## Local Computation

Steffen Lauritzen, University of Oxford<br>Graphical Models, Lecture 13, Michaelmas Term 2010

November 22, 2010

## The general problem

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

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

The potentials $\phi_{C}(x)$ depend on $x_{C}=\left(x_{v}, v \in C\right)$ only.
Basic task to calculate marginal probability

$$
p\left(x_{E}^{*}\right)=\sum_{y_{V \backslash E}} p\left(x_{E}^{*}, y_{V \backslash E}\right)
$$

for $E \subseteq V$ and fixed $x_{E}^{*}$, but sum has too many terms.
A second purpose is to get the prediction
$p\left(x_{v} \mid x_{E}^{*}\right)=p\left(x_{v}, x_{E}^{*}\right) / p\left(x_{E}^{*}\right)$ for $v \in V$.

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 $\mathcal{D}^{m}$.
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;
3. Constructing junction tree: Using MCS, the cliques of $\tilde{\mathcal{G}}$ are found and arranged in a junction tree.
4. Initialization: Assigning potential functions $\phi_{C}$ to cliques.

The complete process above is known as compilation.
Computation is then performed by message passing after observations have been incorporated.

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

$$
\begin{equation*}
\kappa(x)=\frac{\prod_{C \in \mathcal{C}} \phi_{C}\left(x_{C}\right)}{\prod_{S \in \mathcal{S}} \phi_{S}\left(x_{S}\right)} . \tag{1}
\end{equation*}
$$

After incorporation of observations it holds that $p\left(x \mid x_{E}^{*}\right)=\kappa(x) / p\left(x_{E}^{*}\right)$.
The expression (1) will be invariant under the message passing.

## Marginalization

The $A$-marginal of a potential $\phi_{B}$ for $A \subseteq V$ is

$$
\phi_{B}^{\downarrow A}(x)=\phi_{B}^{\downarrow A}\left(x_{A}\right)=\sum_{y_{A \cap B}: y_{A \cap B}=x_{A \cap B}} \phi_{B}(y)
$$

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.

Marginalization satisfies
Consonance For subsets $A$ and $B: \phi^{\downarrow(A \cap B)}=\left(\phi^{\downarrow B}\right)^{\downarrow A}$
Distributivity If $\phi_{C}$ depends on $x_{C}$ only and $C \subseteq B$ :

$$
\left(\phi \phi_{C}\right)^{\downarrow B}=\left(\phi^{\downarrow B}\right) \phi_{C} .
$$

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

## Messages

When $C$ sends message to $D$, the following happens:


Computation is local, involving only variables within cliques.

The expression

$$
\kappa(x)=\frac{\prod_{C \in \mathcal{C}} \phi_{C}\left(x_{C}\right)}{\prod_{S \in \mathcal{S}} \phi_{S}\left(x_{S}\right)}
$$

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

$$
\left(\frac{\phi_{C} \phi_{D}}{\phi_{S}}\right)^{\downarrow D}=\frac{\phi_{D}}{\phi_{S}} \phi_{C}^{\downarrow D}=\frac{\phi_{D}}{\phi_{S}} \phi_{C}^{\downarrow S}
$$

## Second message

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


Now all sets contain the relevant marginal of $\phi=\phi_{C} \phi_{D} / \phi_{S}$ : The separator contains

$$
\phi^{\downarrow S}=\left(\frac{\phi_{C} \phi_{D}}{\phi_{S}}\right)^{\downarrow S}=\left(\phi^{\downarrow D}\right)^{\downarrow S}=\left(\phi_{D} \frac{\phi_{C}^{\downarrow S}}{\phi_{S}}\right)^{\downarrow S}=\frac{\phi_{C}^{\downarrow S} \phi_{D}^{\downarrow S}}{\phi_{S}} .
$$

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.

Two phases:

- CollInfo: messages are sent from leaves towards arbitrarily chosen root $R$.
After Collinfo, the root potential satisfies

$$
\phi_{R}\left(x_{R}\right)=\kappa^{\downarrow R}\left(x_{R}\right)=p\left(x_{R}, x_{E}^{*}\right) .
$$

Basic problem and structure of algorithm Setting up the structure

Two phases:

- CollInfo: messages are sent from leaves towards arbitrarily chosen root $R$.
After Collinfo, the root potential satisfies $\phi_{R}\left(x_{R}\right)=\kappa^{\downarrow R}\left(x_{R}\right)=p\left(x_{R}, x_{E}^{*}\right)$.
- DistInfo: messages are sent from root $R$ towards leaves. After CollInfo and subsequent DistInfo, it holds for all $B \in \mathcal{C} \cup \mathcal{S}$ that $\phi_{B}\left(x_{B}\right)==\kappa^{\downarrow B}\left(x_{B}\right)=p\left(x_{B}, x_{E}^{*}\right)$.

Two phases:

- CollInfo: messages are sent from leaves towards arbitrarily chosen root $R$.
After Collinfo, the root potential satisfies $\phi_{R}\left(x_{R}\right)=\kappa^{\downarrow R}\left(x_{R}\right)=p\left(x_{R}, x_{E}^{*}\right)$.
- DistInfo: messages are sent from root $R$ towards leaves. After CollInfo and subsequent DistInfo, it holds for all $B \in \mathcal{C} \cup \mathcal{S}$ that $\phi_{B}\left(x_{B}\right)==\kappa^{\downarrow B}\left(x_{B}\right)=p\left(x_{B}, x_{E}^{*}\right)$.
- Hence $p\left(x_{E}^{*}\right)=\sum_{x_{S}} \phi_{S}\left(x_{S}\right)$ for any $S \in \mathcal{S}$ and $p\left(x_{v} \mid x_{E}^{*}\right)$ can readily be computed from any $\phi_{S}$ with $v \in S$.

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 $V *=\cup_{C: C \in \mathcal{C} \backslash\{L\}} C$.
We can then think of $L$ and $V^{*}$ forming a junction tree of two cliques with separator $S^{*}=L \cap C^{*}$ where $C^{*}$ is the neighbour of $L$ in the junction tree.
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

$$
\phi_{V^{*}}=\frac{\prod_{C: C \in \mathcal{C} \backslash\{L\}} \phi_{C}}{\prod_{S: S \in \mathcal{S} \backslash\left\{S^{*}\right\}} \phi_{S}} .
$$

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, $\phi_{L}=\kappa^{\swarrow L}$ as desired.

## 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.

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.

Replace sum-marginal with $A$-maxmarginal:

$$
\phi_{B}^{\downarrow A}(x)=\max _{y_{B}: y_{A}=x_{A}} \phi_{B}(y)
$$

Satisfies consonance: $\phi^{\downarrow(A \cap B)}=\left(\phi^{\downarrow B}\right)^{\downarrow A}$ and distributivity: $\left(\phi_{C}\right)^{\downarrow B}=\left(\phi^{\downarrow B}\right) \phi_{C}$, if $\phi_{C}$ depends on $x_{C}$ only and $C \subseteq B$.
CollInfo yields maximal value of density $f$.
DistInfo yields configuration with maximum probability.
Viterbi decoding for HMMs is special case.
Since (1) remains invariant, one can switch freely between maxand sum-propagation.

After Collinfo, the root potential is $\phi_{R}(x) \propto p\left(x_{R} \mid x_{E}\right)$ Modify DistInfo as follows:

1. Pick random configuration $\check{x}_{R}$ from $\phi_{R}$.
2. Send message to neighbours $C$ as $\check{x}_{R \cap C}=\check{x}_{S}$ where $S=C \cap R$ is the separator.
3. Continue by picking $\check{x}_{C}$ according to $\phi_{C}\left(x_{C \backslash S}, \check{x}_{S}\right)$ and send message further away from root.
When the sampling stops at leaves of junction tree, a configuration $\check{x}$ has been generated from $p\left(x \mid x_{E}^{*}\right)$.

## Maximization

The scaling operation on $p$ :

$$
\left(T_{a} p\right)(x) \leftarrow p(x) \frac{n^{\downarrow a}\left(x_{a}\right)}{n p^{\downarrow a}\left(x_{a}\right)}, \quad x \in \mathcal{X}
$$

is potentially very complex, as it cycles through all $x \in \mathcal{X}$, which is huge if $V$ is large. If we exploit a factorization of $p$ w.r.t. a junction tree $\mathcal{T}$ for a decomposable $\mathcal{C} \supseteq \mathcal{A}$

$$
p(x)=\frac{\prod_{C \in \mathcal{C}} \phi_{C}\left(x_{C}\right)}{\prod_{S \in \mathcal{S}} \phi_{S}\left(x_{S}\right)},
$$

we can avoid scaling $p$ and only scale the corresponding factor $\phi_{C^{*}}$ with $a \subseteq C^{*}$ :

$$
\left(T_{a} \phi_{C^{*}}\right)\left(x_{C^{*}}\right) \leftarrow \phi_{C^{*}}\left(x_{C^{*}}\right) \frac{n^{\downarrow a}\left(x_{a}\right)}{n p^{\downarrow a}\left(x_{a}\right)}, \quad x_{C^{*}} \in \mathcal{X}_{C^{*}}
$$

where $p^{\downarrow a}$ is calculated by probability propagation,

The scaling can now be made by changing the $\phi$ 's:

$$
\phi_{B} \leftarrow \phi_{B} \text { for } B \neq C^{*}, \quad \phi_{C^{*}} \leftarrow T_{a} \phi_{C^{*}} .
$$

This can reduce the complexity considerably.
Note that if $a=C$ and $\phi_{a}=n^{\downarrow a}\left(x_{a}\right)$, then $T_{a} \phi_{a}=\phi_{a}$. Hence the explicit formula for the MLE.

