### **Probability Propagation**

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#### Graphical Models, Lecture 9, Michaelmas Term 2011

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Local computation algorithms have been developed with a variety of purposes. For example:

- Kalman filter and smoother
- Solving sparse linear equations;
- Decoding digital signals;
- Estimation in hidden Markov models;
- Peeling in pedigrees;
- Belief function evaluation;
- Probability propagation.

Also dynamic programming, linear programming, optimizing decisions, calculating Nash equilibria in cooperative games, and many others. *List is far from exhaustive!* 

All algorithms are using, explicitly or implicitly, a *graph decomposition* and *a junction tree* or similar to make the computations.

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Factorizing density on  $\mathcal{X} = \times_{v \in V} \mathcal{X}_v$  with V and  $\mathcal{X}_v$  finite:

$$p(x) = \prod_{C \in \mathcal{C}} \phi_C(x).$$

The *potentials*  $\phi_C(x)$  depend on  $x_C = (x_v, v \in C)$  only. Basic task to calculate *marginal* probability

$$p(x_E^*) = \sum_{y_{V\setminus E}} p(x_E^*, y_{V\setminus E})$$

for  $E \subseteq V$  and fixed  $x_E^*$ , but sum has too many terms. A second purpose is to get the prediction  $p(x_v | x_E^*) = p(x_v, x_E^*)/p(x_E^*)$  for  $v \in V$ .

If the initial model is based on a DAG  $\mathcal{D}$ , the first step is to form the *moral graph*  $\mathcal{G} = \mathcal{D}^m$ , exploiting that if P factorizes w.r.t.  $\mathcal{D}$ , it also factorizes w.r.t.  $\mathcal{D}^m$ .

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## A very simple example

Assume

$$p(x, y, z, w) = \phi(x, y)\psi(y, z)\eta(z, w)$$

and assume each of X, Y, Z, and W have, say, 100 states.

The joint state space has thus  $10^8$  states, and to calculate p(x) directly from p(x, y, z, w) by brute force involves  $10^6$  terms in the sum for every x, hence  $10^8$  arithmetic operations are needed.

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we instead may do as follows:

1. Calculate  $\eta^*(z) = \sum_w \eta(z, w)$ , with 10000 additions;

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- 5. Calculate  $\phi^*(x) = \sum_y \phi^*(x, y)$ , with 10000 additions.

Now  $p^*(x) = \phi^*(x)$  so we have done this with only 50000 operations, rather than a million.

Note we have never explicitly formed the product  $p(x, y, z, w) = \phi(x, y)\psi(y, z)\eta(z, w)$ 

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Starting from a DAG  $\mathcal{D}$ , the computational structure is set up in several steps:

 Moralisation: Constructing D<sup>m</sup>, exploiting that if P factorizes over D, it factorizes over D<sup>m</sup>. Skip if starting from an undirected graph.

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- 2. Triangulation: Adding edges to find chordal graph  $\tilde{\mathcal{G}}$  with  $\mathcal{G} \subseteq \tilde{\mathcal{G}}$ . This step is non-trivial (NP-complete) to optimize;

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Starting from a DAG  $\mathcal{D}$ , the computational structure is set up in several steps:

- 1. *Moralisation:* Constructing  $\mathcal{D}^m$ , exploiting that if P factorizes over  $\mathcal{D}$ , it factorizes over  $\mathcal{D}^m$ . Skip if starting from an undirected graph.
- 2. Triangulation: Adding edges to find chordal graph  $\tilde{\mathcal{G}}$  with  $\mathcal{G} \subseteq \tilde{\mathcal{G}}$ . This step is non-trivial (NP-complete) to optimize;
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Computations are executed by *message passing*.

The complete process above is known as *compilation*.

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## Initialization

1. For every vertex  $v \in V$  we find a clique C(v) in the triangulated graph  $\tilde{\mathcal{G}}$  which contains pa(v). Such a clique exists because  $v \cup pa(v)$  are complete in  $\mathcal{D}^m$  by construction, and hence in  $\tilde{\mathcal{G}}$ ;

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- 2. Define potential functions  $\phi_C$  for all cliques C in  $\tilde{\mathcal{G}}$  as

$$\phi_C(x) = \prod_{v:C(v)=C} p(x_v \mid x_{\mathsf{pa}(v)})$$

where the product over an empty index set is set to 1, i.e.  $\phi_C \equiv 1$  if no vertex is assigned to C.

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3. It now holds that

$$p(x) = \prod_{C \in \mathcal{C}} \phi_C(x).$$

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#### Overview

#### This involves following steps

1. *Incorporating observations:* If  $X_E = x_E^*$  is observed, we modify potentials as

$$\phi_{\mathcal{C}}(x_{\mathcal{C}}) \leftarrow \phi_{\mathcal{C}}(x) \prod_{e \in E \cap \mathcal{C}} \delta(x_e^*, x_e),$$

with  $\delta(u, v) = 1$  if u = v and else  $\delta(u, v) = 0$ . Then:

$$p(x \mid X_E = x_E^*) = \frac{\prod_{C \in \mathcal{C}} \phi_C(x_C)}{p(x_E^*)}.$$

Marginals p(x<sup>\*</sup><sub>E</sub>) and p(x<sub>C</sub> | x<sup>\*</sup><sub>E</sub>) are then calculated by a local message passing algorithm.

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## Separators

Between any two cliques C and D which are neighbours in the junction tree their intersection  $S = C \cap D$  is called a *separator*. In fact, the sets S are the minimal separators appearing in any decomposition sequence.

We also assign potentials to separators, initially  $\phi_S \equiv 1$  for all  $S \in S$ , where S is the set of separators. Finally let

$$\kappa(x) = \frac{\prod_{C \in \mathcal{C}} \phi_C(x_C)}{\prod_{S \in \mathcal{S}} \phi_S(x_S)},\tag{1}$$

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and now it holds that  $p(x | x_E^*) = \kappa(x) / p(x_E^*)$ .

The expression (1) will be *invariant* under the message passing.

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# Marginalization

The *A*-marginal of a potential  $\phi_B$  for  $A \subseteq V$  is

$$\phi_B^{\downarrow A}(x) = \phi_B^{\downarrow A}(x_A) = \sum_{y_{A \cap B}: y_{A \cap B} = x_{A \cap B}} \phi_B(y)$$

Since  $\phi_B$  depends on x through  $x_B$  only it is true that if  $B \subseteq V$  is 'small', marginal can be computed easily.

Note that the marginal  $\phi^{\downarrow A}$  depends on  $x_A$  only.

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#### Marginalization satisfies

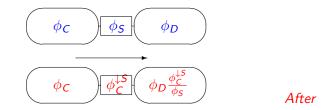
Consonance For subsets A and B:  $\phi^{\downarrow(A\cap B)} = (\phi^{\downarrow B})^{\downarrow A}$ Distributivity If  $\phi_C$  depends on  $x_C$  only and  $C \subseteq B$ :  $(\phi\phi_C)^{\downarrow B} = (\phi^{\downarrow B}) \phi_C$ .

Essentially the distributivity ensures that we can move factors in a sum outside of the summation sign.

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#### Messages

When C sends message to D, the following happens:



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#### **Before**

Computation is *local*, involving only variables within cliques.

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The expression

$$\kappa(\mathbf{x}) = \frac{\prod_{C \in \mathcal{C}} \phi_C(\mathbf{x}_C)}{\prod_{S \in \mathcal{S}} \phi_S(\mathbf{x}_S)}$$

is invariant under the message passing since  $\phi_C \phi_D / \phi_S$  is:

$$\frac{\phi_C \phi_D \frac{\phi_C^{\downarrow S}}{\phi_S}}{\phi_C^{\downarrow S}} = \frac{\phi_C \phi_D}{\phi_S}.$$

After the message has been sent, *D* contains the *D*-marginal of  $\phi_C \phi_D / \phi_S$ .

To see this, calculate

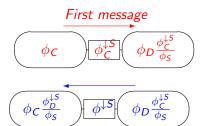
$$\left(\frac{\phi_C\phi_D}{\phi_S}\right)^{\downarrow D} = \frac{\phi_D}{\phi_S}\phi_C^{\downarrow D} = \frac{\phi_D}{\phi_S}\phi_C^{\downarrow S}.$$

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#### Second message

If *D* returns message to *C*, the following happens:



Second message

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Now all sets contain the relevant marginal of  $\phi = \phi_C \phi_D / \phi_S$ : The separator contains

$$\phi^{\downarrow S} = \left(\frac{\phi_C \phi_D}{\phi_S}\right)^{\downarrow S} = (\phi^{\downarrow D})^{\downarrow S} = \left(\phi_D \frac{\phi_C^{\downarrow S}}{\phi_S}\right)^{\downarrow S} = \frac{\phi_C^{\downarrow S} \phi_D^{\downarrow S}}{\phi_S}.$$

C contains

$$\phi_C \frac{\phi^{\downarrow S}}{\phi_C^{\downarrow S}} = \frac{\phi_C}{\phi_S} \phi_D^{\downarrow S} = \phi^{\downarrow C}$$

since, as before

$$\left(\frac{\phi_C\phi_D}{\phi_S}\right)^{\downarrow C} = \frac{\phi_D}{\phi_S}\phi_C^{\downarrow D} = \frac{\phi_C}{\phi_S}\phi_D^{\downarrow S}$$

*Further messages between C and D are neutral!* Nothing will change if a message is repeated.

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Probability Propagation

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Two phases:

► COLLINFO: messages are sent from leaves towards arbitrarily chosen root *R*.

After COLLINFO, the root potential satisfies  $\phi_R(x_R) = \kappa^{\downarrow R}(x_R) = p(x_R, x_E^*).$ 

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After COLLINFO, the root potential satisfies  $\phi_R(x_R) = \kappa^{\downarrow R}(x_R) = p(x_R, x_E^*).$ 

▶ DISTINFO: messages are sent from root *R* towards leaves. After COLLINFO and subsequent DISTINFO, it holds for all  $B \in C \cup S$  that  $\phi_B(x_B) == \kappa^{\downarrow B}(x_B) = p(x_B, x_E^*)$ .

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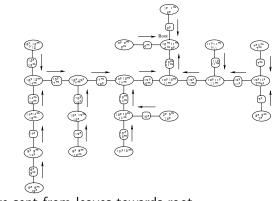
- ▶ DISTINFO: messages are sent from root *R* towards leaves. *After* COLLINFO *and subsequent* DISTINFO, *it holds for all*  $B \in C \cup S$  that  $\phi_B(x_B) == \kappa^{\downarrow B}(x_B) = p(x_B, x_E^*)$ .
- ► Hence  $p(x_E^*) = \sum_{x_S} \phi_S(x_S)$  for any  $S \in S$  and  $p(x_v | x_E^*)$  can readily be computed from any  $\phi_S$  with  $v \in S$ .

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## CollInfo



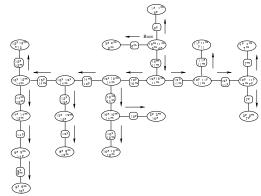
Messages are sent from leaves towards root.

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### DISTINFO



After  $\operatorname{COLLINFO}$ , messages are sent from root towards leaves.

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The correctness of the algorithm is easily established by induction:

We have on the previous overheads shown correctness for a junction tree with only two cliques.

Now consider a leaf clique *L* of the juction tree and let  $V^* = \bigcup_{C: C \in \mathcal{C} \setminus \{L\}} C.$ 

Because the tree is a junction tree, we have  $S^* = L \cap C^* = L \cap V^*$ where  $C^*$  is the neighbour of L in the junction tree. Thus L and  $V^*$  form a junction tree of two cliques with separator  $S^*$ 

After a message has been sent from L to  $V^*$  in the COLLINFO phase,  $\phi_{V^*}$  is equal to the  $V^*$ -marginal of  $\kappa$ .

By induction, when all messages have been sent except the one from the neighbour clique  $C^*$  to L, all cliques other than L contain the relevant marginal of  $\kappa$ , and

$$\phi_{V^*} = \frac{\prod_{C:C \in \mathcal{C} \setminus \{L\}} \phi_C}{\prod_{S:S \in \mathcal{S} \setminus \{S^*\}} \phi_S}$$

Now let,  $V^*$  send its message back to L. To do this, it needs to calculate  $\phi_{V^*}^{\downarrow S^*}$ . But since  $S^* \subseteq C^*$ , and  $\phi_{C^*} = \phi_{V^*}^{\downarrow C^*}$  we have

$$\phi_{V^*}^{\downarrow S^*} = \phi_{C^*}^{\downarrow S^*}$$

and sending a message from  $V^*$  to L is thus equivalent to sending a message from  $C^*$  to L. Thus, after this message has been sent,  $\phi_L = \kappa^{\downarrow L}$  as desired.

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## Alternative scheduling of messages

#### Local control:

Allow clique to send message if and only if it has already received message from all other neighbours. Such messages are *live*.

Using this protocol, there will be one clique who first receives messages from all its neighbours. This is effectively the root R in COLLINFO and DISTINFO.

Additional messages never do any harm (ignoring efficiency issues) as  $\kappa$  is invariant under message passing.

Exactly two live messages along every branch is needed.