CS 726: Programming Assignment 1

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1 Preprocessing

The preprocessing step involves converting the given data into a suitable format for further processing. We have done the following preprocessing steps:

- 1. Clique Potentials: Converted all the cliques and potentials data into a dictionary format. The keys of the dictionary are the cliques and the values are the potentials. If a clique already exists in the dictionary, we multiply the potential with the existing potential.
- 2. **Edges:** Converted all the cliques into a set of tuples, where each tuple consists of two nodes that are connected by an edge.
- 3. **Nodes:** Converted the edge set into a set of all the nodes in the graph.

2 Triangulation

2.1 triangulate_and_get_cliques

Here are some of the functions we have defined for the triangulation and maximum clique finding process:

1. **is_simplicial:** This function checks if a given node is simplicial in the graph. A node is simplicial if the neighbors of the node form a clique.

Algorithm 1 Check if a vertex is simplicial

```
1: function IsSimplicial(adjlist, node)
       neighbors \leftarrow adjlist[node]
2:
       for i \leftarrow 1 to |neighbors| do
3:
           for j \leftarrow i+1 to |neighbors| do
 4:
               if neighbors[j] \notin adjlist[neighbors[i]] then
5:
                   return False
 6:
               end if
 7:
           end for
8:
9:
       end for
       return True
10:
11: end function
```

2. **find_simplicial_vertex:** This function finds a simplicial vertex in the graph. If no simplicial vertex is found, it returns None.

Algorithm 2 Find a simplicial vertex

```
1: function FINDSIMPLICIALVERTEX(adjlist)
2: for node in adjlist do
3: if IsSIMPLICIAL(adjlist, node) then
4: return node
5: end if
6: end for
7: return None
8: end function
```

3. **make_vertex_simplicial:** This function makes a given node simplicial by adding edges between all the neighbors of the node.

Algorithm 3 Make a vertex simplicial

```
1: function MakeVertexSimplicial(adjlist, node)
       neighbors \leftarrow adjlist[node]
2:
       for i \leftarrow 1 to |neighbors| do
3:
4:
           for j \leftarrow i + 1 to |neighbors| do
               if neighbors[j] \notin adjlist[neighbors[i]] then
5:
                  adjlist[neighbors[i]].append(neighbors[j])
6:
                   adjlist[neighbors[j]].append(neighbors[i])
7:
               end if
8:
           end for
9:
       end for
10:
       return adilist
11:
12: end function
```

- 4. **chordal_graph_with_heuristic:** In this function we do the following:
 - (a) Find a simplicial vertex in the graph.
 - (b) If a simplicial vertex is found, take its neighbors and store it in the maximum clique list.
 - (c) If no simplicial vertex is found, take a node based on the heuristic that the node has the minimum degree. Make this node simplicial and take its neighbors and store it in the maximum clique list.
 - (d) Repeat the process until all the nodes are covered.
 - (e) If a clique found is already a subset of a previously found clique, discard it.
 - (f) Return the maximal cliques found.

Algorithm 4 Compute chordal graph with heuristic

```
1: function CHORDALGRAPHWITHHEURISTIC(adjlist)
       chordal\_adjlist \leftarrow deepcopy(adjlist)
2:
       elimination\_order, cliques \leftarrow [], []
3:
4:
       while |elimination\_order| < |adjlist| do
           node \leftarrow \text{FINDSIMPLICIALVERTEX}(chordal\_adjlist)
5:
           if node = None then
6:
               node \leftarrow \arg\min\{|neighbors| : node \in chordal\_adjlist\}
7:
               chordal\_adjlist \leftarrow MakeVertexSimplicial(chordal\_adjlist, node)
8:
           end if
9:
10:
           elimination\_order.append(node)
           clique \leftarrow \{node\} \cup \{n \mid n \in chordal\_adjlist[node], \forall i \in clique, n \in \{node\}\}
11:
   chordal\_adjlist[i]
           cliques.append(clique)
12:
           for neighbor \in chordal\_adjlist[node] do
13:
               chordal\_adjlist[neighbor].remove(node)
14:
15:
           end for
16:
           delete\ chordal\_adjlist[node]
       end while
17:
       return FilterMaximalCliques(cliques)
18:
19: end function
```

3 Junction Tree Construction

3.1 get_junction_tree

In this section, we have defined the following functions for constructing the junction tree:

1. **create_junction_graph**: This function creates a junction graph from the found maximal cliques. We iterate over all the maximal cliques and add an edge between two maximal cliques if they have a common node. We also assign a weight to each edge which is the size of the intersection of the two maximal cliques.

Algorithm 5 Create Junction Graph

```
1: function CreateJunctionGraph(cliques)
         J \leftarrow \{\}
2:
         for C_1, C_2 \in cliques, C_1 \neq C_2 do
3:
              I \leftarrow C_1 \cap C_2
4:
              if I \neq \emptyset then
5:
                  w \leftarrow |I|
6:
                  J[C_1] \leftarrow J[C_1] \cup \{(C_2, w)\}
 7:
                  J[C_2] \leftarrow J[C_2] \cup \{(C_1, w)\}
8:
              end if
9:
         end for
10:
         return J
11:
12: end function
```

2. make_junction_tree: This function creates a junction tree from the junction

graph. We first find the maximum spanning tree of the junction graph using Kruskal's algorithm. This tree is the junction tree.

Algorithm 6 Make Junction Tree

```
1: function MakeJunctionTree(J)
        E \leftarrow \text{sorted edges of } J \text{ by weight (descending)}
        Initialize parent, rank for union-find
3:
        T \leftarrow \{\}
4:
        for (C_1, C_2, w) \in E do
5:
            if FIND(C_1) \neq FIND(C_2) then
6:
                 UNION(C_1, C_2)
7:
                 T[C_1] \leftarrow T[C_1] \cup \{C_2\}
8:
                 T[C_2] \leftarrow T[C_2] \cup \{C_1\}
9:
            end if
10:
        end for
11:
        return T
12:
13: end function
```

3. **get_message_passing_order**: This function gets the order in which the messages should be passed in the junction tree. We do a depth-first search on the junction tree and store the order in which the nodes are visited. Here first a tree is created from the junction tree and then a post-order traversal and a pre-order traversal is done to get the message passing order.

Algorithm 7 Get Message Passing Order

```
1: function GetMessageOrder(T, root)
2:
      Initialize D, P with BFS from root
3:
      C2P, P2C \leftarrow []
4:
      procedure Postorder (node)
          for child \in D[node] do
5:
             Postorder(child)
6:
             C2P.append((child, node))
7:
          end for
8:
      end procedure
9:
      procedure Preorder (node)
10:
          for child \in D[node] do
11:
             P2C.append((node, child))
12:
             Preorder(child)
13:
          end for
14:
      end procedure
15:
      Postorder(root), Preorder(root)
16:
      return C2P + P2C
17:
18: end function
```

3.2 assign_potentials_to_cliques

In this section, we have defined the following functions for assigning potentials to the cliques:

1. **multiply_potentials**: This function takes two potentials and there corresponding cliques and multiplies them to get a new potential and a new clique.

Algorithm 8 Multiply Potentials

```
1: function MultiplyPotentials(P_1, P_2, D_1, D_2)
          D \leftarrow D_1 \cup D_2
 2:
          P_{new} \leftarrow \text{array of size } 2^{|D|} \text{ initialized to None}
 3:
          for val \in \{0, 1\}^{|D|} do
 4:
                A \leftarrow \text{mapping of } D \text{ to } val
 5:
                i_1 \leftarrow \text{index of } A \text{ restricted to } D_1
 6:
               i_2 \leftarrow \text{index of } A \text{ restricted to } D_2
 7:
                i_{new} \leftarrow \text{index of } A \text{ over } D
 8:
                P_{new}[i_{new}] \leftarrow P_1[i_1] \times P_2[i_2]
 9:
          end for
10:
          return (P_{new}, D)
11:
12: end function
```

After this we iterate over all the maximal cliques and for each clique, we find all the clique potentials that are subsets of the maximal clique. We multiply all these potentials to get the potential for the maximal clique.

Algorithm 9 Compute Maximum Clique Potentials

```
1: MCP \leftarrow \{\}
                                                                    2:\ VC \leftarrow \{\}
                                                                            ▶ Tracks visited cliques
 3: CA \leftarrow \{\}

⊳ Stores assigned cliques

 4: for MC \in max\_cliques do
        SC \leftarrow \{\}
                                                                           \triangleright Subset cliques of MC
 5:
 6:
        CA[MC] \leftarrow []
        for C \in clique\_potentials do
 7:
            if C \subseteq MC and C \notin VC then
 8:
                SC \leftarrow SC \cup \{C\}
 9:
                VC \leftarrow VC \cup \{C\}
10:
                CA[MC] \leftarrow CA[MC] \cup \{C\}
11:
            end if
12:
        end for
13:
14:
        (P, D) \leftarrow (clique\_potentials[first(SC)], first(SC))
        for C \in SC[1:] do
15:
            (P, D) \leftarrow \text{MULTIPLYPOTENTIALS}(P, clique\_potentials[C], D, C)
16:
        end for
17:
        USC \leftarrow \bigcup SC
                                                                          ▶ Union of subset cliques
18:
        LN \leftarrow MC - USC
                                                                                 ▶ Remaining nodes
19:
20:
        for N \in LN do
21:
            (P, D) \leftarrow \text{MULTIPLYPOTENTIALS}(P, [1, 1], D, \{N\})
22:
        end for
        MCP[MC] \leftarrow P
23:
24: end for
```

4 Marginal Probability

4.1 get_z_value

In this section, we have defined the following functions for finding the Z value:

1. **create_empty_message_dict**: This function creates an empty message dictionary for all the cliques in the junction tree. The dictionary has the sender clique as the key and the value is a dictionary with the receiver clique as the key and its value is the message from the sender clique to the receiver clique.

Algorithm 10 Create Empty Message Dictionary

```
1: function CreateEmptyMessageDict(J)
2:
        M \leftarrow \{\}
       for N \in J do
3:
            M[N] \leftarrow \{\}
 4:
            for N' \in J[N] do
5:
               M[N][N'] \leftarrow \text{None}
 6:
            end for
 7:
       end for
8:
9:
       return M
10: end function
```

2. **multiply_messages**: This function takes a potential of the clique or a precomputed value (potential is already multiplied with some messages) and a message to be multiplied as input and it multiplies them to get a new potential.

Algorithm 11 Multiply Messages

```
1: function MultiplyMessages(P, M, N, D)
 2:
           P' \leftarrow \text{copy of } P
           for val \in \{0,1\}^{|N|} do
 3:
                A \leftarrow \text{mapping of } N \text{ to } val
 4:
                i_m \leftarrow \text{index of } A \text{ restricted to } D
 5:
                i_p \leftarrow \text{index of } A \text{ over } N
 6:
                \overset{\scriptscriptstyle{P}}{P'}[i_p] \leftarrow P'[i_p] \times M[i_m]
 7:
 8:
           end for
           return P'
 9:
10: end function
```

- 3. **condense_message**: This function takes a potential and the nodes to be marginalized on and marginalizes the potential to get a new potential.
- 4. **message_passing_opt_order**: This function takes the message passing order and the junction tree and passes the messages in the optimal order. It updates the message dictionary with the new messages.
- 5. **calc_z**: This function calculates the Z value using the fully updated message dictionary. We simply choose any maximal clique and marginalize it on all it component nodes to get the Z value.

Algorithm 12 Condense Message

```
1: function CondenseMessage(P, N, C, S)
 2:
         P' \leftarrow []
         for va\ddot{l} \in \{0,1\}^{|C|} do
 3:
              sum\_val \leftarrow 0
 4:
              for val' \in \{0,1\}^{|N|-|C|} do
 5:
                  A \leftarrow \text{merge of } C \mapsto val \text{ and } S \mapsto val'
 6:
                  i \leftarrow \text{index of } A \text{ over } N
 7:
                  sum\_val \leftarrow sum\_val + P[i]
 8:
              end for
 9:
              Append sum\_val to P'
10:
         end for
11:
12:
         return P'
13: end function
```

Algorithm 13 Calculate Partition Function Z

```
1: function CALCZ(M, P)

2: N \leftarrow \text{first key in } P

3: Z \leftarrow P[N]

4: for N' \in M[N] do

5: Z \leftarrow \text{MULTIPLYMESSAGES}(Z, M[N'][N], N, N \cap N')

6: end for

7: Z \leftarrow \text{CONDENSEMESSAGE}(Z, N, [], N)

8: return Z[0]

9: end function
```

Algorithm 14 Message Passing with Optimized Order

```
1: function MessagePassingOptOrder(J, P, O)
        M \leftarrow \text{CreateEmptyMessageDict}(J)
2:
3:
        for (C, N) \in O do
            P' \leftarrow \text{copy of } P[C]
4:
            for N' \in J[C] \setminus \{N\} do
5:
                P' \leftarrow \text{MultiplyMessages}(P', M[N'][C], C, C \cap N')
6:
            end for
7:
            D \leftarrow C \setminus N
8:
            S \leftarrow C \setminus D
9:
            M[C][N] \leftarrow \text{CondenseMessage}(P', C, S, D)
10:
        end for
11:
        return M
13: end function
```

4.2 compute_marginals

In this section, we have defined the following functions for computing the marginals:

- 1. multiply_messages: Same as defined before
- 2. **condense_message**: Same as defined before

After this we iterate over each node. For each node we find a maximal clique that contains the node. We then multiply all the messages from the maximal clique to the node to get the marginal probability.

Algorithm 15 Compute Marginals

```
1: M \leftarrow \text{list of size } |N| \text{ initialized to } [0,0]
 2: for i, n in N do
         C \leftarrow \text{first clique in } C_{max} \text{ containing } n
         P \leftarrow \text{copy of } P[C]
 4:
         for N' \in J[C] do
              P \leftarrow \text{MULTIPLYMESSAGES}(P, M_{dict}[N'][C], C, C \cap N')
 6:
 7:
         end for
         P \leftarrow \text{CondenseMessage}(P, C, \{n\}, C \setminus \{n\})
 8:
         M[i][0] \leftarrow P[0]/Z
 9:
         M[i][1] \leftarrow P[1]/Z
10:
11: end for
12: return M
```

5 MAP Assignment

In this section we have to find the MAP assignment. This can be done by putting k=1 in the top k assignments function (compute_top_k).

6 Top k Assignments

In this section, we have defined the following functions for computing the top k assignments:

- 1. create_empty_message_dict: Same as defined before
- 2. **multiply_messages**: This is similar to the previous function but it also keeps track of the assignments and potential values for each assignment.

Algorithm 16 Multiply Messages

```
1: function MULTIPLYMESSAGES(potential, message, node, mesg_depends_on)
2:
       potential\_new \leftarrow empty list
3:
       for val in all combinations of [0, 1] for node do
           assignmt \leftarrow map \ node \ to \ val
4:
5:
           targ\_idx \leftarrow index from assignmt for mesg\_depends\_on
           node\_idx \leftarrow index from assignmt for node
6:
           for pot_assqn in potential[node_idx] do
 7:
              for mesg\_assgn in message[targ\_idx] do
8:
                  if assignments match on mesq_depends_on then
9:
                      new\_assqn \leftarrow combine\ pot\_assqn\ and\ mesq\_assqn
10:
                      Append new\_assgn to potential\_new[node\_idx]
11:
                  end if
12:
              end for
13:
           end for
14:
       end for
15:
       return potential_new
16:
17: end function
```

- 3. **condense_message**: Similar to the previous function but it also keeps track of the top k assignments and potential values for each assignment.
- 4. **message_passing_opt_order_topk**: This function is similar to the previous function but it also keeps track of the top k assignments and potential values for each assignment.

Finally, we take a sample maximal clique and multiply all the messages from the maximal clique to the node to get the top k assignments.

Algorithm 17 Condense Message

```
1: function CondenseMessage(potential, node, compl_to_topk_on, to_topk_on)
2:
       new\_potential \leftarrow empty list
       for val in all combinations of [0, 1] for compl_to_topk_on do
3:
           topk\_things \leftarrow \text{empty list}
 4:
           for val1 in all combinations of [0, 1] for to_topk_on do
5:
               assignmt \leftarrow combine \ val \ and \ val 1
6:
               idx \leftarrow index from assignmt for node
 7:
               for pot\_assgn in potential[idx] do
8:
9:
                   Update pot\_assqn with val1
10:
                   Append pot_assqn to topk_things
               end for
11:
           end for
12:
           Sort topk\_things and keep top k
13:
           Append topk\_things to new\_potential
14:
       end for
15:
16:
       return new\_potential
17: end function
```

Algorithm 18 Message Passing with Optimal Order and Top-K

```
1: function MESSAGEPASSINGOPTORDERTOPK(junc_tree, potentials, opt_order)
       message\_dict \leftarrow CreateEmptyMessageDict(junc\_tree)
2:
       for (m_clique, neigh) in opt_order do
3:
           potn\_message \leftarrow initialize \text{ with } potentials[m\_clique]
4:
           for neigh1 in junc_tree[m_clique] do
5:
6:
              if neigh1 \neq neigh then
                  potn\_message \leftarrow MultiplyMessages(potn\_message,
 7:
                     message\_dict[neigh1][m\_clique], m\_clique,
8:
                     intersection of m\_clique and neigh1)
9:
               end if
10:
           end for
11:
           message\_dict[m\_clique][neigh] \leftarrow CondenseMessage(
12:
13:
             potn_message, m_clique,
             difference of m\_clique and neigh,
14:
             intersection)
15:
       end for
16:
       {f return}\ message\_dict
17:
18: end function
```

Algorithm 19 Sampling and Returning Top-K Assignments

```
1: message\_dict \leftarrow MessagePassingOptOrderTopK(
      junction_tree, max_clique_potentials, opt_order)
3: sample\_node \leftarrow first node in max\_cliques
4: sample\_node\_potential \leftarrow initialize with max\_clique\_potentials[sample\_node]
5: for neigh in junction_tree[sample_node] do
       sample\_node\_potential \leftarrow MultiplyMessages(
6:
             sample\_node\_potential, message\_dict[neigh][sample\_node],
7:
             sample_node, intersection of sample_node and neigh)
8:
9: end for
10: top_k\_assignments \leftarrow CondenseMessage(
      sample\_node\_potential, sample\_node, [], sample\_node)
12: top\_k\_dict\_list \leftarrow empty list
13: for assgn in top\_k\_assignments[0] do
       assign\_list \leftarrow sorted values from <math>assgn[1]
       dict\_entry \leftarrow \{
15:
             "assignment": assign\_list,
16:
17:
             "probability": assgn[0]/z
18:
       Append dict_entry to top_k_dict_list
19:
20: end for
21: return top_k_dict_list
```

Contributions

- Deeptanshu Malu: Primarily responsible for:
 - 1. Triangulation implementation and testing.
 - 2. Junction Graph Construction and validation.
 - 3. Development and optimization of message and potential multiplication/condensation for Marginal Probability, Z Value, and Top k Assignments.
 - 4. Implementation of the Message Passing Algorithm.
- Deevyanshu Malu: Primarily responsible for:
 - 1. Triangulation implementation and testing.
 - 2. Junction Graph Construction and validation.
 - 3. Implementation of the potential assignment to cliques.
 - 4. Development of the algorithm for determining the optimal message passing order.
 - 5. Development and optimization of message and potential multiplication/condensation for Top k Assignments.

- Neel Rambhia: Primarily responsible for:
 - 1. Triangulation implementation and testing.
 - 2. Junction Graph Construction and validation.
 - 3. Implementation of the potential assignment to cliques.
 - 4. Development and optimization of message and potential multiplication/condensation for Marginal Probability, Z Value, and Top k Assignments.

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