Probabilistic Machine Learning:
7. Probabilistic Graphical Models - part 1

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The presentation has been inspired and in some parts totally based on

1. Pattern Recognition and Machine Learning, Christopher M. Bishop [1] Chapter 8. Graphical Models

Table of Contents

Pre-reading

There was nothing to read.

Table of Contents

Table of Contents

Chain rule – recap

By the *chain rule* of probability, we can always represent a *joint distribution* as follows, using any ordering of the variables:

$$P(x_{1:V}) = P(x_1)P(x_2|x_1)P(x_3|x_2,x_1)P(x_4|x_1,x_2,x_3)\dots P(x_V|x_{1:V-1}) \quad (1)$$

, where V is the number of variables, and where we have dropped the conditioning on the fixed parameters θ for brevity. The problem with this expression is that it becomes more and more complicated to represent the conditional distributions $P(x_t|x_{1:t-1})$ as t gets large.

Example I

Bishop p.361-362 [1]

Let us consider a situation when some variables are independent of each other and the join distribution factorizes into the following form

$$P(x_{1:7}) = P(x_1)P(x_2)P(x_3)P(x_4|x_1, x_2, x_3)P(x_5|x_1, x_3)P(x_6|x_4)P(x_7|x_4, x_5) \tag{2}$$

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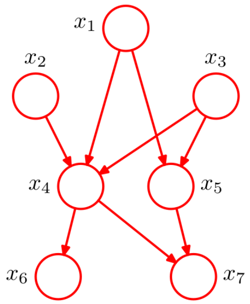

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 362*

Directed Graphical Model

The joint distribution defined by a graph is given by the *product, over all of the nodes of the graph, of a conditional distribution for each node conditioned on the variables corresponding to the parents of that node* in the graph. Thus, for a graph with K nodes, the joint distribution is given by

$$\mathrm{P}(\boldsymbol{x}) = \prod_{k=1}^{K} \mathrm{P}(x_k|\mathrm{pa}_k), \tag{3}$$

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The directed graphs are subject to an important restriction – there must be *no directed cycles*, in other words there are no closed paths within the graph such that we can move from node to node along links following the direction of the arrows and end up back at the starting node. Such graphs are called *directed acyclic graphs*, or *DAG*s.

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This is equivalent to the statement that there exists an ordering of the nodes such that there are no links that go from any node to any lower numbered node.

Example – Bayesian Regression

Let us consider the Bayesian Regression model that consist of coefficients vector β and obervations vector $\boldsymbol{y} = (y_1, \ldots, y_N)^\top$ and the noise variance σ^2 which we all consider *random variables*.

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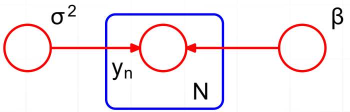

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 363*

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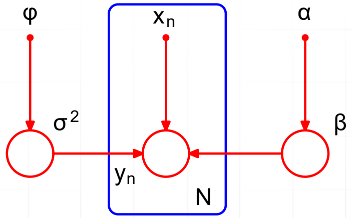

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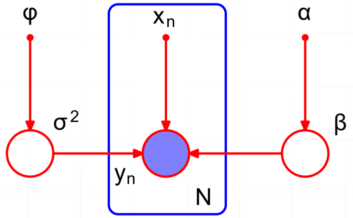
Example – Bayesian Regression

If we additionally mark the observed variables we get



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Suppose we are given a new input value $\hat{x}$ and we wish to find the corresponding probability distribution for $\hat{y}$ conditioned on the observed data. The corresponding joint distribution of all of the random variables in this model, conditioned on the deterministic parameters, is then given by

$$P(\hat{y}, \mathbf{y}, \beta, \sigma^2 | \hat{x}, \mathbf{x}, \alpha, \varphi) = P(\hat{y} | \hat{x}, \beta, \sigma^2) P(\sigma^2 | \varphi) P(\beta | \alpha) \prod_{n=1}^{N} P(y_n | x_n, \beta, \sigma^2) \tag{6}$$

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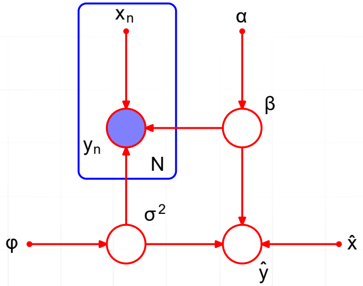
which is equivalent to



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Example – Mixture Model

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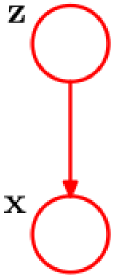
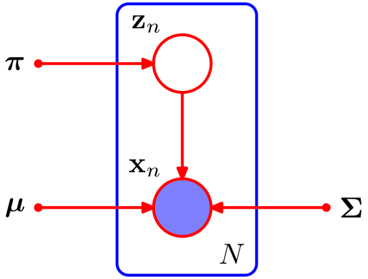
This is how it looks like as directed graphical model:



Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 431*

Example – Mixture Model

And here with all the non-random parameters:



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    5. Online tools such as Lucidchart, draw.io, Google Docs Draw, etc.

Table of Contents

Markov Random Fields

A *Markov random field*, also known as a *Markov network* or an *undirected graphical model*, has a set of nodes each of which corresponds to a variable or group of variables, as well as a set of links each of which connects a pair of nodes. The *links are undirected*, that is they do not carry arrows.

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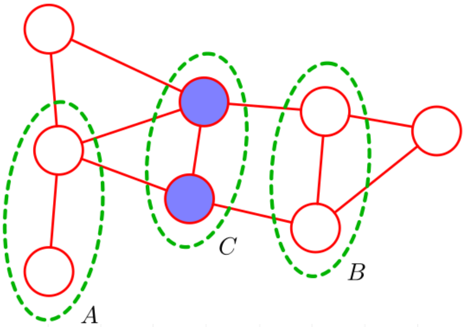

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 384*

Markov Random Fields

Conditional independence

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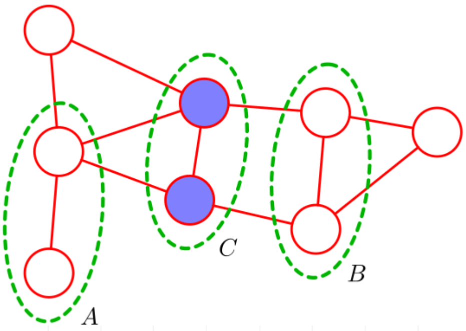
It turns out the situation here is easier. Consider the following undirected model:



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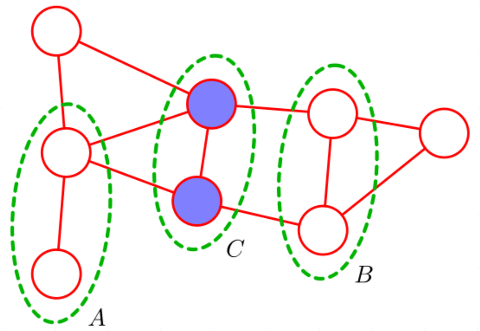

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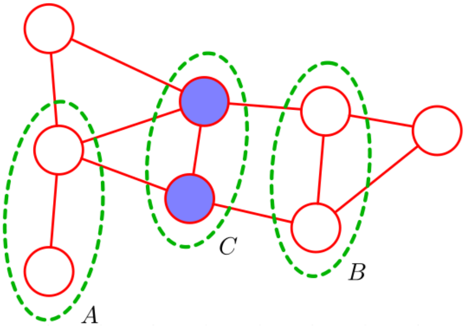
Three sets of nodes are identified – A, B and C. Mind that as a special case, they could consist of single elements. We want to test if

$$A \perp\!\!\!\perp B | C \tag{9}$$

holds.

Markov Random Fields

Conditional independence



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To test it we consider *all possible paths* that connect nodes in set *A* to nodes in set *B*. If all such paths *pass through one or more nodes in set* C, then all such paths are *blocked* and so the conditional independence property holds.

Markov Random Fields

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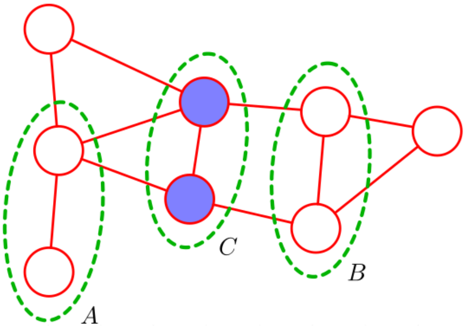

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An alternative way to view the conditional independence test is to imagine *removing all nodes in set C* from the graph together with any links that connect to those nodes. We then ask *if there exists a path that connects any node in A to any node in B*. If there are no such paths, then the conditional independence property must hold.

Markov blanket – recap

Directed models

Consider a joint distribution $\mathrm{P}(x_1, \ldots, x_D)$ of a model consisting of D nodes, and consider the conditional distribution of a particular node x_i conditioned on all of the remaining variables $\boldsymbol{x}_{j \neq i}$.

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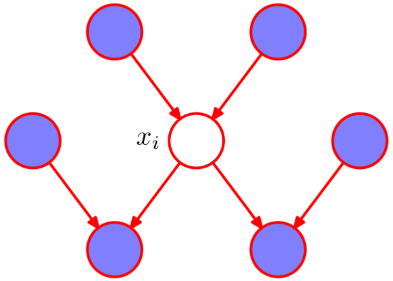
The conditionals $\mathrm{P}(x_k|\mathrm{pa}_k)$ will depend on the children of x_i as well as on the *co-parents*, in other words variables corresponding to parents of node x_k other than node x_i due to head-to-head.

Markov blanket – recap

Directed models

The set of nodes comprising the parents, the children and the co-parents is called the *Markov blanket*.

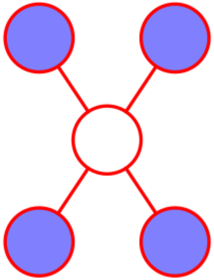


Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 383*

Markov blanket

Undirected models

For an undirected graph, the Markov blanket of a node x_i consists of the set of neighbouring nodes.



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$$P(x_i, x_j|\boldsymbol{x}_{\setminus\{i,j\}}) = P(x_i|\boldsymbol{x}_{\setminus\{i,j\}})P(x_j|\boldsymbol{x}_{\setminus\{i,j\}}) \tag{11}$$

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The factorization of the joint distribution must therefore be such that x_i and x_j do not appear in the same *factor*.
We define the factors in the decomposition of the joint distribution to be functions of the variables in the *cliques*. In fact, we can consider functions of the *maximal cliques*, without loss of generality, because other cliques must be subsets of maximal cliques.

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In eq. 13 we have assumed that $\mathbf{x}$ comprises discrete variables, but the framework is equally applicable to continuous variables, or a combination of the two, in which the summation is replaced by the appropriate combination of summation and integration.

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4. For evaluating local marginal probabilities we can work with the unnormalized joint distribution and then *normalize the marginals explicitly at the end*. Provided the marginals only involves a small number of variables, the evaluation of their normalization coefficient will be feasible.

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In such a case it is convenient to express then as exponentials, so that

$$\psi_C(\mathbf{x}_C) = \exp(-E(\mathbf{x}_C)), \tag{15}$$

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The *Hammersley-Clifford theorem* [2] states that such formulation of the factorization of the joint probability distribution is correct.

Relation of directed and undirected models

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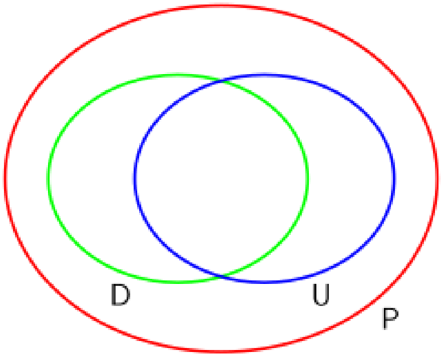
If it is the case that every conditional independence property of the distribution is reflected in the graph, and vice versa, then the graph is said to be a *perfect map* for that distribution. A perfect map is therefore both an I map and a D map.

Relation of directed and undirected models



Credit: *Pattern Recognition and Machine Learning*, *Christopher M. Bishop p. 392*

Figure: Venn diagram illustrating the set of all distributions *P* over a given set of variables, together with the set of distributions *D* that can be represented as a *perfect map* using a directed graph, and the set *U* that can be represented as a perfect map using an undirected graph.

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The graphical framework can be extended in a consistent way to graphs that include *both directed and undirected links*. These are called *chain graphs* [3], and contain the directed and undirected graphs considered so far as special cases. Although such graphs can represent a broader class of distributions than either directed or undirected alone, *there remain distributions for which even a chain graph cannot provide a perfect map*. Chain graphs are not discussed further in this course.

Table of Contents

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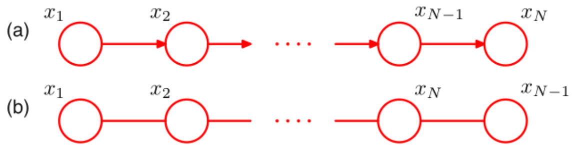
Specifically, we shall see that many algorithms can be expressed in terms of the propagation of *local messages* around the graph.

In this part of the lecture we will focus primarily on techniques for *exact inference*, and later we shall consider a number of *approximate inference* algorithms.

Inference on a chain

Consider the undirected graph in *Figure (b)* consisting of N nodes. The directed chain can be transformed into an equivalent undirected chain. Because the directed graph does not have any nodes with more than one parent, this does not require the addition of any extra links, and the directed and undirected versions of this graph express exactly the same set of conditional independence statements.



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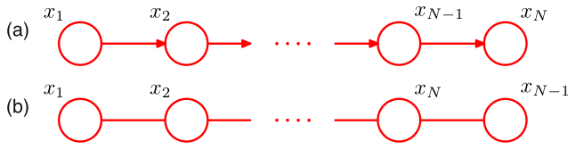

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The joint distribution takes the form

$$P(\mathbf{x}) = \frac{1}{Z}\psi_{1,2}(x_1, x_2)\psi_{2,3}(x_2, x_3)\cdots\psi_{N-1,N}(x_{N-1}, x_N) \tag{16}$$

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But by by exploiting the factorization we can rearrange the order of the summations and the multiplications to allow the required marginal to be evaluated much more efficiently.

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at first to obtain a function of x_{N-1} which can be integrated out by a summation that additionally involves only $\psi_{N-2,N-1}(x_{N-2}, x_{N-1})$.

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Similarly we can proceed from “the left side”.

Inference on a chain

Finally we end up with the following form:

$$p(x_n) = \frac{1}{Z} \underbrace{\left[\sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \cdots \left[\sum_{x_2} \psi_{2,3}(x_2, x_3) \left[\sum_{x_1} \psi_{1,2}(x_1, x_2) \right] \right] \cdots \right]}_{\mu_\alpha(x_n)} \underbrace{\left[\sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \cdots \left[\sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N) \right] \cdots \right]}_{\mu_\beta(x_n)} . \qquad (8.52)$$

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 396*

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Mind that if the graph had been fully connected, there would have been no conditional independence properties, and we would have been forced to work directly with the full joint distribution.

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The potential function Z can be easily evaluated by summing the right-hand side of eq. 20 over all states of x_n, an operation that requires only $\mathrm{O}(K)$ computation.

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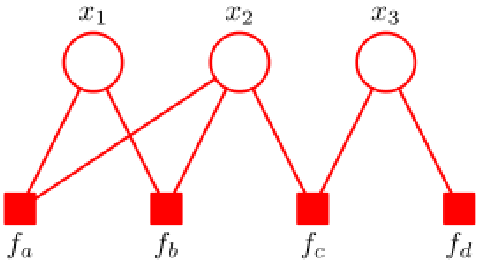
Directed graphs, represent special cases of eq. 21 in which the factors $f_s(x_s)$ are local conditional distributions. Similarly, undirected graphs, are a special case in which the factors are potential functions over the maximal cliques. The normalizing coefficient $1/Z$ can be viewed as a factor defined over the empty set of variables.

Factor graphs

In a factor graph, there is a node (depicted as usual by a circle) for every variable in the distribution, as was the case for directed and undirected graphs. There are also *additional nodes (depicted by small squares) for each factor $f_s(x_s)$* in the joint distribution. Finally, there are *undirected links connecting each factor node to all of the variables nodes on which that factor depends.*

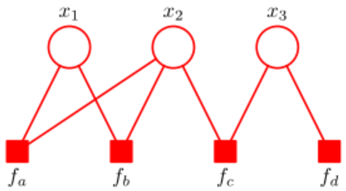


Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 400*

Figure: Factor graph corresponding to $P(\mathbf{x}) = f_a(x_1, x_2)f_b(x_1, x_2)f_c(x_2, x_3)f_d(x_3)$

Factor graphs

Example I



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Note that there are two factors $f_a(x_1, x_2)$ and $f_b(x_1, x_2)$ that are defined over the same set of variables.

Factor graphs

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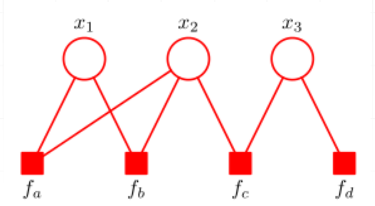

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In an undirected graph, the product of two such factors would simply be lumped together into the same clique potential. Similarly, $f_c(x_2, x_3)$ and $f_d(x_3)$ could be combined into a single potential over x_2 and x_3.

Factor graphs

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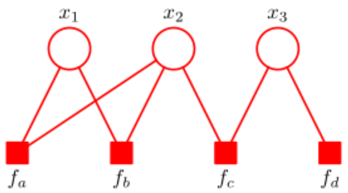

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In an undirected graph, the product of two such factors would simply be lumped together into the same clique potential. Similarly, $f_c(x_2, x_3)$ and $f_d(x_3)$ could be combined into a single potential over x_2 and x_3.
The factor graph, however, keeps such factors explicit and so is able to convey more detailed information about the underlying factorization.

Factor graphs

Example II

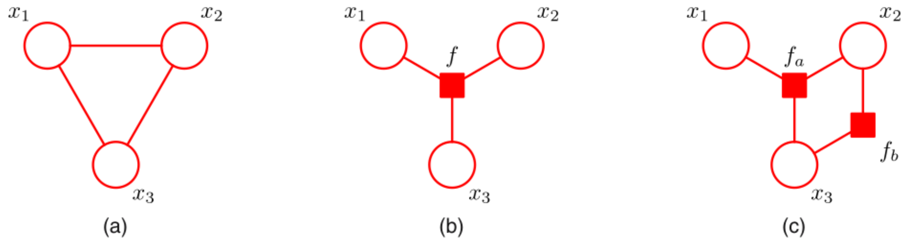

Figure 8.41 (a) An undirected graph with a single clique potential $\psi(x_1, x_2, x_3)$. (b) A factor graph with factor $f(x_1, x_2, x_3) = \psi(x_1, x_2, x_3)$ representing the same distribution as the undirected graph. (c) A different factor graph representing the same distribution, whose factors satisfy $f_a(x_1, x_2, x_3) f_b(x_1, x_2) = \psi(x_1, x_2, x_3)$.

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 400*

Factor graphs

Construction

Undirected graph Create variable nodes corresponding to the nodes in the original undirected graph, and then create additional factor nodes corresponding to the maximal cliques x_s. The factors $f_s(x_s)$ are then set equal to the clique potentials. Note that there may be several different factor graphs that correspond to the same undirected graph.

Factor graphs

Construction

Undirected graph Create variable nodes corresponding to the nodes in the original undirected graph, and then create additional factor nodes corresponding to the maximal cliques x_s. The factors $f_s(x_s)$ are then set equal to the clique potentials. Note that there may be several different factor graphs that correspond to the same undirected graph.

Drirected graphs Create variable nodes in the factor graph corresponding to the nodes of the directed graph, and then create factor nodes corresponding to the conditional distributions, and then finally add the appropriate links. Again, there can be multiple factor graphs all of which correspond to the same directed graph.

Trees

We have seen that exact inference on a graph comprising a *chain of nodes* can be performed efficiently in time that is *linear in the number of nodes*, using an algorithm that can be interpreted in terms of *messages passed along the chain*. More generally, inference can be performed efficiently using local message passing on a broader class of graphs called *trees*.

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Undirected graph Tree is defined as a graph in which there is one, and only one, path between any pair of nodes. Such graphs therefore *do not have loops*.

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If we convert a directed tree into an undirected graph, we see that the *moralization step* will not add any links as *all nodes have at most one parent*, and as a consequence the corresponding moralized graph will be an undirected tree.

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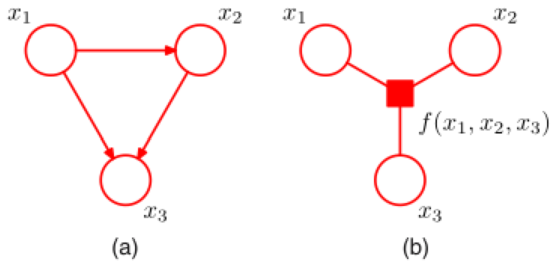
In fact, *local cycles in a directed graph* due to *links connecting parents of a node* can be removed on conversion to a factor graph by defining the appropriate factor function.

Figure 8.44 (a) A fragment of a directed graph having a local cycle. (b) Conversion to a fragment of a factor graph having a tree structure, in which $f(x_1, x_2, x_3) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)$.



Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 400*

Polytree

If there are *nodes in a directed graph that have more than one parent*, but there is still *only one path (ignoring the direction of the arrows) between any two nodes*, then the graph is a called a *polytree*.

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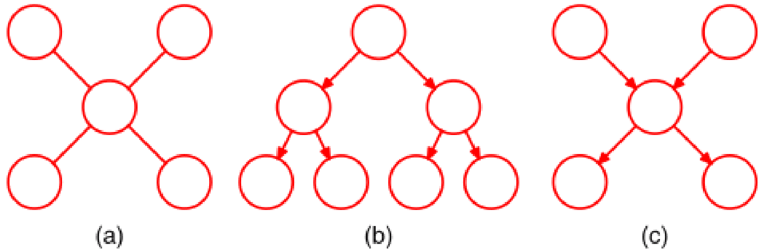

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 399*

Figure: Examples of tree-structured graphs, showing (a) an undirected tree, (b) a directed tree, and (c) a directed polytree.

Polytree

Example

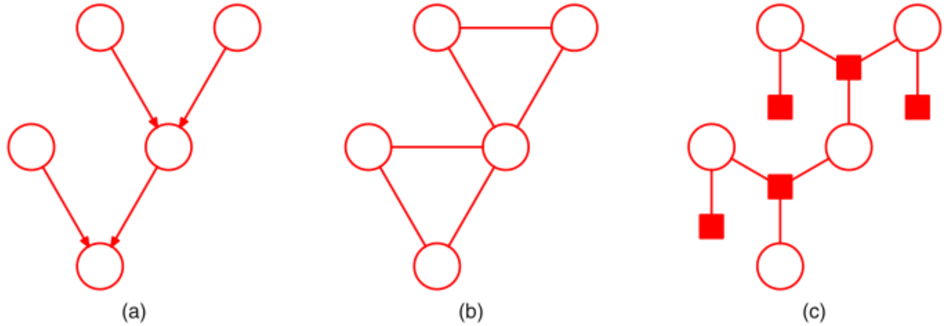

Figure 8.43 (a) A directed polytree. (b) The result of converting the polytree into an undirected graph showing the creation of loops. (c) The result of converting the polytree into a factor graph, which retains the tree structure.

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 402*

The sum-product algorithm

We shall now make use of the *factor graph framework* to derive a powerful class of *efficient*, *exact* inference algorithms that are applicable to *tree-structured graphs*.

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We begin by considering the problem of *finding the marginal* $P(x)$ for particular variable node x. For the moment, we shall suppose that *all of the variables are hidden*. By definition, the marginal is obtained by summing the joint distribution over all variables except x,

$$P(x) = \sum_{\boldsymbol{x} \setminus x} P(\boldsymbol{x}). \tag{22}$$

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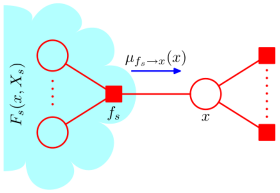
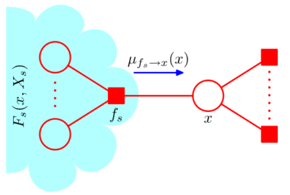
The idea is to substitute $P(x)$ using the *factor graph expression* $P(\boldsymbol{x}) = \prod_s f_s(\boldsymbol{x}_s)$ and then interchange summations and products in order to obtain an efficient algorithm.

The sum-product algorithm



Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 404*

The sum-product algorithm



Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 404*

The joint distribution can be written as a product of the form

$$P(\boldsymbol{x}) = \prod_{s \in \mathrm{ne}(x)} F_S(x, X_s), \tag{23}$$

where $\mathrm{ne}(x)$ denotes the set of factor nodes that are neighbours of x, X_s denotes the set of all variables in the *subtree* connected to the variable nodes x via the factor node f_s, and $F_s(x, X_s)$ represent the *product of all the factors in the group* associated with factor f_s.

The sum-product algorithm

Substituting eq. 23 into 22 and *interchanging the sums and products*, we obtain

$$P(x) = \prod_{s \in \mathrm{ne}(x)} \left[\sum_{X_s} F_S(x, X_s) \right] \tag{24}$$

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Here we introduce *message functions from factor nodes to variable factor nodes*

$$\mu_{f_s \to x}(x) = \sum_{X_s} F_S(x, X_s) \tag{25}$$

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The required marginal P(x) is given by the product of all the incoming messages arriving

at node x.

The sum-product algorithm

How to get *messages*?

The sum-product algorithm

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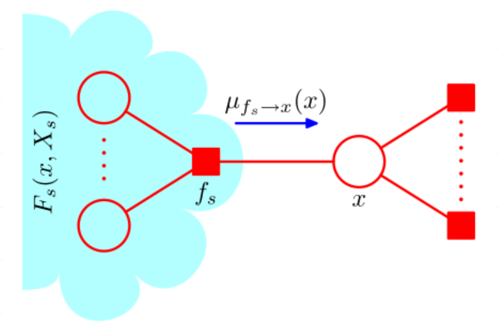
Let us recall



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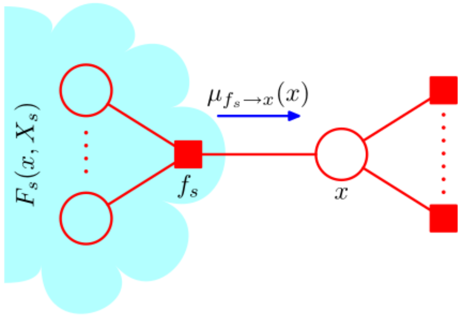


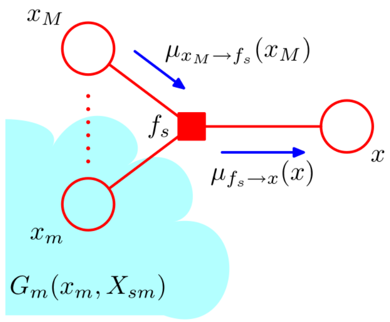
Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 404*

Note that each factor $F_s(x, X_s)$ is described by a *(sub-)graph* of factors and so can itself be factorized!

The sum-product algorithm

In particular, we can write

$$F_s(x, X_s) = f_s(x, x_1, \dots, x_M) G_1(x_1, X_{s1}) \cdots G_M(x_M, X_{sM}) \tag{26}$$



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Combining equations gives us

$$\begin{aligned} \mu_{f_s \to x}(x) &= \sum_{x_1} \ldots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m \in \mathrm{ne}(f_s) \setminus x} \left[\sum_{X_{xm}} G_m(x_m, X_{sm}) \right] \\ &= \sum_{x_1} \ldots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m \in \mathrm{ne}(f_s) \setminus x} \mu_{x_m \to f_s}(x_m) \qquad (8.66) \end{aligned}$$

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where $\mathrm{ne}(f_s)$ denotes the set of variable nodes that are neighbours of the factor node f_s.

The sum-product algorithm

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$$\mu_{x_m\to f_s}(x_m) = \sum_{X_s m} G_m(x_m, X_{sm}) \tag{28}$$

The sum-product algorithm

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$$\mu_{x_m\to f_s}(x_m) = \sum_{X_sm} G_m(x_m, X_{sm}) \qquad (28)$$

It is important to note that a factor node can send a message to a variable node once it has received incoming messages from all other neighbouring variable nodes.

The sum-product algorithm

We have therefore introduced *two distinct kinds of message*, those that go from factor nodes to variable nodes, and those that go from variable nodes to factor nodes. In each case, we see that messages passed along a link are always *a function of the variable associated with the variable node that link connects to*.

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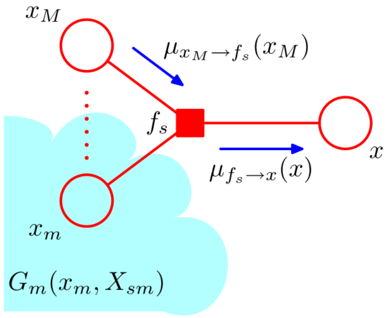

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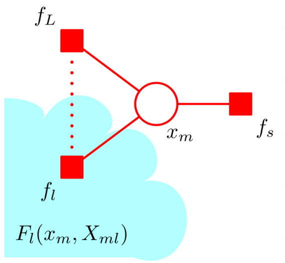

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 406*

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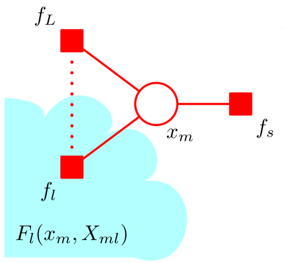

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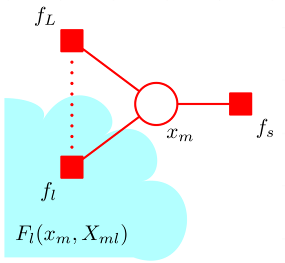

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 406*

Finally, we derive an expression for evaluating the *messages from variable nodes to factor nodes*, again by making use of the (sub-)graph factorization.
The term $G_m(x_m, X_{sm})$ associated with node x_m is given by a product of terms $F_l(x_m, X_{ml})$ each associated with one of the factor nodes $f_l$that is linked to node x_m (excluding node f_s), so that

$$G_m(x_m, X_{sm}) = \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml}) \tag{29}$$

The sum-product algorithm

By putting eq. 29 into 28 and *interchanging the sums and products*, we obtain

$$\mu_{x_m \to f_s}(x_m) = \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} \left[\sum_{X_{ml}} F_l(x_m, X_{ml}) \right] = \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} \mu_{f_l \to x_m}(x_m) \tag{30}$$

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Similarly, if the leaf node is a *factor node*, then the message sent should be

$$\mu_{f \to x}(x) = f(x) \tag{32}$$

The sum-product algorithm

Recall the original goal – calculate the marginal for variable node x, and that this marginal is given by the *product of incoming messages along all of the links arriving at that node*. Each of these messages can be *computed recursively* in terms of other messages.

In order to start this recursion, we can view the node x as the *root* of the tree and *begin at the leaf nodes*.
If the leaf node is a *variable node*, then the message that it sends along its *one and only link* is given by

$$\mu_{x \to f}(x) = 1. \tag{31}$$

Similarly, if the leaf node is a *factor node*, then the message sent should be

$$\mu_{f \to x}(x) = f(x) \tag{32}$$

When all nodes will send their messages sequentially we can evaluate the marginal of intrest – Px. For an inductive proof check [1] p.407.

The sum-product algorithm

Rethinking

Now suppose we wish to find the *marginals for every variable node in the graph*.

The sum-product algorithm

Rethinking

Now suppose we wish to find the *marginals for every variable node in the graph*. This could be done by simply running the above algorithm *afresh for each such node*. However, this would be *very wasteful* as many of the required computations would be repeated.

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Yes, we can!

The sum-product algorithm

All marginals

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- Propagate messages from the leaves to the root as before. At this point, the root node will have received messages from all of its neighbours.
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The sum-product algorithm

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- By now, a message will have passed in both directions across every link in the graph, and every node will have received a message from all of its neighbours.

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Again a simple inductive proof can be found in [1].

The sum-product algorithm

All marginals – example

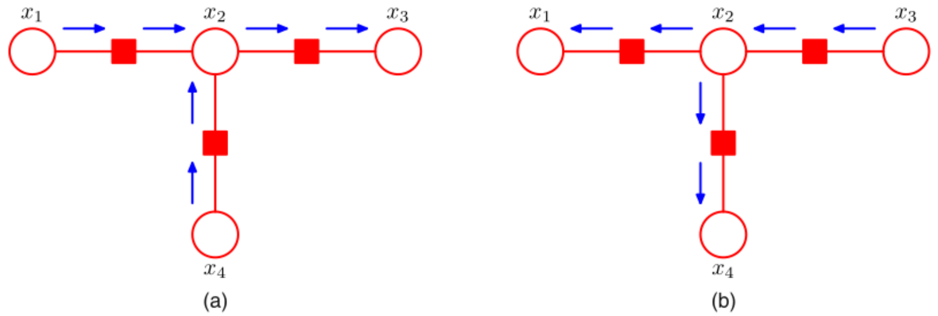

Figure 8.52 Flow of messages for the sum-product algorithm applied to the example graph in Figure 8.51. (a) From the leaf nodes x_1 and x_4 towards the root node x_3. (b) From the root node towards the leaf nodes.

Credit: *Pattern Recognition and Machine Learning, Christopher M. Bishop p. 410*

The sum-product algorithm

Marginals of all nodes in factors

Suppose we wish to find the *marginal distributions* $P(\boldsymbol{x}_s)$ associated with the sets of variables belonging to each of the factors.

The sum-product algorithm

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It is easy to see that the marginal associated with a factor is given by the *product of messages arriving at the factor node and the local factor at that node*

$$P(\boldsymbol{x}_s) = f_s(\boldsymbol{x}_s) \prod_{i \in \mathrm{ne}(f_s)} \mu_{x_i \to f_s}(x_i) \tag{33}$$

The sum-product algorithm

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If the factors are *parameterized functions* and we wish to *learn the values of the parameters* using the *EM algorithm*, then these marginals are precisely the quantities we will need to calculate in the E step.

The sum-product algorithm

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- How about normalization? In case of directed graphs and conditional probabilities everything is properly normalized. For undirected graphs and arbitraty energy functions we end up with unnormalized probabilities. Can we normalize them efficiently?

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Both questions has been answered in [1] Chapter 8.4.4 The sum-product algorithm p.407-411

The sum-product algorithm

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This can be done with the *max-sum algorithm* which has a lot in common with the sum-product algorithm. If you are interested in this subject please check [1] Chapter 8.4.5 The max-sum algorithm p.411-415.

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[1] Christopher M. Bishop. *Pattern Recognition and Machine Learning*. Springer, 2006.

[2] Peter Clifford. “Markov random fields in statistics”. In: ().

[3] S. L. Lauritzen and N. Wermuth. “Graphical Models for Associations between Variables, some of which are Qualitative and some Quantitative”. In: *Ann. Statist.* 17.1 (Mar. 1989), pp. 31–57.