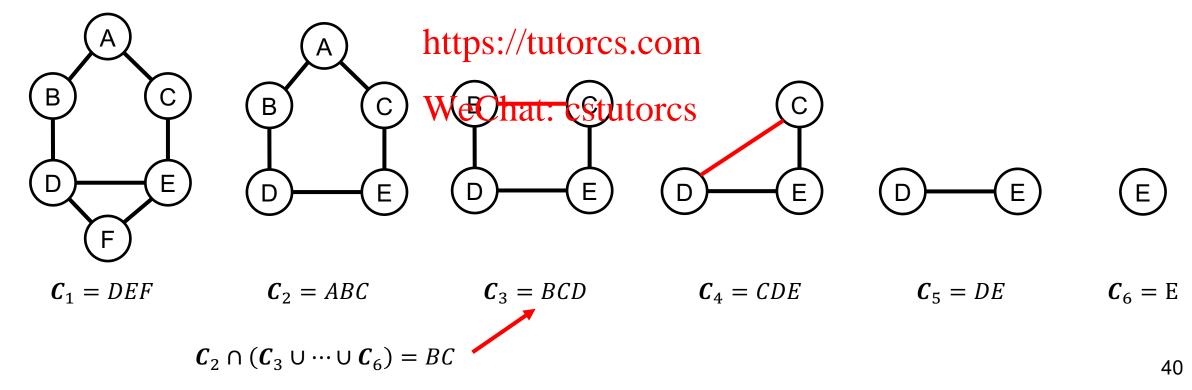
Running Intersection Property

- Let C_i ,..., C_n be the cluster sequence induced by applying elimination order π to graph G.
 - For every i < n, the variables $C_i \cap (C_{i+1} \cup \cdots \cup C_n)$ are contained in some cluster C_j where j > i
 - This is known as the running site rection property of the aust er sequence



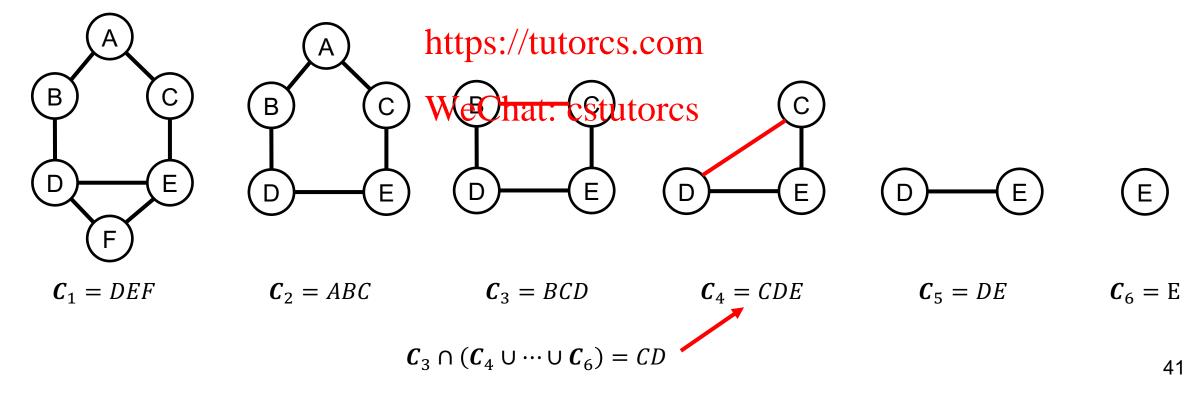
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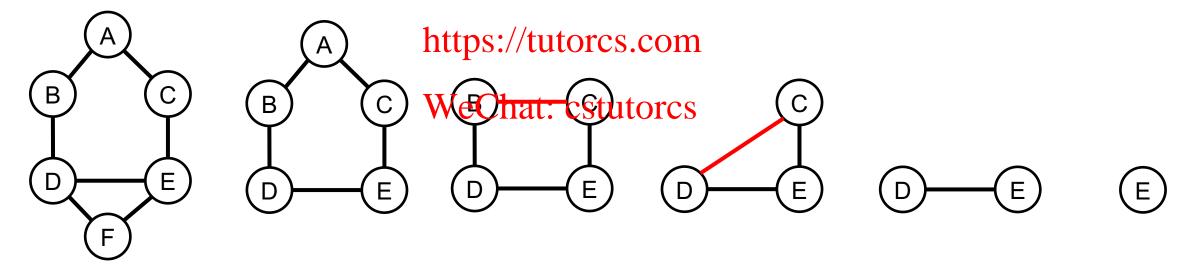
- Nonmaximal clusters are the ones contained in previous clusters of the sequence
 - We can remove a nonmaximal cluster from the sequence

 $C_2 = ABC$

 $C_1 = DEF$

- But we must reorder the sequence to maintain the running intersection property (RIP)
- Keeping the RIP is important with the least of the result of the least of the lea

 $C_3 = BCD$



 $C_4 = CDE$

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 $\boldsymbol{C}_6 = \mathbf{E}$

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$$C_1 = DEF$$

$$C_2 = ABC$$

WeChateGestutorcs
$$C_4 = CDE$$

$$C_5 = DE$$

$$C_6 = E$$

Remove
$$C_5$$
 Move C_1 to C_5 position

$$C_2 = ABC$$

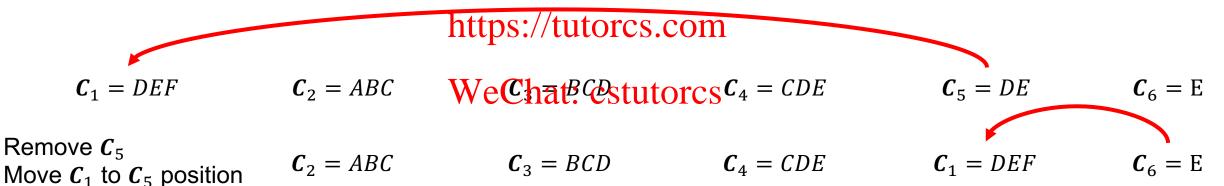
$$C_3 = BCD$$

$$C_A = CDE$$

$$C_1 = DEF$$

$$\boldsymbol{C}_6 = \mathbf{E}$$

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 - But we must reorder the sequence to maintain the running intersection property (RIP)
 - Keeping the RIP is important Name and i Ptoliginal Exhaust Pto a jointree later

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$$C_1 = DEF$$

$$C_2 = ABC$$

WeChateCostutorcs $C_4 = CDE$

$$C_5 = DE$$

$$C_6 = E$$

Remove
$$C_5$$
 Move C_1 to C_5 position

$$C_2 = ABC$$

$$C_3 = BCD$$

$$C_4 = CDE$$

$$C_1 = DEF$$

$$\boldsymbol{C}_6 = \mathbf{E}$$

Remove
$$C_6$$

$$C_2 = ABC$$

$$C_3 = BCD$$

$$C_4 = CDE$$

$$C_1 = DEF$$

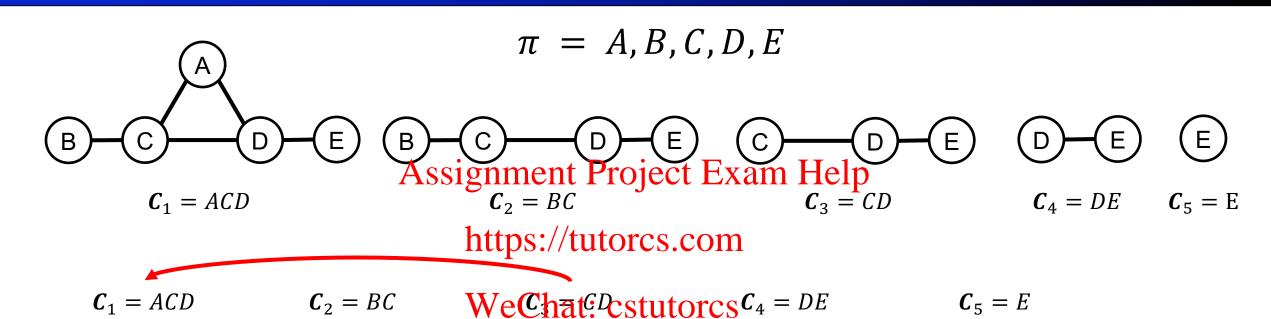
$$C_1 = ABC$$

$$\boldsymbol{C}_2 = BCD$$

$$C_3 = CDE$$

$$C_4 = DEF$$

Nonmaximal Clusters: Another Example



Remove
$$C_3$$

Move C_1 to C_3 position

$$C_2 = BC$$

$$C_1 = ACD$$

$$C_4 = DE$$

$$C_5 = E$$

Remove
$$C_5$$

$$C_2 = BC$$

$$C_1 = ACD$$

$$C_4 = DE$$

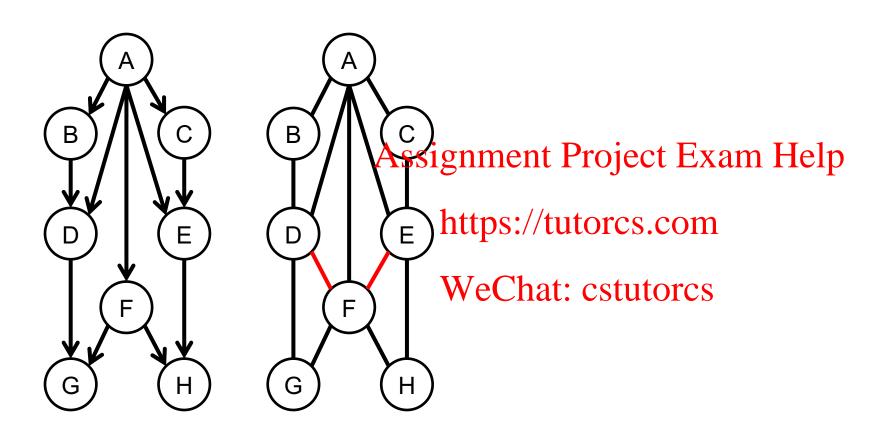
```
C_1, \dots, C_n \leftarrow maximal cluster sequence induced by elimination order \pi
T \leftarrow \{\boldsymbol{C}_n\}
for i \leftarrow n-1, ..., 1 do
           T \leftarrow T \cup \{\boldsymbol{C}_i\}
           add Assignmenta Project Exam Help_{+1} \cup \cdots \cup c_n
return T
                       https://tutorcs.com
                        \boldsymbol{C}_2 = BCD \boldsymbol{C}_3 = CDE \boldsymbol{C}_4 = DEF
C_1 = ABC
                       WeChat: cstutorcs
                               CDE
                                                    BCD
                                                                       ABC
```

```
C_1, \dots, C_n \leftarrow maximal cluster sequence induced by elimination order \pi
T \leftarrow \{\boldsymbol{C}_n\}
for i \leftarrow n-1, ..., 1 do
           T \leftarrow T \cup \{\boldsymbol{C}_i\}
           add Assignmenta Project Exam Help_{+1} \cup \cdots \cup c_n
return T
                       https://tutorcs.com
                         \boldsymbol{C}_2 = BCD \boldsymbol{C}_3 = CDE \boldsymbol{C}_4 = DEF
C_1 = ABC
                       WeChat: cstutercs<sub>4</sub> = DE
                                                     BCD
                                                                         ABC
```

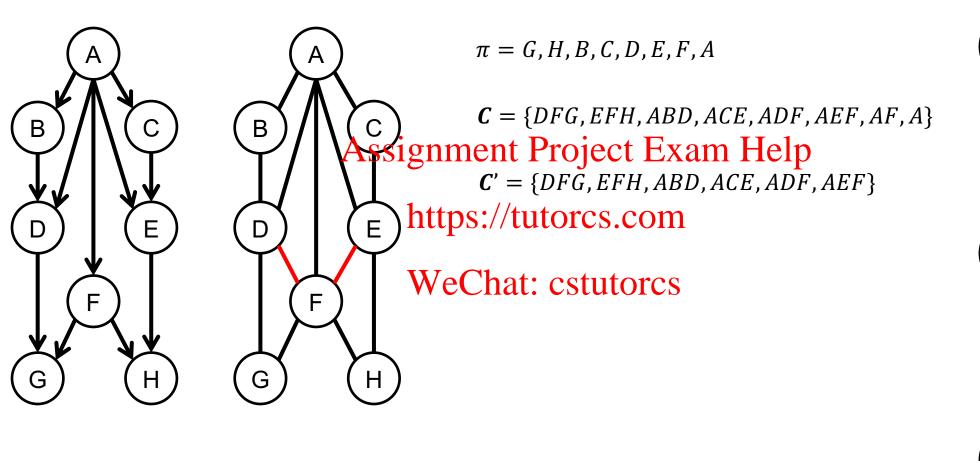
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           T \leftarrow T \cup \{\boldsymbol{C}_i\}
           add Assignmenta Project Exam Help_{+1} \cup \cdots \cup c_n
return T
https://tutorcs.com
c_1 = ABC
c_2 = BCD
c_3 = CDE
c_4 = DEF
                 c<sub>2</sub> \WeChat: Estutores
                                                    BCD
                                                                       ABC
```

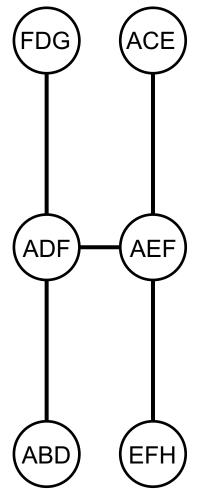
```
C_1, \dots, C_n \leftarrow maximal cluster sequence induced by elimination order \pi
         T \leftarrow \{\boldsymbol{C}_n\}
         for i \leftarrow n-1, \dots, 1 do
                    T \leftarrow T \cup \{\boldsymbol{C}_i\}
                    add Assignmenta Project Exam Help_{+1} \cup \cdots \cup c_n
         return T
         https://tutorcs.com
c_1 = ABC
c_2 = BCD
c_3 = CDE
c_4 = DEF
c_1 \cap (c_2 \cup ... \cup c_4) = BC WeChat: cstutorcs
                                                                                ABC
                                                             BCD
```

Elimination Orders to Jointrees: Example

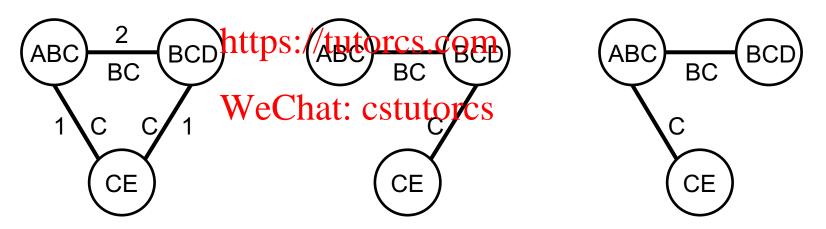


Elimination Orders to Jointrees: Example





```
C_1, ..., C_n \leftarrow maximal cluster sequence induced by elimination order \pi G_c \leftarrow cluster graph of C_1, ..., C_n G_c^{MST} \leftarrow maximum spanning tree of G_c return G_c^{MST} Assignment Project Exam Help
```

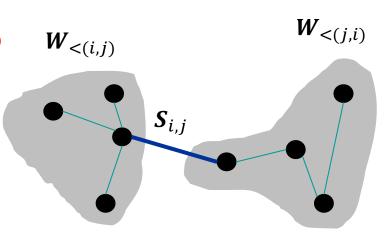


A cluster graph is a complete weighted undirected graph with cost $|C_i \cap C_j|$ assigned to each edge $C_i - C_j$

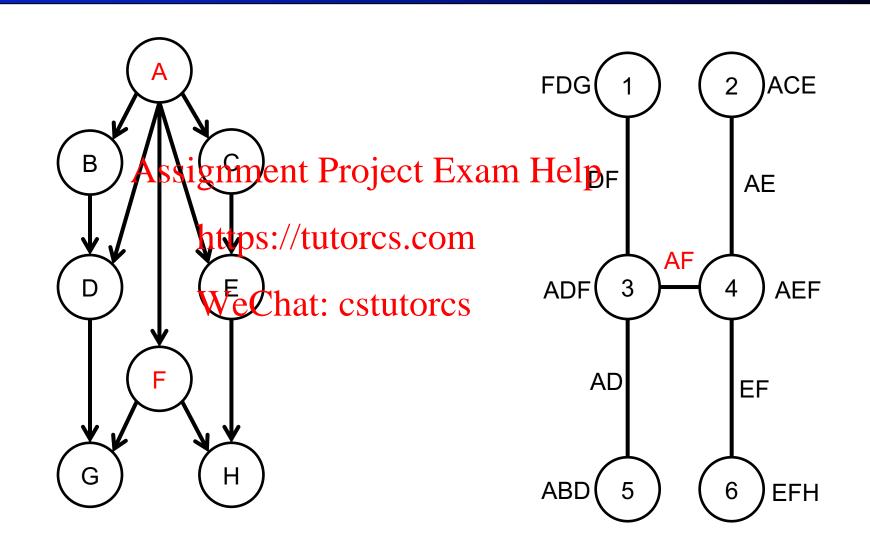
Jointrees and Independence

- For an edge (i, j) be the set of all variables that appear only on the C_i side of the jointree T, let
 - $W_{<(i,j)}$ be the set of all variables that appear only of the C_i side of T
 - $W_{<(j,i)}$ be the set of all variables that C_j be the set of all variables that C_j side of T We Chat: cstutores
 - lacktriangle Variables on both sides are in the separation $oldsymbol{S}_{i,j}$
- Then

$$W_{<(i,j)}\perp W_{<(j,i)}|S_{i,j}$$



Jointrees and Independence



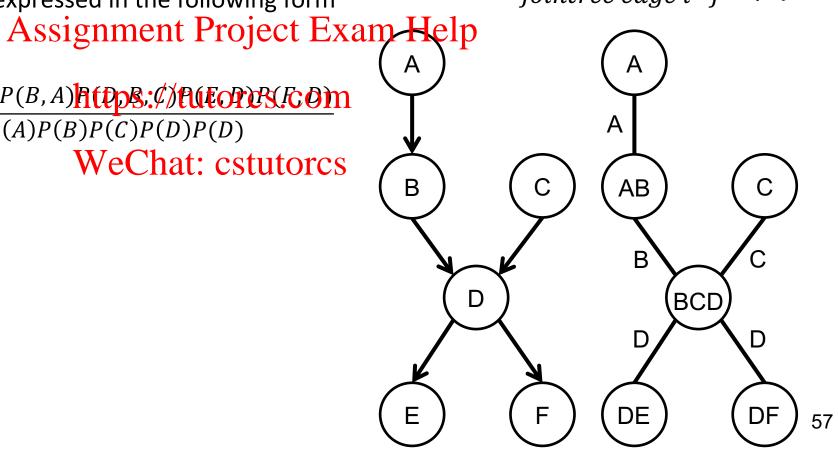
Jointrees as a Factorization Tool

Given a probability distribution P(X) induced by a graph and given a corresponding jointree

The distribution can be expressed in the following form

 $P(X) = \frac{\prod_{jointree\ node\ i} P(\mathbf{C}_i)}{\prod_{jointree\ edge\ i-j} P(\mathbf{C}_i \cap \mathbf{C}_j)}$

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Conclusion

- In this lecture we formalized several concept related to VE and FE
- We defined polynomial time width-preserving algorithms to convert
 - Elimination orders to Acintgennent Project Exam Help
 - Jointrees to elimination orders
- Me also discussed approaches to find optimal prefixes and treewidth lower bound
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 - These algorithms have practical implications since they can be used with heuristics and search methods
- Tasks
 - Read Chapter 9 from the textbook (Darwiche)