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Probabilistic Graphical Model

Session # 11: Approximate Inference and MAP Inference

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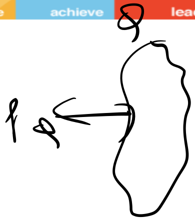
Constrained Optimization Problem



- Define a target class Q of **easy** distributions Q.
- Then search for an instance within that class that is the **best** approximation to P_Φ.
- Queries can then be answered using inference on Q rather than on P_Φ.
- This approach reformulates the inference task as one of optimizing an objective function over the class Q.
- This problem falls into the category of **constrained optimization**.

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Exact Inference as an Optimization Problem

- Factorized distribution

$$P_{\Phi}(X) = \frac{1}{Z} \prod_{\varphi \in \Phi} \varphi(U_{\varphi})$$

- $U_{\varphi} = Scope[\varphi] \subseteq X$ are scope of each factor φ in the distribution P_{Φ}.
- Queries about the distribution P_{Φ} include queries about marginal probabilities of variables and queries about the partition function Z.
- Exact inference finds a set of calibrated beliefs that represent $P_{\Phi}(X)$.
- We can view exact inference as searching over the set of distributions over the set of distributions Q that are representable by the cluster tree to find a distribution Q^* that matches P_{Φ}.

Exact Inference as an Optimization Problem

- Searching for a calibrated distribution that is as close as possible to P_Φ.
- Aim is to avoid performing inference with the distribution P_Φ.
- **Relative Entropy** or **KL Divergence** is used as a distance measure to find an approximation Q to P_Φ, such that the relative entropy is minimized.

Relative Entropy

- Relative entropy between two distributions P_1 and P_2

$$D(P_1 || P_2) = E_{P_1}\left[\ln \frac{P_1(X)}{P_2(X)}\right]$$

$$\int \ln \frac{P_1(x)}{P_2(x)} P_1(x)\, dx$$

- $D \geq 0$
- $D = 0$ if and only if $P_1 = P_2$.
- Relative entropy is non-symmetric.

$$D(P_1 || P_2) \neq D(P_2 || P_1)$$

Exact Inference as an Optimization Problem

- Goal is to search for a distribution Q that minimizes $D(Q||P_\Phi)$.
- Suppose the clique tree structure T for P_Φ satisfies running intersection property and family preservation property.

$$Q = \underbrace{\{\beta_i : i \in V_T\}}\ \cup\ \underbrace{\{\mu_{i,j} : (i-j) \in E_T\}}$$

$$\boxed{P_\Phi(X) = \frac{\prod \phi}{\prod \mu}}$$

$$Q(X) = \frac{\prod_{i \in V_T} \beta_i(C_i)}{\prod_{i \in E_T} \mu_{i,j}(S_{i,j})}$$

- Due to calibration requirement we have

$$\beta_i[c_i] = Q(c_i)$$

$$\mu_{i,j}[s_{i,j}] = Q(S_{i,j})$$

- Seach for a Q that is representable by a set of beliefs over the cliques and sepsets in a particular clique tree structure T.

Exact Inference as an Optimization Problem

$\int \ln\left[Q/P\right] Q(x)$

- CTree-Optimize-KL: $-D(Q||P_\Phi) \sim -D(P_\Phi||Q)$ $\int \ln \frac{P_\Phi(x)}{Q(x)} P_\Phi$

  Find $Q = \{\beta_i : i \in V_T\} \cup \{\mu_{i,j} : (i - j) \in E_T\}$

  Maximizing $-D(Q||P_\Phi) = 0$ $Q = P_\Phi$

  subject to $\mu_{i,j}[s_{i,j}] = \sum_{C_i - S_{i,j}} \beta_i[c_i]$ $\forall (i-j) \in E_T,\ \forall s_{i,j} \in Val(S_{i,j})$

  $\sum_{c_i} \beta_i[c_i] = 1$ $\forall i \in V_T$

  Q as the objective function

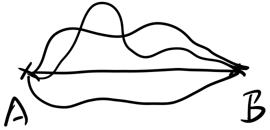
- Optimization problem CTree-Optimize-KL has a unique solution

$$-\int Q(x) \ln \Phi(x) = H_{\Phi}(X)$$

Exact Inference as an Optimization Problem

$$P_\Phi = \frac{1}{Z}\tilde{P}_\Phi$$

- Applying Relative entropy equation in P_Φ



Calculus of Variations

$$\rightarrow D(Q||P_\Phi) = \ln Z - F[\tilde{P}_\Phi, Q]$$

$$F[\tilde{P}_\Phi, Q] = \sum_{\varphi \in \Phi} E_Q[\ln \varphi] + H_Q(X)$$

$$D(Q||P_\Phi) \geq 0$$

$$\ln Z \geq F[\tilde{P}_\Phi, Q]$$

functional $\rightarrow f(Q)$ = scalar value

$f(x)$ = function of a variable

- $F[\tilde{P}_\Phi, Q]$ is called the **energy functional.**
- The first term is called the **energy term**.
- The second term is called the **entropy term**.
- Minimizing the relative entropy is equivalent to maximizing the energy functional.

Exact Inference as an Optimization Problem

$\min f(x, y, z)$

s.t $g(x, y, z) = c$

Lagrange multiplier

$\Rightarrow \nabla f(x, y, z) = \lambda \nabla g(x, y, z)$

- CTree-Optimize:

Find $\quad Q = \{\beta_i : i \in V_T\} \cup \{\mu_{i,j} : (i - j) \in E_T\}$

Maximizing $\quad F[\tilde{P}_\Phi, Q]$

subject to $\quad \mu_{i,j}[s_{i,j}] = \sum_{C_i - S_{i,j}} \beta_i[c_i] \quad \forall (i - j) \in E_T,\ \forall s_{i,j} \in Val(S_{i,j})$

$$\sum_{c_i} \beta_i[c_i] = 1 \qquad \forall i \in V_T$$

$$\beta_i(c_i) \geq 0 \qquad \forall i \in V_T;\ c_i \in Val(C_i)$$

Fixed-point characterisation

We need first the concept of Lagrange multipliers since we will convert the given <u>constrained optimization problem</u> to an unconstrained one.

To understand the derivation in the book, we need Lagrange multipliers + functionals ⇒ out of scope

Fixed-point characterisation

Setting up Lagrange multiplier equations for the constrained optimization problem and finding stationary points leads to the same sort of equations as the message passing algorithm

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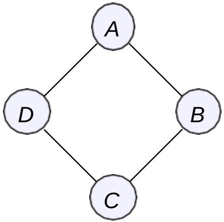
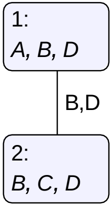
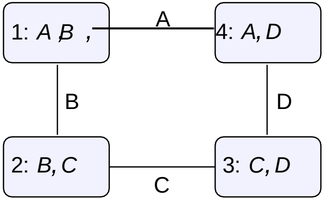
Propagation-Based Approximation

- Use the same message propagation as in exact inference.
- Use Cluster graph instead of clique tree.
- The cluster graph contains loops (undirected cycles), such graphs are often called **loopy**.
- The BP algorithm is called **Loopy belief propagation**, since it uses propagation steps used by algorithms for Markov trees, but applied to networks with loops.

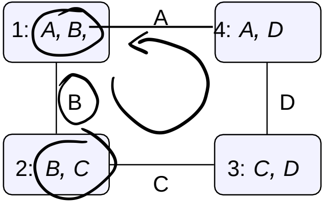


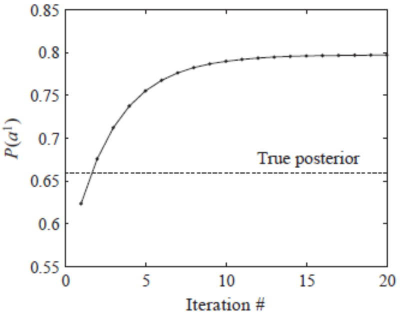




Propagation-Based Approximation

- Message propagation process may not converge in two passes, since information from one pass will circulate and affect the next round.
- In some cases, the propagation of beliefs may not converge at all.
- An example run of loopy belief propagation is given below.





What happens if we use CTree-BU-Update?

Let us propagate messages in the order $\mu_{12}, \mu_{23}, \mu_{34}, \mu_{41}$

In the first message μ_{12}, the cluster AB passes information to cluster BC using a marginal distribution on B.

What happens if we use CTree-BU-Update?

Suppose all clusters favour consensus joint assignments

$\beta_1(a^0, b^0)$ and $\beta_1(a^1, b^1)$ much larger than $\beta_1(a^0, b^1)$ and $\beta_1(a^1, b^0)$

If μ_{12} strengthens the belief that $B = b^1$,

then μ_{23} strengthens the belief that $C = c^1$

What happens if we use CTree-BU-Update?

Going around the loop, cluster AB will get a message that strengthens the belief that $A = a'$

This message will be treated as being independent of the initial propagation when it is not so. ⇒ This procedure overestimates the marginal probability of A

Cluster-graph Belief Propagation

We say that U satisfies the running intersection property if, whenever there is a variable X such that X ∈ C_i and X ∈ C_j , then there is a single path between C_i and C_j for which X ∈ S_e for all edges e in the path

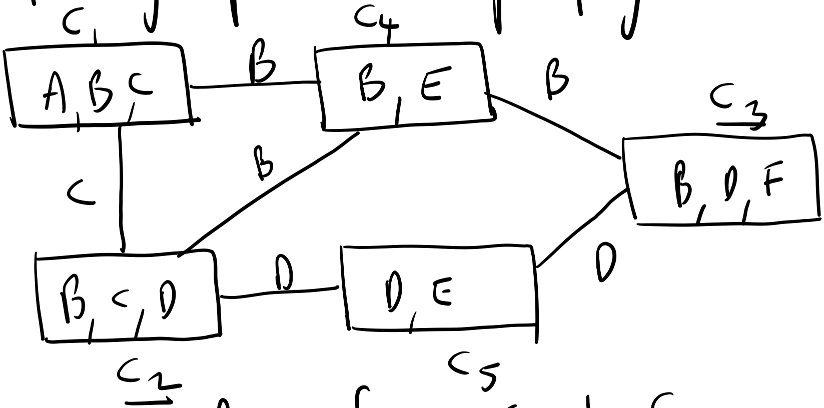
This is a <u>generalized running intersection</u> <u>property</u>

Cluster-graph belief propagation

There is only a single path in which information about X can flow in the graph.

- All clusters must agree on a marginal distribution of X.
- At most one path means information about X cannot endlessly cycle in a loop.

Cluster-graph belief propagation



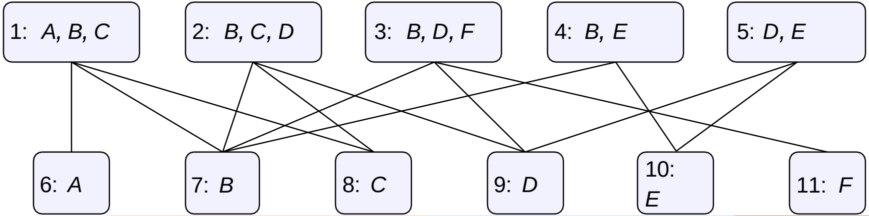
Two paths from C_3 to C_2

Cluster-graph belief propagation

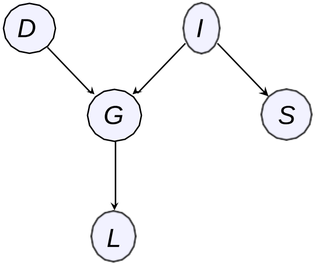
- The first path from C_3 to C_2 goes through C_4 and propagates information about B
- The second path from C_2 to C_3 goes through C_5 and propagates information about D
- We can still get circular reasoning
- For edge i-j connecting C_i, C_j $\sum_{C_i - S_{i,j}} \beta_i = \sum_{C_j - S_{i,j}} \beta_j$

Bethe Cluster Graph

- Bethe cluster graph, uses a bipartite graph.
- The first layer graph consists of "large" clusters, with one cluster for each factor φ in Φ, whose scope is $Scope[\varphi]$.
- These clusters satisfy the family-preservation property.
- The second layer consists of "small" univariate clusters, one for each random variable.
- Place an edge between each univariate cluster X on the second layer and each cluster in the first layer that includes X ; the scope of this edge is X itself.



MAP and Variable Elimination



$$\max_{S,I,D,L,G} P(D, I, G, S, L)$$

$$= \max_{L,G}[\varphi_L(L, G)] \cdot \mathrm{Max}_D[\varphi_D(D) \cdot T_2(G, D)]$$

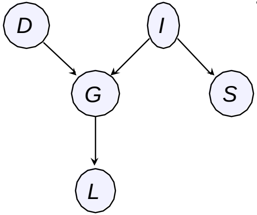
$$= \max_{L,G}[\varphi_L(L, G)] \cdot T_3(G)$$

$$= \max_{G}[T_3(G)] \cdot \max_L[\varphi_L(L, G)]$$

$$= \max_{G}[T_3(G)] \cdot T_4(G)$$

$$= \boxed{T_5(\theta)}$$

MAP and Variable Elimination



Step	Variable eliminated	Factors used	Intermediate factor	New factor
1	S	$\varphi_S(S, I)$	$\psi_1(I, S)$	$T_1(I)$
2	I	$\varphi_I(I) \cdot \varphi_G(G, I, D) \cdot T_1(I)$	$\psi_2(G, I, D)$	$T_2(G, D)$
3	D	$\varphi_D(D) \cdot T_2(G, D)$	$\psi_3(G, D)$	$T_3(G)$
4	L	$\varphi_L(L, G)$	$\psi_4(L, G)$	$T_4(G)$
5	G	$T_3(G) \cdot T_4(G)$	$\psi_5(G)$	$T_5(\theta)$

Now choose the maximizing value x_i^* for X_i.

g^*

MAP, Variable Elimination and Traceback

$\max P(b/a)$

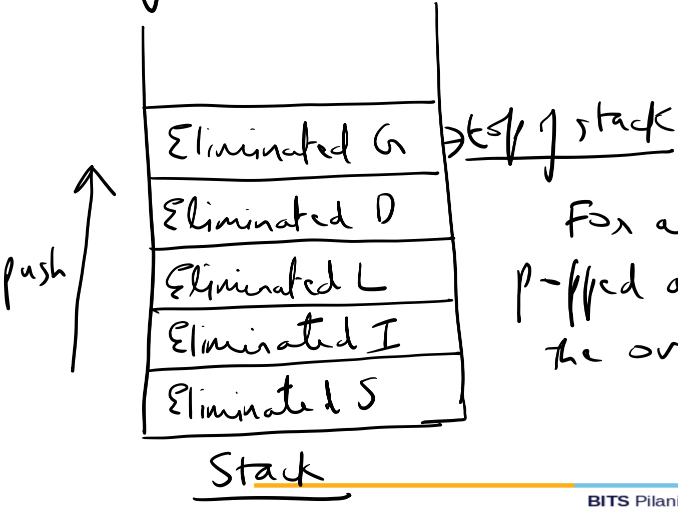
- Determine a conditional maximizing value – their maximizing value given the values of the variables that have not yet been eliminated.
- Pick the value of the final variable.
- Then go back and pick the values of the other variables accordingly.
- For the last variable eliminated X, the factor for the value x contains the probability of the most likely assignment that contains $X = x$.
- This process is called **traceback** of the solution.

$a^* \to \max P(b/a^*)$

MAP, Variable Elimination and Traceback

Step	Variable eliminated	Factors used	Intermediate factor	New factor	Traceback
1	S	$\varphi_S(S, I)$	$\psi_1(I, S)$	$\tau_1(I)$	$s^* = arg\ \max_s \psi_1(i^*, s)$
2	I	$\varphi_I(I) \cdot \varphi_G(G, I, D) \cdot \tau_1(I)$	$\psi_2(G, I, D)$	$\tau_2(G, D)$	$i^* = arg\ \max_i \psi_2(g^*, d^*, i)$ d^*
3	D	$\varphi_D(D) \cdot \tau_2(G, D)$	$\psi_3(G, D)$	$\tau_3(G)$	$= arg\ \max_d \psi_3(g^*, d)$
4	L	$\varphi_L(L, G)$	$\psi_4(L, G)$	$\tau_4(G)$	$l^* = arg\ \max_l \psi_4(g^*, l)$
5	G	$\tau_3(G) \cdot \tau_4(G)$	$\psi_5(G)$	$\tau_5(\theta)$	$g^* = arg\ \max_g \psi_5(g)$

Think of it like a stack....



For assignment the stack is popped and variables assigned in the order $G^* \to D^* \to L^* \to I^* \to S^*$

MAP and Variable Elimination Algorithm

$X_1 = S,\ X_2 = I,\ X_3 = L,\ X_4 = D,\ X_5 = G$

Procedure Max-Product-VE (
  Φ, // Set of factors over $\boldsymbol{X}$
  $\prec$ // Ordering on $\boldsymbol{X}$
)

Let $X_1, \ldots, X_k$ be an ordering of $\boldsymbol{X}$ such that
  $X_i \prec X_j$ iff $i < j$
  for $i = 1, \ldots, k$
    $(\Phi, \phi_{X_i}) \leftarrow$ Max-Product-Eliminate-Var(Φ, X_i)
  $\boldsymbol{x}^* \leftarrow$ Traceback-MAP$(\{\phi_{X_i} : i = 1, \ldots, k\})$
  return $\boldsymbol{x}^*, \Phi$ // Φ contains the probability of the MAP

Procedure Max-Product-Eliminate-Var (
  Φ, // Set of factors
  Z // Variable to be eliminated
)

$\Phi' \leftarrow \{\phi \in \Phi : Z \in Scope[\phi]\}$
  $\Phi'' \leftarrow \Phi - \Phi'$
  $\psi \leftarrow \prod_{\phi \in \Phi'} \phi$
  $\tau \leftarrow \max_Z \psi$
  return $(\Phi'' \cup \{\tau\}, \psi)$

2

Procedure Traceback-MAP (
  $\{\phi_{X_i} : i = 1, \ldots, k\}$
)

for $i = k, \ldots, 1$
  $\boxed{\boldsymbol{u}_i \leftarrow (x^*_{i+1}, \ldots, x^*_k)\langle Scope[\phi_{X_i}] - \{X_i\}\rangle}$
  // The maximizing assignment to the variables eliminated after X_i
  $x^*_i \leftarrow \arg\max_{x_i} \phi_{X_i}(x_i, \boldsymbol{u}_i)$
  // x^*_i is chosen so as to maximize the corresponding entry in the factor, relative to the previous choices $\boldsymbol{u}_i$
return $\boldsymbol{x}^*$

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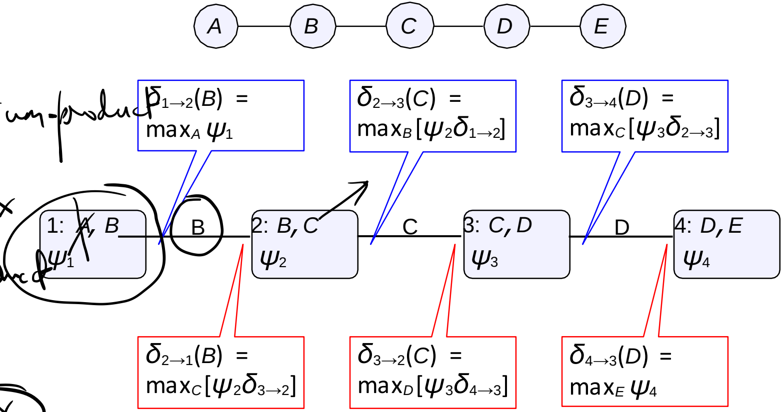
MAP using Belief Propagation

Same as sum-product except
sum → max



sum product

$\sum_A \psi_1$

max

MAP using Belief Propagation

- An exact solution to the MAP problem via a variable elimination procedure is intractable.
- Use message passing procedures in cluster graphs to compute approximate max-marginals.
- These pseudo-max-marginals can be used for selecting an assignment.
- The task has two parts: computing the max-marginals and decoding them to extract a

  MAP assignment.

$$\psi(C_i) = \psi_i \cdot \prod \delta_{k->i}$$

$$\tau(S_{i,j}) = \max_{C_i - S_{i,j}} \psi(C_i)$$

MAP using Belief Propagation

- For each clique C_i , and each assignment c_i to C_i ,

$$\beta_i(c_i) = MaxMarg_{P_\Phi}(c_i)$$

- Any two adjacent cliques must agree on their sepset. The cliques are said to be max-calibrated.

Σ Σ

$$\boxed{\max_{C_i - S_{i,j}} \beta_i = \max_{C_j - S_{i,j}} \beta_j = \mu_{ij}(S_{i,j})}$$

- The beliefs in a clique tree resulting from an upward and downward pass of the max-product clique tree algorithm are max-calibrated.

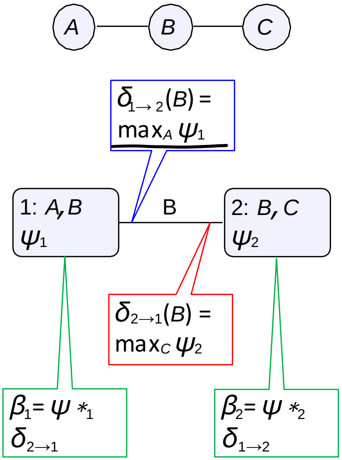
MAP using Belief Propagation

- The assignment ξ^* has the local optimal assignment property ξ^* given a max-calibrated set of beliefs $\beta_i(C_i)$, if for each clique

$$\xi^*(C_i) \in \boxed{\arg\max_{C_i} \beta_i(c_i)}$$

- The task of finding a locally optimal assignment ξ^* given a max-calibrated set of beliefs is called the decoding task.

MAP + BP – Most Likely Assignment – Example



ψ_1		
	a^1b^1	3
	a^2b^1	-1
	a^1b^2	0
	a^2b^2	1

ψ_2		
	b^1c^1	4
	b^1c^2	-1
	b^2c^1	1
	b^2c^2	2

$\delta_{1\to2}$		
	b^1	3
	b^2	1

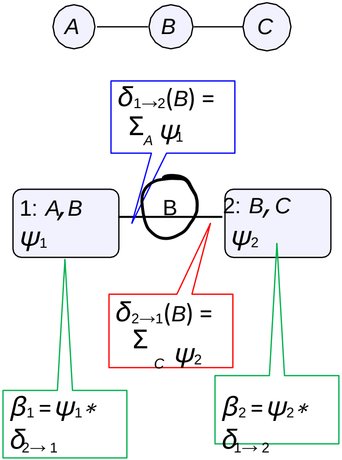
$\delta_{2\to1}$		
	b^1	4
	b^2	2

β_1		
	a^1b^1	3*4 = 12
	a^2b^1	-1*4 = -4
	a^1b^2	0*2 = 0
	a^2b^2	1*2 = 2

β_2		
	b^1c^1	4*3 = 12
	b^1c^2	-1*3 = -3
	b^2c^1	1*1 = 1
	b^2c^2	2*1 = 2

Most Likely assignment = (a^1, b^1, c^1)

MAP + BP – Calibration – Example



β_1		
	a^1b^1	3*4 = 12
	a^2b^1	-1*4 = -4
	a^1b^2	0*2 = 0
	a^2b^2	1*2 = 2

β_2		
	b^1c^1	4*3 = 12
	b^1c^2	-1*3 = -3
	b^2c^1	1*1 = 1
	b^2c^2	2*1 = 2

$\max_A \beta_1$		
	b^1	12
	b^2	2

=

$\max_C \beta_2$		
	b^1	12
	b^2	2