Gates: A graphical notation for mixture models

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Abstract

Gates are a new notation for representing mixture models and context-sensitive independence in factor graphs. Factor graphs provide a natural representation for message-passing algorithms, such as expectation propagation. However, message passing in mixture models is not well captured by factor graphs unless the entire mixture is represented by one factor, because the message equations have a containment structure. Gates capture this containment structure graphically, allowing both the independences and the message-passing equations for a model to be readily visualized. Different variational approximations for mixture models can be understood as different ways of drawing the gates in a model. We present general equations for expectation propagation and variational message passing in the presence of gates.

1 Introduction

Graphical models, such as Bayesian networks and factor graphs [1], are widely used to represent and visualise fixed dependency relationships between random variables. Graphical models are also commonly used as data structures for inference algorithms since they allow independencies between variables to be exploited, leading to significant efficiency gains. However, there is no widely used notation for representing *context-specific* dependencies, that is, dependencies which are present or absent conditioned on the state of another variable in the graph [2]. Such a notation would be necessary not only to represent and communicate context-specific dependencies, but also to be able to exploit context-specific independence to achieve efficient and accurate inference.

A number of notations have been proposed for representing context-specific dependencies, including: case factor diagrams [3], contingent Bayesian networks [4] and labeled graphs [5]. None of these has been widely adopted, raising the question: what properties would a notation need, to achieve widespread use? We believe it would need to be:

- simple to understand and use,
- flexible enough to represent context-specific independencies in real world problems,
- usable as a data structure to allow existing inference algorithms to exploit context-specific independencies for efficiency and accuracy gains,
- usable in conjunction with existing representations, such as factor graphs.

This paper introduces the *gate*, a graphical notation for representing context-specific dependencies that we believe achieves these desiderata. Section 2 describes what a gate is and shows how it can be used to represent context-specific independencies in a number of example models. Section 3 motivates the use of gates for inference and section 4 expands on this by showing how gates can be used within three standard inference algorithms: Expectation Propagation (EP), Variational Message Passing (VMP) and Gibbs sampling. Section 5 shows how the placement of gates can tradeoff cost versus accuracy of inference. Section 6 discusses the use of gates to implement inference algorithms.

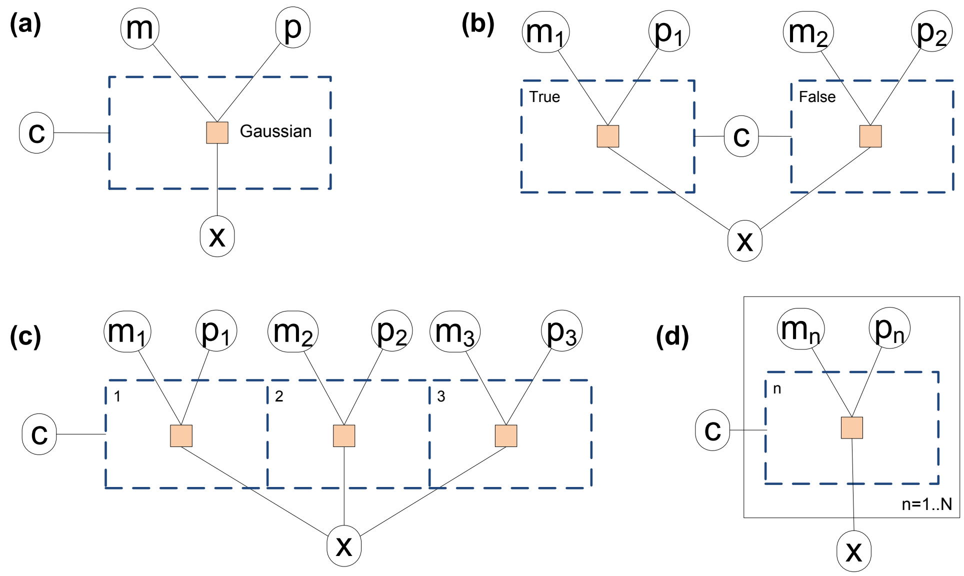

Figure 1: **Gate examples** (a) The dashed rectangle indicates a gate containing a Gaussian factor, with selector variable c. (b) Two gates with different key values used to construct a mixture of two Gaussians. (c) When multiple gates share a selector variable, they can be drawn touching with the selector variable connected to only one of the gates. (d) A mixture of N Gaussians constructed using both a gate and a plate. For clarity, factors corresponding to variable priors have been omitted.

2 The Gate

A gate encloses part of a factor graph and switches it on or off depending on the state of a latent selector variable. The gate is on when the selector variable has a particular value, called the *key*, and off for all other values. A gate allows context-specific independencies to be made explicit in the graphical model: the dependencies represented by any factors inside the gate are present only in the context of the selector variable having the key value. Mathematically, a gate represents raising the contained factors to the power zero if the gate is off, or one if it is on:

$$\left(\prod_i f_i(x)\right)^{\delta(c=key)}$$

where c is the selector variable. In diagrams, a gate is denoted by a dashed box labelled with the value of *key*, with the selector variable connected to the box boundary. The label may be omitted if c is boolean and *key* is *true*. Whilst the examples in this paper refer to factor graphs, gate notation can also be used in both directed Bayesian networks and undirected graphs.

A simple example of a gate is shown in figure 1a. This example represents the term $\mathcal{N}(x; m, p^{-1})^{\delta(c=true)}$ so that when c is true the gate is on and x has a Gaussian distribution with mean m and precision p. Otherwise, the gate is off and x is uniformly distributed (since it is connected to nothing).

By using several gates with different key values, multiple components of a mixture can be represented. Figure 1b shows how a mixture of two Gaussians can be represented using two gates with different key values, true and false. If c is true, x will have distribution $\mathcal{N}(m_1, p_1^{-1})$, otherwise x will have distribution $\mathcal{N}(m_2, p_2^{-1})$. When multiple gates have the same selector variable but different key values, they can be drawn as in figure 1c, with the gate rectangles touching and the selector variable connected to only one of the gates. Notice that in this example, an integer selector variable is used and the key values are the integers 1,2,3.

For large homogeneous mixtures, gates can be used in conjunction with plates [6]. For example, figure 1d shows how a mixture of N Gaussians can be represented by placing the gate, Gaussian factor and mean/precision variables inside a plate, so that they are replicated N times.

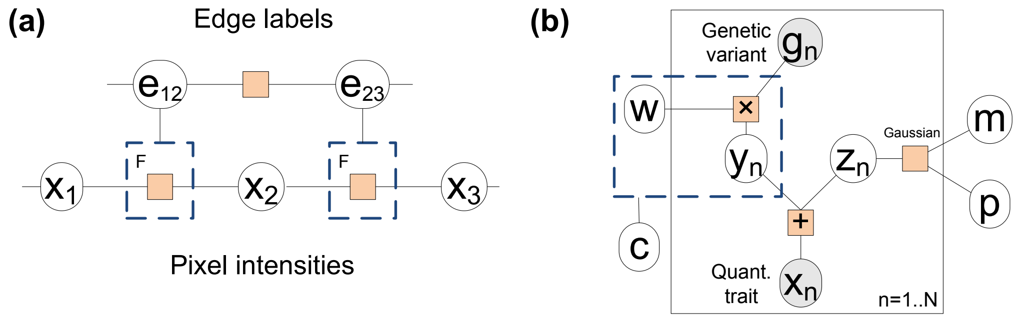

Figure 2: **Examples of models which use gates** (a) A line process where neighboring pixel intensities are independent if an edge exists between them. It illustrates how gates convey the context-specific independencies present in a model. (b) Testing for dependence between a genetic variant g_n and an observed quantitative trait x_n. The selector variable c encodes whether the linear dependency represented by the structure inside the gate is present or absent.

Gates may be nested inside each other, implying a conjunction of their conditions. To avoid ambiguities, gates cannot partially overlap, nor can a gate contain its own selector variable.

Gates can also contain variables, as well as factors. Such variables have the behaviour that, when the gate is off, they revert to having a default value of false or zero, depending on the variable type. Mathematically, a variable inside a gate represents a Dirac delta when the gate is off: $\delta(x)^{1-\delta(c=key)}$ where $\delta(x)$ is one only when x has its default value. Figure 2b shows an example where variables are contained in gates – this example is described in the following section.

2.1 Examples of models with gates

Figure 2a shows a *line process* from [7]. The use of gates makes clear the assumption that two neighboring image pixels x_i and x_j have a dependency between their intensity values, unless there is an edge e_{ij} between them. An opaque three-way factor would hide this context-specific independence.

Gates can also be used to test for independence. In this case the selector variable is connected only to the gate, as shown in the example of figure 2b. This is a model used in functional genomics [8] where the aim is to detect associations between a genetic variant g_n and some quantitative trait x_n (such as height, weight, intelligence etc.) given data from a set of N individuals. The binary selector variable c switches on or off a linear model of the genetic variant's contribution y_n to the trait x_n, across all individuals. When the gate is off, y_n reverts to the default value of 0 and so the trait is explained only by a Gaussian-distributed background model z_n. Again, the gate makes it clear that x_n only depends on g_n if c is true. Inferring the posterior distribution of c allows associations between the genetic variation and the trait to be detected.

3 How gates arise from message-passing on mixture models

A driving force in the popularity of factor graphs is their tight relationship with message passing algorithms. Factor graph notation arises naturally when describing message passing algorithms, such as the sum-product algorithm. Similarly, the gate notation arises naturally when considering the behavior of message passing algorithms on mixture models.

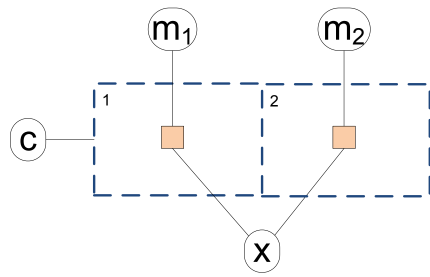

Figure 3: A simple mixture model

As a motivating example, consider the mixture model of figure 3. The joint distribution is:

$$p(x, c, m_1, m_2) = p(c)p(m_1)p(m_2)f(x|m_1)^{\delta(c-1)}f(x|m_2)^{\delta(c-2)} \tag{1}$$

where f is the Gaussian distribution. If we apply mean-field approximation to this model, we obtain the following fixed-point system:

$$q(c = k) \propto p(c = k) \exp\left(\sum_x q(x) \sum_{m_k} q(m_k) \log f(x|m_k)\right) \tag{2}$$

$$q(m_k) \propto p(m_k) \exp\left(\sum_x q(x) \log f(x|m_k)\right)^{q(c=k)} \tag{3}$$

$$q(x) \propto \prod_k \exp\left(\sum_{m_k} q(m_k) \log f(x|m_k)\right)^{q(c=k)} \tag{4}$$

These updates can be interpreted as message-passing combined with "blurring" (raising to a power between 0 and 1). For example, the update for $q(m_k)$ can be interpreted as (message from prior)$\times$(blurred message from f). The update for $q(x)$ can be interpreted as (blurred message from m_1)$\times$(blurred message from m_2). Blurring occurs whenever a message is sent from a factor having a random exponent to a factor without that exponent. Thus the exponent acts like a container, affecting all messages that pass out of it. Hence, we use a graphical notation where a gate is a container, holding all the factors switched by the gate. Graphically, the blurring operation then happens whenever a message leaves a gate. Messages passed into a gate and within a gate are unchanged.

This graphical property holds true for other algorithms as well. For example, if we apply fully-factorized expectation propagation to this model, we obtain the following messages:

$$m_{f\to c}(c = k) = \sum_x \sum_{m_k} p(m_k)f(x|m_k) \tag{5}$$

$$m_{f\to m_k}(m_k) \propto \text{proj}\left[p(c \neq k)m_{f\to c}(c \neq k)p(m_k) + p(c = k)f(x|m_k)p(m_k)\right]/p(m_k) \tag{6}$$

$$= \text{blur}_k[f(x|m_k), p(m_k)] \tag{7}$$

$$m_{c\to x}(x) \propto \text{blur}_1\left[\sum_{m_1} p(m_1)f(x|m_1), 1\right] \text{blur}_2\left[\sum_{m_2} p(m_2)f(x|m_2), 1\right] \tag{8}$$

$$\text{where } \text{blur}_k[h, q] = \text{proj}\left[p(c \neq k)m_{f\to c}(c \neq k)q + p(c = k)hq\right]/q \tag{9}$$

This has a similar form as the mean-field equations, with a modified definition of blurring. In this paper, $\text{proj}[p]$ means the unique exponential-family member whose sufficient statistics match p [9]:

$$\text{proj}[p] = \underset{q}{\text{argmin}}\, KL(p \,||\, q) \tag{10}$$

where the minimization is over the distribution family of interest. For example, if we want $q(x)$ to be Gaussian then $\mathrm{proj}[p(x)]$ in (9) returns a Gaussian whose mean and variance match the distribution $p(x)$ (after normalization of $p(x)$).

In (8), the two gates containing $f(x|m_1)$ and $f(x|m_2)$ have been treated as separate factors. Another approach, which is more accurate for EP, is to treat these two gates as one factor. This leads to the same updates except $m_{c\to x}$ is now:

$$m_{c\to x}(x) = \mathrm{proj}\left[p(c=1)\sum_{m_1} p(m_1)f(x|m_1) + p(c=2)\sum_{m_2} p(m_2)f(x|m_2)\right] \tag{11}$$

which is the exact marginal for x.

3.1 Why gates are not equivalent to 'pick' factors

It is possible to rewrite this model so that the f factors do not have exponents, and therefore would not be in gates. However, this will necessarily change the approximation. This is because the blurring effect caused by exponents operates in one direction only, while the blurring effect caused by intermediate factors is always bidirectional. For example, suppose we try to write the model using a factor $\mathtt{pick}(x|c, h_1, h_2) = \delta(x - h_1)^{\delta(c-1)}\delta(x - h_2)^{\delta(c-2)}$. We can introduce latent variables (h_1, h_2) so that the model becomes $p(x, c, m_1, m_2, h_1, h_2) = p(c)p(m_1)p(m_2)f(h_1|m_1)f(h_2|m_2)\mathtt{pick}(x|c, h_1, h_2)$ (see figure 4a) . The `pick` factor will correctly blur the downward messages from (m_1, m_2) to x. However, the `pick` factor will also blur the message upward from x before it reaches the factor f, which is incorrect.

Another approach is to pick from (m_1, m_2) before reaching the factor f, so that the model becomes $p(x, c, m_1, m_2, m) = p(c)p(m_1)p(m_2)f(x|m)\mathtt{pick}(m|c, m_1, m_2)$ (see figure 4b) . In this case, the message from x to f is not blurred, and the upward messages to (m_1, m_2) are blurred, which is correct. However, the downward messages from (m_1, m_2) to f are blurred before reaching f, which is incorrect.

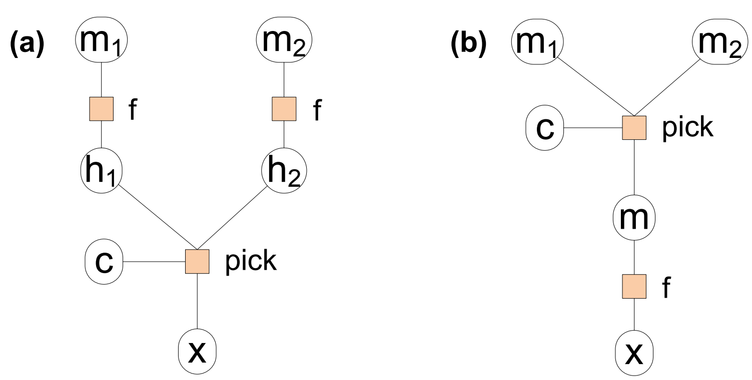

Figure 4: Two different ways of writing figure 3a without gates. Both lead to problems in message-passing.

3.2 Variables inside gates

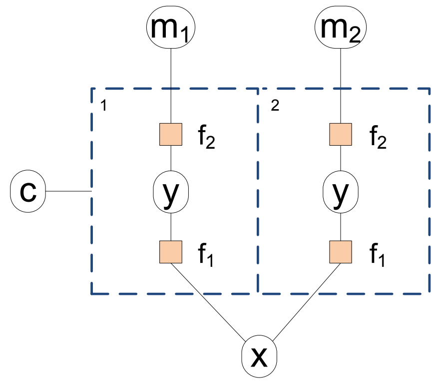

Figure 5: A mixture model with a variable inside the gates

Now consider an example where it is natural to consider a variable to be inside a gate. The model is:

$$p(x, c, m_1, m_2, y) = p(c)p(m_1)p(m_2) \prod_k (f_1(x|y) f_2(y|m_k))^{\delta(c-k)} \tag{12}$$

as depicted in figure 5. If we use a structured variational approximation where y is conditioned on c, then the fixed-point equations are [10]:

$$q(c = k) \propto p(c = k) \exp\left(\sum_x q(x) \sum_y q(y|c = k) \log f_1(x|y)\right)$$
$$\exp\left(\sum_y q(y|c = k) \sum_{m_k} q(m_k) \log f_2(y|m_k)\right) \exp\left(-\sum_y q(y|c = k) \log q(y|c = k)\right) \tag{13}$$

$$q(y|c = k) \propto \exp\left(\sum_x q(x) \log f_1(x|y)\right) \exp\left(\sum_{m_k} q(m_k) \log f_2(y|m_k)\right) \tag{14}$$

$$q(m_k) \propto p(m_k) \exp\left(\sum_y q(y|c = k) \log f_2(y|m_k)\right)^{q(c=k)} \tag{15}$$

$$q(x) \propto \prod_k \exp\left(\sum_y q(y|c = k) \log f_1(x|y)\right)^{q(c=k)} \tag{16}$$

Notice that only the messages to x and m_k are blurred; the messages to and from y are not blurred. Thus we can think of y as sitting inside the gate. The message from the gate to c can be interpreted as the evidence for the submodel containing f_1, f_2, and y.

The factor $f_1(x|y)$ does not depend on k, so we could rewrite the model into an equivalent one where f_1 does not have an exponent:

$$p(x, c, m_1, m_2, y) = p(c)p(m_1)p(m_2) f_1(x|y) \prod_k (f_2(y|m_k))^{\delta(c-k)} \tag{17}$$

If we do this, then the update for $q(x)$ becomes:

$$q(x) \propto \exp\left(\sum_y (\sum_k q(y|c = k) q(c = k)) \log f_1(x|y)\right) \tag{18}$$

which is equivalent to (16). The other updates are also the same.

4 Inference with gates

In the previous section, we explained why the gate notation arises when performing message passing in some example mixture models. In this section, we describe how gate notation can be generally incorporated into Variational Message Passing [11], Expectation Propagation [12] and Gibbs Sampling [7] to allow each of these algorithms to support context-specific independence.

For reference, Table 1 shows the messages needed to apply standard EP or VMP using a fully factorized approximation $q(\mathbf{x}) = \prod_i q(x_i)$. See appendices A and B for a full explanation of this table. Notice that VMP uses different messages to and from deterministic factors, that is, factors which have the form $f_a(x_i, \mathbf{x}_{a\setminus i}) = \delta(x_i - h(\mathbf{x}_{a\setminus i}))$ where x_i is the derived child variable. Different VMP messages are also used to and from such deterministic derived variables. For both algorithms the marginal distributions are obtained as $q(x_i) = \prod_a m_{a\to i}(x_i)$, except for derived child variables in VMP where $q(x_i) = m_{\text{par}\to i}(x_i)$. The (approximate) model evidence is obtained by a product of contributions, one from each variable and each factor. Table 1 shows these contributions for each algorithm, with the exception that deterministic factors and their derived variables contribute 1 under VMP.

When performing inference on models with gates, it is useful to employ a *normalised form* of gate model. In this form, variables inside a gate have no links to factors outside the gate, and a variable outside a gate links to at most one factor inside the gate. Both of these requirements can be achieved by splitting a variable into a copy inside and a copy outside the gate, connected by an equality factor inside the gate. A factor inside a gate should not connect to the selector of the gate; it should be

Alg.	**Type**	**Variable to factor** $m_{i\to a}(x_i)$	**Factor to variable** $m_{a\to i}(x_i)$
EP	Any	$\prod_{b\neq a} m_{b\to i}(x_i)$	$\dfrac{\text{proj}\left[\sum_{\mathbf{x}_a\setminus x_i}\left(\prod_{j\in a} m_{j\to a}(x_j)\right) f_a(\mathbf{x}_a)\right]}{m_{i\to a}(x_i)}$
VMP	Stochastic	$\prod_{a\ni i} m_{a\to i}(x_i)$	$\exp\left[\sum_{\mathbf{x}_a\setminus x_i}\left(\prod_{j\neq i} m_{j\to a}(x_j)\right)\log f_a(\mathbf{x}_a)\right]$
	Det. to parent	$\prod_{b\neq a} m_{b\to i}(x_i)$	$\exp\left[\sum_{\mathbf{x}_{a\setminus(i,\text{ch})}}\left(\prod_{k\neq(i,\text{ch})} m_{k\to a}(x_k)\right)\log \hat{f}_a(\mathbf{x}_a)\right]$ where $\hat{f}_a(\mathbf{x}_a) = \sum_{x_{\text{ch}}} m_{\text{ch}\to a}(x_{\text{ch}}) f_a(\mathbf{x}_a)$
	Det. to child	$m_{\text{par}\to i}(x_i)$	$\text{proj}\left[\sum_{\mathbf{x}_a\setminus x_i}\left(\prod_{j\neq i} m_{j\to a}(x_j)\right) f_a(\mathbf{x}_a)\right]$

Alg.	**Evidence for variable** x_i	**Evidence for factor** f_a
EP	$s_i = \sum_{x_i}\prod_a m_{a\to i}(x_i)$	$s_a = \frac{\sum_{\mathbf{x}_a}\left(\prod_{j\in a} m_{j\to a}(x_j)\right) f_a(\mathbf{x}_a)}{\sum_{\mathbf{x}_a}\prod_{j\in a} m_{j\to a}(x_j) m_{a\to j}(x_j)}$
VMP	$s_i = \exp(-\sum_{x_i} q(x_i)\log q(x_i))$	$s_a = \exp\left(\sum_{\mathbf{x}_a}\left(\prod_{j\in a} m_{j\to a}(x_j)\right)\log f_a(\mathbf{x}_a)\right)$

Table 1: **Messages and evidence computations for EP and VMP** The top part of the table shows messages between a variable x_i and a factor f_a. The notation $j \in a$ refers to all neighbors of the factor, $j \neq i$ is all neighbors except i, par is the parent factor of a derived variable, and ch is the child variable of a deterministic factor. The $\text{proj}[p]$ operator returns an exponential-family distribution whose sufficient statistics match p. The bottom part of the table shows the evidence contributions for variables and factors in each algorithm.

given the key value instead. In addition, gates should be *balanced* by ensuring that if a variable links to a factor in a gate with selector variable c, the variable also links to factors in gates keyed on all other values of the selector variable c. This can be achieved by connecting the variable to uniform factors in gates for any missing values of c. This has no impact on computational cost since the uniform factors involve no computation; it is only a convenience in describing the algorithm. After balancing, each gate is part of a *gate block* – a set of gates activated by different values of the same condition variable. See appendix C for details.

4.1 Variational Message Passing with gates

VMP can be augmented to run on a gate model in normalised form, by changing only the messages out of the gate and by introducing messages from the gate to the selector variable. Messages sent between nodes inside the gate and messages into the gate are unchanged from standard VMP. The variational distributions for variables inside gates are implicitly conditioned on the gate selector, as at the end of section 3. In the following, an individual gate is denoted g, its selector variable c and its key k_g.

The messages out of a gate are modified as follows:

- The message from a factor f_a inside a gate g with selector c to a variable outside g is the usual VMP message, raised to the power $m_{c\to g}(c = k_g)$, except in the following case.
- Where a variable x_i is the child of a number of deterministic factors inside a gate block G with selector variable c, the variable is treated as derived and the message is a moment-matched average of the individual VMP messages. Then the message to x_i is

$$m_{G\to i}(x_i) = \text{proj}\left[\sum_{g\in G} m_{c\to g}(c = k_g) m_{g\to i}(x_i)\right] \tag{19}$$

  where $m_{g\to i}(x_i)$ is the usual VMP message from the unique parent factor in g and proj is a moment-matching projection onto the exponential family.

The message from a gate g to its selector variable c is a product of evidence messages from the contained nodes:

$$m_{g\to c}(c = k_g) = \prod_{a\in g} s_a \prod_{i\in g} s_i, \qquad\qquad m_{g\to c}(c \neq k_g) = 1 \tag{20}$$

where s_a and s_i are the VMP evidence messages from a factor and variable, respectively (Table 1). The set of contained factors includes any contained gates, which are treated as single factors by the containing gate. Deterministic variables and factors send evidence messages of 1, except where a deterministic factor f_a parents a variable x_i outside g. Instead of sending $s_a = 1$, the factor sends:

$$s_a = \exp\left(\sum_{x_i} m_{a\to i}(x_i) \log m_{i\to a}(x_i)\right) \tag{21}$$

The child variable x_i outside the gate also has a different evidence message:

$$s_i = \exp\left(-\sum_{x_i} m_{G\to i}(x_i) \log m_{i\to a}(x_i)\right) \tag{22}$$

where $m_{G\to i}$ is the message from the parents (19) and $m_{i\to a}$ is the message from x_i to any parent. To allow for nested gates, we must also define an evidence message for a gate:

$$s_g = \left(\prod_{a\in g} s_a \prod_{i\in g} s_i\right)^{q(c=k_g)} \tag{23}$$

These rules are derived by considering the behavior of VMP on an equivalent model that does not use gates. For compactness, define a *merge variable* to be a variable x_i that is the child of of a number of deterministic factors inside a gate block. Define $\mathrm{exists}(x_i)$ to be the indicator for node x_i to exist, i.e. the product of $\delta(c_g - k_g)$ for all gates g that x_i is contained in. Note that a gate selector variable can be a derived variable. However the gate it selects cannot be its parent factor.

Starting from a gate model in normalised form, the gates are removed as follows:

1. Replace each factor $f_a(\mathbf{x}_a)$ with $f'_a(\mathbf{x}_a, \mathbf{c}_a) = f_a(\mathbf{x}_a)^{\mathrm{exists}(f_a)}$ where $\mathbf{c}_a$ is the set of condition variables for f_a to exist.
2. For each merge variable x_i, replace x_i's parents with a single deterministic factor given by multiplying the parents together.
3. Erase all gates, promoting all variables to the top level. This defines an equivalent ungated model.

To get good results on this ungated model, the approximation $q(\mathbf{x})$ should not be fully factorized but rather have the form $\prod_i q(x_i|\mathrm{exists}(x_i))$. If x_i is a merge variable with parents inside a gate block with selector variable c_i, then the term for x_i should be $q(x_i|\mathrm{exists}(x_i), c_i)$. (Note that $\mathrm{exists}(x_i)$ includes $\mathrm{exists}(c_i)$ since x_i and c_i must be in the same gate.) Running structured VMP on this ungated model leads to the rules given above, where $q(x_i)$ above actually represents $q(x_i|\mathrm{exists}(x_i))$.

4.2 Expectation Propagation with gates

As with VMP, EP can support gate models in normalised form by making small modifications to the message-passing rules. Once again, messages between nodes inside a gate are unchanged. Recall that, following gate balancing, all gates are part of gate blocks. In the following, an individual gate is denoted g, its selector variable c and its key k_g.

The messages into a gate are as follows:

- The message from a selector variable to each gate in a gate block G is the same. It is the product of all messages into the variable excluding messages from gates in G.
- The message from a variable to each neighboring factor inside a gate block G is the same. It is product of all messages into the variable excluding messages from any factor in G.

Let $\mathrm{nbrs}(g)$ be the set of variables outside of g connected to some factor in g. Each gate computes an intermediate evidence-like quantity s_g defined as:

$$s_g = \prod_{a \in g} s_a \prod_{i \in g} s_i \prod_{i \in \mathrm{nbrs}(g)} s_{ig} \qquad \text{where } s_{ig} = \sum_{x_i} m_{i \to g}(x_i) m_{g \to i}(x_i) \tag{24}$$

where $m_{g \to i}$ is the usual EP message to x_i from its (unique) neighboring factor in g. The third term is used to cancel the denominators of s_a (see definition in Table 1). Given this quantity, the messages out of a gate may now be specified:

- The combined message from all factors in a gate block G with selector variable c to a variable x_i is the weighted average of the messages sent by each factor:

$$m_{G \to i}(x_i) = \frac{\mathrm{proj}\left[\sum_{g \in G} m_{c \to g}(c = k_g) s_g s_{ig}^{-1} m_{g \to i}(x_i) m_{i \to g}(x_i)\right]}{m_{i \to g}(x_i)} \tag{25}$$

  (Note $m_{i \to g}(x_i)$ is the same for each gate g.)
- The message from a gate block G to its selector variable c is:

$$m_{G \to c}(c = k_g) = \frac{s_g}{\sum_{g \in G} s_g} \tag{26}$$

Finally, the evidence contribution of a gate block with selector c is:

$$s_c = \frac{\sum_{g \in G} s_g}{\prod_{i \in \mathrm{nbrs}(g)} \sum_{x_i} m_{i \to g}(x_i) m_{G \to i}(x_i)} \tag{27}$$

These rules are derived by considering the behavior of EP on an equivalent model that does not use gates. The idea is to consider each gate block as a monolithic factor, as in the derivation of (11). When calculating the messages out of this factor, we apply EP recursively to the gate body. This is possible due to the gate balancing transformation which ensures the set of connected variables is the same for all cases, and the link-removal transformation which ensures that inner variables can be summed out.

When a gate block is considered as a monolithic factor $f_G(c, \mathbf{x}_G)$ where $\mathbf{x}_G = \mathrm{nbrs}(G)$, we have the formula:

$$f_G(c, \mathbf{x}_G) = \prod_{g \in G} f_g(\mathbf{x}_G)^{\delta(c - k_g)} \tag{28}$$

where $f_g(\mathbf{x}_G)$ is the product of all factors in gate g, summed over all variables $\mathbf{x}_g$ inside gate g:

$$f_g(\mathbf{x}_G) = \sum_{\mathbf{x}_g} \prod_{a \in g} f_a(\mathbf{x}_a) \tag{29}$$

Given incoming messages for the gate, $m_{i \to g}(x_i)$ for all $x_i \in \mathbf{x}_G$, the EP message from f_G to c is:

$$m_{G \to c}(c = k_g) = Z_G^{-1} \sum_{\mathbf{x}_G} f_g(\mathbf{x}_G) \prod_i m_{i \to g}(x_i) \tag{30}$$

where Z_G^{-1} is an arbitrary scale factor. Expanding the definition of f_g and locally applying the EP evidence formula gives $m_{G \to c}(c = k_g) = Z_G^{-1} s_g$. To make $m_{G \to c}(c)$ a normalized distribution over c, the appropriate scale factor is:

$$Z_G = \sum_{g \in G} s_g \tag{31}$$

The EP message from f_G to $x_i \in \mathbf{x}_G$ is:

$$m_{G \to i}(x_i) = \frac{\mathrm{proj}\left[\sum_{g \in G} m_{c \to g}(c = k_g) r_g(x_i)\right]}{m_{i \to g}(x_i)} \tag{32}$$

$$\text{where } r_g(x_i) = \sum_{\mathbf{x}_G \backslash x_i} f_g(\mathbf{x}_G) \prod_j m_{j \to g}(x_j) \tag{33}$$

Expanding the definition of f_g and locally applying the EP evidence formula to the right-hand side gives $r_g(x_i) = s_g s_{ig}^{-1} m_{g \to i}(x_i) m_{i \to g}(x_i)$ as in (25). The evidence contribution s_G for the gate block is the usual formula for the evidence contribution of a factor, specialized to (28):

$$s_G = \frac{\sum_{g \in G} m_{c \to g}(k_g) \sum_{\mathbf{x}_G} f_g(\mathbf{x}_G) \prod_i m_{i \to g}(x_i)}{\left(\sum_{g \in G} m_{c \to g}(k_g) m_{G \to c}(k_g)\right) \prod_{i \in \mathrm{nbrs}(G)} m_{i \to g}(x_i) m_{G \to i}(x_i)} \tag{34}$$

$$= \frac{\sum_{g \in G} m_{c \to g}(k_g) s_g}{\left(\sum_{g \in G} m_{c \to g}(k_g) m_{G \to c}(k_g)\right) \prod_{i \in \mathrm{nbrs}(G)} m_{i \to g}(x_i) m_{G \to i}(x_i)} \tag{35}$$

$$= \frac{Z_G}{\prod_{i \in \mathrm{nbrs}(G)} m_{i \to g}(x_i) m_{G \to i}(x_i)} \tag{36}$$

4.3 Gibbs sampling with gates

Gibbs sampling can easily extend to gates which contain only factors. Gates containing variables require a facility for computing the evidence of a submodel, which Gibbs sampling does not provide. Note also that Gibbs sampling does not support deterministic factors. Thus the graph should only be normalised up to these constraints. The algorithm starts by setting the variables to initial values and sending these values to their neighboring factors. Then for each variable x_i in turn:

1. Query each neighboring factor for a conditional distribution for x_i. If the factor is in a gate that is currently off, replace with a uniform distribution. For a gate g with selector x_i, the conditional distribution is proportional to s for the key value and 1 otherwise, where s is the product of all factors in g.
2. Multiply the distributions from neighboring factors together to get the variable's conditional distribution. Sample a new value for the variable from its conditional distribution.

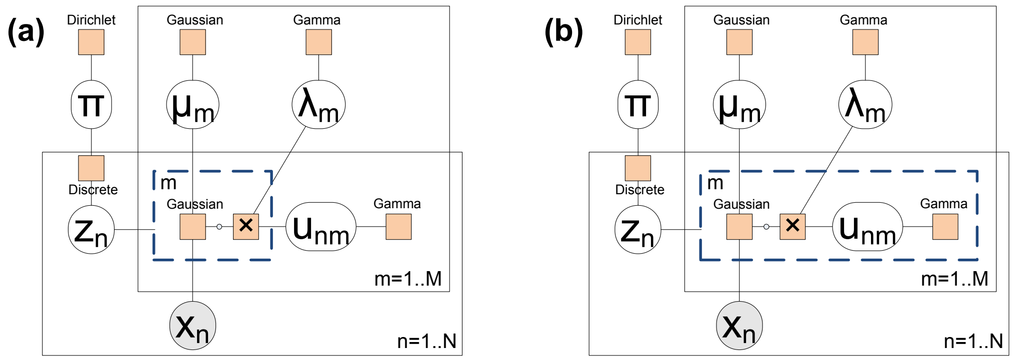

Figure 6: **Student-t mixture model using gates** (a) Model from [13] (b) Structured approximation suggested by [14], which can be interpreted as enlarging the gate.

5 Enlarging gates to increase approximation accuracy

Gates induce a structured approximation as in [10], so by moving nodes inside or outside of gates, you can trade off inference accuracy versus cost. Because one gate of a gate block is always on, any node (variable or factor) outside a gate block G can be equivalently placed inside each gate of G. This increases accuracy since a separate set of messages will be maintained for each case, but it may increase the cost.

For example, Archambeau and Verleysen [14] suggested a structured approximation for Student-t mixture models, instead of the factorised approximation of [13]. Their modification can be viewed as a gate enlargement (figure 6). By enlarging the gate block to include u_{nm}, the blurring between the multiplication factor and u_{nm} is removed, increasing accuracy. This comes at no additional cost since u_{nm} is only used by one gate and therefore only one message is needed per n and m.

6 Discussion and conclusions

Gates have proven very useful to us when implementing a library for inference in graphical models. By using gates, the library allows mixtures of arbitrary sub-models, such as mixtures of factor analysers. Gates are also used for computing the evidence for a model, by placing the entire model in a gate with binary selector variable b. The log evidence is then the log-odds of b, that is, $\log P(b = \text{true}) - \log P(b = \text{false})$. Similarly, gates are used for model comparison by placing each model in a different gate of a gate block. The marginal over the selector gives the posterior distribution over models.

Graphical models not only provide a visual way to represent a probabilistic model, but they can also be used as a data structure for performing inference on that model. We have shown that gates are similarly effective both as a graphical modelling notation and as a construct within an inference algorithm.

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A Summary of Variational Message Passing

This section describes how to fit a fully factorized approximation $q(\mathbf{x}) = \prod_i q(x_i)$ using Variational Message Passing (VMP) [11]. VMP distinguishes between four kinds of nodes in a factor graph:

- Deterministic factors, which have the form $f_a(x_i, \mathbf{x}_{a\setminus i}) = \delta(x_i - h(\mathbf{x}_{a\setminus i}))$.
- Stochastic factors (all other factors)
- Stochastic variables (children of stochastic factors)
- Derived variables (children of deterministic factors)

Deterministic factors and derived variables come in pairs, each deterministic factor having a designated derived child variable and each derived variable having a designated deterministic parent factor. For each of these four node types, VMP describes how to compute (1) the outgoing messages and (2) the evidence contribution.

For a stochastic variable x_i, the incoming messages are functions $m_{a\to i}(x_i)$, one from each neighboring factor f_a. The outgoing message $m_{i\to a}(x_i)$ to any neighbor f_a is the marginal of x_i, computed as the product of all incoming messages:

$$q(x_i) \propto \prod_{a \ni i} m_{a\to i}(x_i) \tag{37}$$

$$m_{i\to a}(x_i) = q(x_i) \tag{38}$$

The evidence contribution is $s_i = \exp(-\sum_{x_i} q(x_i) \log q(x_i))$.

For a derived variable x_i, VMP distinguishes between the incoming message $m_{\text{par}\to i}(x_i)$ from the parent factor f_{par} and the incoming messages $m_{b\to i}(x_i)$ from the other factors. The outgoing message $m_{i\to\text{par}}(x_i)$ to the parent factor is the product of messages from the other factors:

$$m_{i\to\text{par}}(x_i) = \prod_{b\neq\text{par}} m_{b\to i}(x_i) \tag{39}$$

The outgoing message $m_{i\to b}(x_i)$ to a child factor is the message from the parent factor:

$$m_{i\to b}(x_i) = m_{\text{par}\to i}(x_i) \tag{40}$$

The evidence contribution is 1.

For a stochastic factor $f_a(\mathbf{x}_a)$, the incoming messages are functions $m_{i\to a}(x_i)$, one from each neighboring variable x_i. The outgoing message $m_{a\to i}(x_i)$ is the logarithmic average of the factor over the other variables:

$$m_{a\to i}(x_i) \propto \exp\left(\sum_{\mathbf{x}_a\setminus x_i} \left(\prod_{j\neq i} m_{j\to a}(x_j)\right) \log f_a(\mathbf{x}_a)\right) \tag{41}$$

The evidence contribution is $s_a = \exp\left(\sum_{\mathbf{x}_a} \left(\prod_{j\in a} m_{j\to a}(x_j)\right) \log f_a(\mathbf{x}_a)\right)$.

For a deterministic factor $f_a(x_{\text{ch}}, \mathbf{x}_{a\setminus\text{ch}})$, VMP distinguishes between the incoming message $m_{\text{ch}\to a}(x_{\text{ch}})$ from the child variable and the incoming messages $m_{j\to a}(x_j)$ from the other variables. The outgoing message $m_{a\to\text{ch}}(x_{\text{ch}})$ to the child variable is the average of the factor over the other variables, projected onto the approximating family of x_{ch}:

$$m_{a\to\text{ch}}(x_{\text{ch}}) = \text{proj}\left[\sum_{\mathbf{x}_a\setminus x_{\text{ch}}} \left(\prod_{j\neq\text{ch}} m_{j\to a}(x_j)\right) f_a(\mathbf{x}_a)\right] \tag{42}$$

The outgoing message $m_{a\to j}(x_j)$ to a parent variable is the logarithmic average, over the other parent variables, of the factor averaged over the child variable:

$$m_{a\to j}(x_j) \propto \exp\left(\sum_{\mathbf{x}_a\setminus(x_i, x_{\text{ch}})} \left(\prod_{k\neq(i,\text{ch})} m_{k\to a}(x_k)\right) \log\left(\sum_{x_{\text{ch}}} m_{\text{ch}\to a}(x_{\text{ch}}) f_a(\mathbf{x}_a)\right)\right) \tag{43}$$

Because $f_a(\mathbf{x}_a) = \delta(x_{\text{ch}} - h(\mathbf{x}_{a\setminus\text{ch}}))$, the inner term $\sum_{x_{\text{ch}}} m_{\text{ch}\to a}(x_{\text{ch}}) f_a(\mathbf{x}_a)$ reduces to $m_{\text{ch}\to a}(h(\mathbf{x}_{a\setminus\text{ch}}))$. The evidence contribution is 1.

B Summary of Expectation Propagation

This section describes how to fit a fully factorized approximation $q(\mathbf{x}) = \prod_i q(x_i)$ using Expectation Propagation (EP) [12, 9]. EP only distinguishes between two node types: factors and variables. Deterministic factors are not treated specially. For each node type, EP describes how to compute (1) the outgoing messages and (2) the evidence contribution.

For a variable x_i, the incoming messages are functions $m_{a\to i}(x_i)$, one from each neighboring factor f_a. The approximate marginal distribution is proportional to the product of incoming messages:

$$q(x_i) \propto \prod_{a\ni i} m_{a\to i}(x_i) \tag{44}$$

The outgoing message $m_{i\to a}(x_i)$ to f_a is proportional to the product of all incoming messages except from f_a:

$$m_{i\to a}(x_i) \propto \prod_{b\neq a} m_{b\to i}(x_i) \tag{45}$$

The evidence contribution for x_i is:

$$s_i = \sum_{x_i} \prod_a m_{a\to i}(x_i) \tag{46}$$

For a factor f_a, the incoming messages are functions $m_{i\to a}(x_i)$, one from each neighboring variable x_i. The outgoing message $m_{a\to i}(x_i)$ is proportional to the moment-matched projection of the factor averaged over the other variables:

$$m_{a\to i}(x_i) \propto \frac{\mathrm{proj}\left[\sum_{\mathbf{x}_a\setminus x_i}\left(\prod_{j\in a} m_{j\to a}(x_j)\right) f_a(\mathbf{x}_a)\right]}{m_{i\to a}(x_i)} \tag{47}$$

The evidence contribution is:

$$s_a = \frac{\sum_{\mathbf{x}_a}\left(\prod_{j\in a} m_{j\to a}(x_j)\right) f_a(\mathbf{x}_a)}{\sum_{\mathbf{x}_a}\prod_{j\in a} m_{j\to a}(x_j) m_{a\to j}(x_j)} \tag{48}$$

The approximate model evidence is the product of contributions from all variables and factors: $\prod_a s_a \prod_i s_i$. Note that this formula is invariant to any rescaling of the messages.

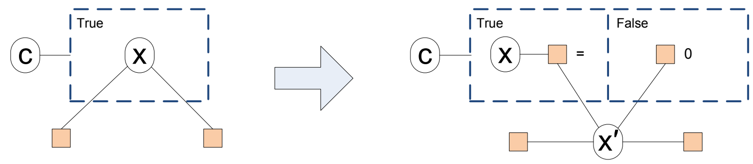
C Transformation to normal form

C.1 Removing links to variables inside gates

This section describes how to transform a factor graph into an equivalent model where a variable inside a gate does not link to any factors outside the gate. This transformation ensures that if a gate g_1 contains the selector variable of another gate g_2, then g_1 also contains g_2. Thus the state of a gate can be uniquely determined from the value of its selector variable.

Suppose the variable x is inside a gate g and linked to some factors f_a outside g. Just outside of g, create a variable x' and link the outer factors f_a to x' instead of x. Inside g, place a deterministic factor $f_=(x, x') = \delta(x' = x)$. Alongside g, create a complementary gate $\bar{g}$. (A complementary gate is a gate which is open when g is closed, and vice versa.) Inside $\bar{g}$, place a deterministic factor $f_0(x') = \delta(x' = 0)$ that constrains its argument to be zero.

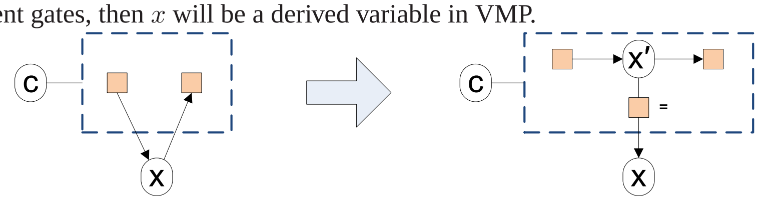
For VMP, if x is a derived variable and one of the factors f_a was x's parent, then f_a becomes a parent of x', and x's parent is now $f_=$. Otherwise $f_=$ and f_0 are the parents of x'. In either case, x' treated by VMP as a derived variable.



C.2 Reduction of gate crossings

This section describes how to transform a factor graph into an equivalent model where a variable outside a gate links to at most one factor inside the gate. This transformation is useful to reduce the number of gate-crossing edges and thereby avoid blurring of messages, as well as to convert stochastic variables into derived variables.

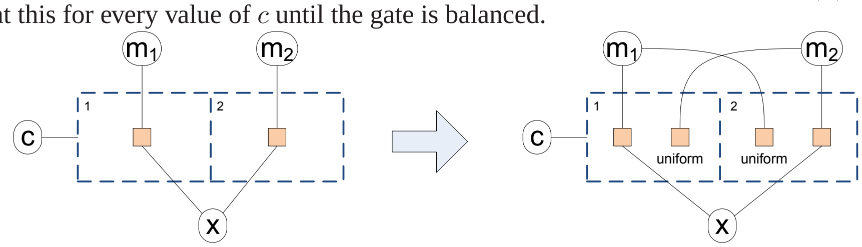
Suppose the variable x is outside a gate g and linked to some factors f_a inside g. Inside g, create a new variable x' and link it to all the factors f_a instead of x. Inside g, add a deterministic factor $f_=(x, x') = \delta(x' = x)$. If one of the factors f_a was x's parent, then f_a becomes the parent of x', and x's parent is now $f_=$. Note that x's parent is now deterministic. If this transformation is done to all of x's parent gates, then x will be a derived variable in VMP.



C.3 Gate balancing

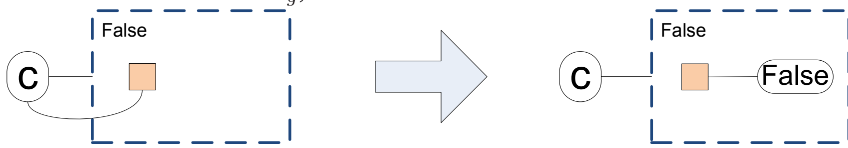
This section describes how to transform a factor graph into an equivalent model where gates are *balanced* in the sense that if a gate g with selector variable c links to a variable x outside g then for *every* value of c there is a gate linking to x.

Suppose variable x links to gate g_1 with condition $c = k_1$, but does not link to any gate when $c = k_2$. Then create a new gate g_2 with condition $c = k_2$ and place a uniform factor $f(x) = 1$ inside it. Repeat this for every value of c until the gate is balanced.



C.4 Removing links to selectors

This section describes how to transform a factor graph into an equivalent model where the selector variable of a gate g has no neighbors inside g. Suppose selector variable c connects to factor f inside g. If the gate has key k_g, then factor f will only be active if $c = k_g$. So f can equivalently be connected to a constant with value k_g, instead of c.



D Converting case-factor diagrams to gates

A case-factor diagram (CFD) is a compact way to encode a set of constraints on Boolean variables. It has the following syntax:

```
D ::= 0 | 1 | case(x,D1,D2) | factor(D1,D2)
```

In this notation, "0" means an impossible state, i.e. "fail", "1" means that all unassigned variables are false, "x" stands for any Boolean variable, and "D1" and "D2" are sub-diagrams. For example, this CFD states that exactly one of (x, y, z) is true:

```
case(x,1, case(y,1, case(z,1,0)))
```

The size of this CFD is linear in the number of variables, which is a big improvement over the usual factor graph notation for that constraint.

To illustrate the complexities of CFDs, consider the constraint "an even number of variables are true" over the set $x_1, ..., x_n$. We can encode this using the following recursion:

$$\mathrm{EVEN}_0 = 1 \tag{49}$$

$$\mathrm{ODD}_0 = 0 \tag{50}$$

$$\mathrm{EVEN}_i = \mathrm{case}(x_i, \mathrm{ODD}_{i-1}, \mathrm{EVEN}_{i-1}) \qquad i = 1, ..., n \tag{51}$$

$$\mathrm{ODD}_i = \mathrm{case}(x_i, \mathrm{EVEN}_{i-1}, \mathrm{ODD}_{i-1}) \qquad i = 1, ..., n \tag{52}$$

The final CFD is then EVEN_n. In this CFD, the subexpression EVEN_{i-1} appears twice. However, these appearances are mutually exclusive since in one case x_i is false and in the other x_i is true.

It turns out that any case-factor diagram can be encoded as a gated factor graph with only a constant factor increase in the number of nodes. The general transformation is as follows. Each unique subexpression in the CFD is given a Boolean variable v_{expr} which is true iff the expression is reached in the CFD. Each v_{expr} is fed by an OR factor. The OR factor has one input always set to false, so that the variable is false if never used. The other inputs correspond to each use of the expression in the CFD. Because a node in a CFD can be reached in at most one way, at most one of these inputs will be true. In addition to the OR factor, we connect v_{expr} as follows:

- v_0 is constrained to be false.
- v_1 is not constrained.
- $v_{\mathrm{factor}(D1,D2)}$ is connected to $\mathrm{or}(v_{D1})$ and $\mathrm{or}(v_{D2})$.
- $v_{\mathrm{case}(x,D1,D2)}$ is connected to a gate surrounding two fresh variables x' and $\bar{x}'$ with a NOT factor between them. x' is connected to $\mathrm{or}(v_{D1})$ and $\bar{x}'$ is connected to $\mathrm{or}(v_{D2})$. Additionally, x' is connected to v_x (not $\mathrm{or}(v_x)$) via an equality constraint $f_=(x', v_x)$ which sits inside the gate.
- For the top-level expression D of the CFD, constrain v_D to be true.

The graph that results from this transformation can be simplified a bit. For example, v_1 and all edges leading to v_1 can be dropped since v_1 is unconstrained. Since v_0 is always false, it can be dropped and all edges leading to v_0 can be replaced with *false* constraints. Since v_D is always true, it can be dropped and the *true* constraint propagated forward to its children.