# **CS726** Programming Assignment – 1 Report

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# 1 Triangulation

This step is implemented in the function triangulate\_and\_get\_cliques. We first check if the graph is already triangulated, using the function whether\_triangulated described below:

### Algorithm 1 Check if Graph is already Triangulated

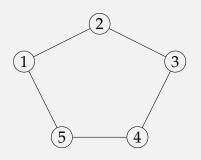
```
    cycles ← Find all cycles in graph
    for each cycle in cycles do
    if length of cycle ≥ 4 then
    if there is no shortcut (vertices connected by non-cycle edge) then
    return False
    end if
    end for
    return True
```

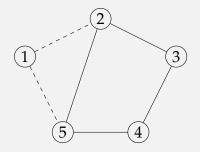
If the graph is already triangulated, we directly proceed with extracting the maximal cliques. If the graph is not triangulated, we first triangulate it using the minimum degree heuristic, as described in the pseudocode below:

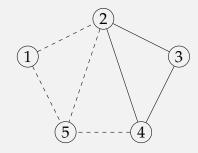
#### **Algorithm 2** Triangulation Process

```
1: vertices_left ← Set of all vertices
   while vertices_left is not empty do
      vertex ← Vertex in vertices_left with minimum degree
3:
      for each pair (i, j) of neighbours of vertex do
4:
5:
          if the graph does not contain an edge between i and j then
             Add edge (i, j) to the original graph
6:
          end if
7:
      end for
8:
9:
      Remove vertex from vertices_left
      Update graph by removing vertex and updating degrees and edges
10:
11: end while
```

The figure below shows the run of the triangulation algorithm on an example graph:

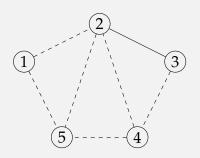


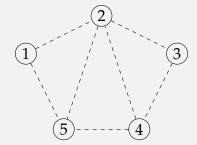


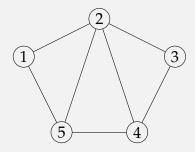


Step 1: Initial Graph

Step 2: Select 1, add (5,2), remove 1 Step 3: Select 5, add (4,2), remove 5







Step 4: Select 4, remove 4

Step 5: Select 2, remove 2

Final Triangulated Graph

Once we obtain the triangulated graph, we extract the maximal cliques from it using the function get\_maximal\_cliques, which uses the Bron-Kerbosch algorithm described below:

### Algorithm 3 Bron–Kerbosch Algorithm for Finding Maximal Cliques

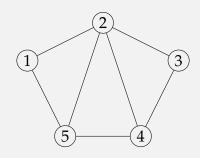
```
1: procedure BRON_KERBOSCH(current_clique, candidates, excluded, maximal_cliques)
      if candidates is empty and excluded is empty then
2:
          Add current_clique to maximal_cliques
3:
4:
          return
      end if
5:
      for each vertex v in candidates do
6:
          Bron_Kerbosch(current_clique \cup \{v\},
7:
                candidates \cap Neighbors(v),
8:
                excluded \cap Neighbors(v),
9:
                maximal_cliques)
10:
11:
          Remove v from candidates
          Add v to excluded
12:
      end for
13:
14: end procedure
```

# 2 **Junction Tree Construction**

This step is implemented in the get\_junction\_tree function. We use the maximal cliques obtained after the triangulation process to create the junction tree while maintaining the running intersection property. Each clique in this tree retains its assigned potential values. Consider the given triangulated graph:

### Algorithm 4 Constructing a Junction Tree from Maximal Cliques

```
Require: Set of maximal cliques C
Ensure: Junction tree satisfying the running intersection property
 1: Initialize an empty priority queue T
    for all pairs (C_1, C_2) in C do
        Compute the intersection set S = C_1 \cap C_2
 3:
        if S \neq \emptyset then
 4:
            Compute weight w = |S|
 5:
            Push (-w, C_1, C_2) onto T (negative weight for max heap)
 6:
        end if
 7:
 8: end for
 9:
10: Initialize parent[C] = C and rank[C] = 0 for all C \in C
11:
12: function FINDPARENT(C)
        if parent[C] \neq C then
13:
            parent[C] \leftarrow FindParent(parent[C])
14:
        end if
15:
        return parent [C]
16:
17: end function
18:
19: function UNION(C_1, C_2)
20:
        root_1 \leftarrow FindParent(C_1)
        root_2 \leftarrow FindParent(C_2)
21:
22:
        if root_1 \neq root_2 then
            if rank[root_1] > rank[root_2] then
23:
                parent[root_2] \leftarrow root_1
24:
            else if rank[root_2] > rank[root_1] then
25:
               parent[root_1] \leftarrow root_2
26:
27:
            else
                parent[root_2] \leftarrow root_1
28:
               rank[root_1] \leftarrow rank[root_1] + 1
29:
            end if
30:
            return True
31:
        end if
32:
        return False
33:
34: end function
35:
36: Initialize an empty set MST (Minimum Spanning Tree)
37: while T is not empty do
        Pop (w, C_1, C_2) from T
38:
        if UNION(C_1, C_2) then
39:
40:
            Add edge (C_1, C_2) to MST
        end if
41:
42: end while
43: return MST
```



Final Triangulated Graph

From the triangulated graph, we obtain the maximal cliques:

$$C_1 = \{1, 2, 5\}, \quad C_2 = \{2, 3, 4\}, \quad C_3 = \{2, 4, 5\},$$

The intersection sets are as follows:

$$C_1 \cap C_3 = \{2,5\}, \quad |C_1 \cap C_3| = 2$$
  
 $C_1 \cap C_2 = \{2\}, \quad |C_1 \cap C_2| = 1$   
 $C_3 \cap C_2 = \{2,4\}, \quad |C_3 \cap C_2| = 2$ 

We construct edges with weights corresponding to intersection sizes:

$$(C_1, C_3, 2), (C_3, C_2, 2), (C_1, C_2, 1)$$

Using Kruskal's algorithm:

- 1. Sort edges:  $(C_1, C_3, 2)$ ,  $(C_3, C_2, 2)$ ,  $(C_1, C_2, 1)$ .
- 2. Add  $(C_1, C_3)$  (weight 2).
- 3. Add  $(C_3, C_2)$  (weight 2).
- 4. Ignore  $(C_1, C_2)$  (weight 1) as it would form a cycle.

#### **Final Junction Tree:**

$$C_1 \leftrightarrow C_3 \leftrightarrow C_2$$

$$C_1 \qquad \qquad C_3 \qquad \qquad C_2$$

For any two cliques  $C_i$  and  $C_j$  containing the same variable X, all cliques along the unique path in the tree must contain X. This holds for all intersections.

# 3 Marginal Probability

Here is the pseudocode for sharing messages between the maximal cliques of the graph.

# Computing the partition function

Firstly, we show how to calculate the Z value for the given graph. So, we first select a root node and then perform a depth-first search (DFS) to calculate the depth of each maximal clique (node in the junction tree). Then, we send messages from the deepest leaves till the root node. Finally, we calculate the partition function using the root clique potential and the received messages. (Messages are being sent again from root to the internal nodes and finally to the leaves, to be used in the next step of computing marginal probabilities.)

### **Algorithm 5** Computation of Partition Function Z

```
Require: Graphical Model with maximal cliques and potentials
Ensure: Partition function Z
 1: Construct the junction tree JT from maximal cliques
 2: Initialize adjacency list JT_{adj} from JT
 3: Select a root clique C_{root}
 4: Initialize depth map with C<sub>root</sub> at depth 0
 5: function DFS(node, parent, depth)
       for each child in JT_{adi}[node] do
 6:
           if child \neq parent then
 7:
               Update depth map
 8:
               Call DFS on child with depth +1
 9:
           end if
10:
       end for
11:
12: end function
13: Perform DFS from C_{root}
   function SENDMESSAGE(C_{from}, C_{to})
14:
       Compute separator set S = C_{from} \cap C_{to}
15:
       Initialize message vector M of size 2^{|S|}
16:
       Modify clique potential based on incoming messages
17:
18:
       for each state assignment in C_{from} do
19:
           Compute corresponding separator index
           Aggregate message value
20:
       end for
21:
       Store message M(C_{from} \rightarrow C_{to})
22:
23: end function
24: Initialize messages dictionary
25: Initialize clique potentials
26: for each clique from deepest to root do
27:
       Send messages to parent cliques
28: end for
29: for each clique from root to leaves do
       Send messages to child cliques
30:
31: end for
32: Compute partition function Z using root clique potential and received messages
33: return Z
```

### Computing the marginal probabilities

Here is the pseudocode for computing the marginal probabilities in the graphical model using message passing. We get the partition function Z from the previous step and use it to normalize the marginal probabilities. We iterate over each variable in the graphical model and find the maximal clique containing it. We then extract the potential function for the clique (using the messages received from neighboring cliques) and compute the marginal probability for the variable. (For every variable, we need to do this only for one clique containing it, as the marginal probability will be the same in all maximal cliques containing the variable.)

```
Algorithm 6 Computation of Marginal Probabilities
```

```
Require: Graphical Model with maximal cliques, clique potentials, and messages
Ensure: Marginal probabilities for each variable
 1: Initialize adjacency list for junction tree
 2: Retrieve partition function Z using previously computed values
 3: Initialize marginal probability list M with zeros
 4: for each variable X_i in the graphical model do
 5:
       Find a maximal clique C containing X_i
       Extract the potential function for clique C
 6:
       for each neighboring clique C' of C do
 7:
           Compute separator set S = C \cap C'
 8:
           Retrieve message M(C' \rightarrow C)
 9:
           for each assignment in C do
10:
              Identify corresponding index in S
11:
12:
              Multiply message values with clique potential
           end for
13:
       end for
14:
       Compute marginal probability for X_i
15:
       Normalize values using Z
16:
17: end for
18: return M
```

# 4 Finding the Most Probable Assignment

Here is the pseudocode for finding the top-K most probable assignments in the graphical model. The value of the partition function Z is used from the previous step. Similar to the previous step, we do a DFS to calculate the depth of each maximal clique. We then send messages from the deepest leaves to the root node. This time the messages which are being send are of a different format, and they contain the following two values:

- The union of all sets of variables seen so far (from its descendants and including itself).
- Mapping between the assignments of the variables in the union set, and the corresponding product of potentials.

Moreover, to optimize, we are not sending all the assignments in the message, but only the top-K most probable assignments, where top-K is being performed over all the variables present in the current maximal clique, but not in the descendants. Finally, we send a message from the root node to "None", which basically collects the assignments of all the variables in the graphical model. We then normalize the probabilities and return the top-K most probable assignments.

### Algorithm 7 Compute the Top-K Most Probable Assignments in the Graphical Model

```
1: junction_t ree \leftarrow getJunctionTree()
2: junction\_tree\_adj\_list \leftarrow
3: for each edge (a, b) in junction_tree do
       junction\_tree\_adj\_list[a] \leftarrow junction\_tree\_adj\_list[a] \cup b
5:
       junction\_tree\_adj\_list[b] \leftarrow junction\_tree\_adj\_list[b] \cup a
6: end for
7: root \leftarrow select a maximal clique as root
8: depth\_map[root] \leftarrow 0
9: procedure DFS(node, parent, depth)
       for each child in junction_tree_adj_list[node] do
10:
11:
           if child \neq parent then
12:
               depth\_map[child] \leftarrow depth
               DFS(child, node, depth + 1)
13:
           end if
14:
       end for
15:
16: end procedure
17: DFS(root, None, 1)
18: procedure SENDMESSAGE(from_clique, to_clique, parent_map, clique_potentials, messages)
19:
       variables\_seen \leftarrow all variables in from\_clique
       for each neighbor in parent_map[from_clique] do
20:
           if neighbor \neq to\_clique and (neighbor, from\_clique) \in messages then
21:
               variables\_seen \leftarrow variables\_seen \cup variables in messages[(neighbor, from\_clique)]
22:
           end if
23:
       end for
24:
       Initialize message_to_send with all entries set to 1
25:
       for each possible assignment in message_to_send do
26:
27:
           Compute index in from_potential
           Multiply with clique potential and incoming messages
28:
29:
       end for
       Store message in messages[(from_clique, to_clique)]
30:
31: end procedure
32: messages \leftarrow \{\}
33: clique\_potentials \leftarrow getCliquePotentials()
34: max\_depth \leftarrow max depth in depth\_map
35: for depth = max\_depth to 0 do
       for each clique with depth d = depth do
36:
           Identify parent clique(s)
37:
           for each parent p do
38:
               SENDMESSAGE(clique, p, junction_tree_adj_list, clique_potentials, messages)
39:
           end for
40:
       end for
41:
42: end for
43: SENDMESSAGE(root, None, junction_tree_adj_list, clique_potentials, messages)
44: Normalize probabilities and sort assignments
45: return top-k assignments
```