These are exercises for self-study and exam preparation. All material is examinable unless otherwise mentioned.

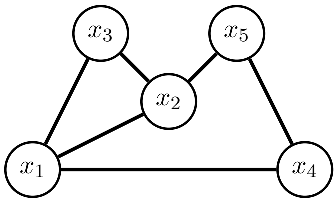
Exercise 1. ***Visualising and analysing Gibbs distributions via undirected graphs***

We here consider the Gibbs distribution

$$p(x_1, \ldots, x_5) \propto \phi_{12}(x_1, x_2)\phi_{13}(x_1, x_3)\phi_{14}(x_1, x_4)\phi_{23}(x_2, x_3)\phi_{25}(x_2, x_5)\phi_{45}(x_4, x_5)$$

(a) *Visualise it as an undirected graph.*

Solution. We draw a node for each random variable x_i. There is an edge between two nodes if the corresponding variables co-occur in a factor.



(b) *What are the neighbours of x_3 in the graph?*

Solution. The neighbours are all the nodes for which there is a single connecting edge. Thus: $\text{ne}(x_3) = \{x_1, x_2\}$. (Note that sometimes, we may denote $\text{ne}(x_3)$ by ne_3.)

(c) *Do we have $x_3 \perp\!\!\!\perp x_4 \mid x_1, x_2$?*

Solution. Yes. The conditioning set $\{x_1, x_2\}$ equals ne_3, which is also the Markov blanket of x_3. This means that x_3 is conditionally independent of all the other variables given $\{x_1, x_2\}$, i.e. $x_3 \perp\!\!\!\perp x_4, x_5 \mid x_1, x_2$, which implies that $x_3 \perp\!\!\!\perp x_4 \mid x_1, x_2$. (One can also use graph separation to answer the question.)

(d) *What is the Markov blanket of x_4?*

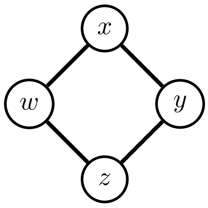
Solution. The Markov blanket of a node in a undirected graphical model equals the set of its neighbours: $\text{MB}(x_4) = \text{ne}(x_4) = \text{ne}_4 = \{x_1, x_5\}$. This implies, for example, that $x_4 \perp\!\!\!\perp x_2, x_3 \mid x_1, x_5$.

(e) *On which minimal set of variables A do we need to condition to have $x_1 \perp\!\!\!\perp x_5 \mid A$?*

Solution. We first identify all trails from x_1 to x_5. There are three such trails: (x_1, x_2, x_5), (x_1, x_3, x_2, x_5), and (x_1, x_4, x_5). Conditioning on x_2 blocks the first two trails, conditioning on x_4 blocks the last. We thus have: $x_1 \perp\!\!\!\perp x_5 \mid x_2, x_4$, so that $A = \{x_2, x_4\}$.

Exercise 2. ***Factorisation and independencies for undirected graphical models***

Consider the undirected graphical model defined by the following graph, sometimes called a diamond configuration.



(a) *How do the pdfs/pmfs of the undirected graphical model factorise?*

Solution. The maximal cliques are (x, w), (w, z), (z, y) and (x, y). The undirected graphical model thus consists of pdfs/pmfs that factorise as follows

$$p(x, w, z, y) \propto \phi_1(x, w)\phi_2(w, z)\phi_3(z, y)\phi_4(x, y) \tag{S.1}$$

(b) *List all independencies that hold for the undirected graphical model.*

Solution. We can generate the independencies by conditioning on progressively larger sets. Since there is a trail between any two nodes, there are no unconditional independencies. If we condition on a single variable, there is still a trail that connects the remaining ones. Let us thus consider the case where we condition on two nodes. By graph separation, we have

$$w \perp\!\!\!\perp y \mid x, z \qquad x \perp\!\!\!\perp z \mid w, y \tag{S.2}$$

These are all the independencies that hold for the model, since conditioning on three nodes does not lead to any independencies in a model with four variables.

Exercise 3. ***Factorisation from the Markov blankets***

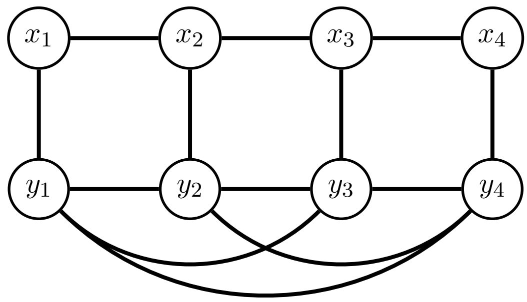
For a distribution $p(x_1, \ldots, x_4, y_1, \ldots, y_4)$, we are given the following Markov blankets for the x-variables:

$$MB(x_1) = \{x_2, y_1\} \qquad MB(x_2) = \{x_1, x_3, y_2\} \qquad MB(x_3) = \{x_2, x_4, y_3\} \qquad MB(x_4) = \{x_3, y_4\} \tag{1}$$

Without inserting more independencies than those specified by the Markov blankets, draw the graph over which p factorises and state the factorisation. (Assume that p is positive for all possible values of its variables).

Solution. The Markov blankets of a variable are its neighbours in the graph. But since we are only given the Markov blankets on the x-variables and for the y-variables, and are not allowed to insert additional independencies, we must assume that each y_i is connected to all the other $y's$. For example, if we didn't connect y_1 and y_4 we would assert the additional independency $y_1 \perp\!\!\!\perp y_4 \mid x_1, x_2, x_3, x_4, y_2, y_3$.

We thus have a graph as follows:



The factorisation thus is

$$p(x_1, \ldots, x_4, y_1, \ldots, y_4) = \frac{1}{Z} g(y_1, \ldots, y_4) \prod_{i=1}^{3} m_i(x_i, x_{i+1}) \prod_{i=1}^{4} g_i(x_i, y_i), \tag{S.3}$$

where the $m_i(x_i, x_{i+1})$, $g_i(x_i, y_i)$ and $g(y_1, \ldots, y_4)$ are positive factors. We have a Markov chain for the x_i, but only a single factor for (y_1, y_2, y_3, y_4) to avoid inserting independencies beyond those specified by the given Markov blankets.

Exercise 4. ***Undirected graphical model with pairwise potentials***

We here consider Gibbs distributions where the factors only depend on two variables at a time. The probability density or mass functions over d random variables $x_1, \ldots, x_d$ then take the form

$$p(x_1, \ldots, x_d) \propto \prod_{i \leq j} \phi_{ij}(x_i, x_j)$$

Such models are sometimes called pairwise Markov networks.

(a) *Let $p(x_1, \ldots, x_d) \propto \exp\left(-\frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{b}^\top \mathbf{x}\right)$ where $\mathbf{A}$ is symmetric and $\mathbf{x} = (x_1, \ldots, x_d)^\top$. What are the corresponding factors ϕ_{ij} for $i \leq j$?*

Solution. Denote the (i, j)-th element of $\mathbf{A}$ by a_{ij}. We have

$$\mathbf{x}^\top \mathbf{A}\mathbf{x} = \sum_{ij} a_{ij} x_i x_j \tag{S.4}$$

$$= \sum_{i<j} 2a_{ij} x_i x_j + \sum_i a_{ii} x_i^2 \tag{S.5}$$

where the second line follows from $\mathbf{A}^\top = \mathbf{A}$. Hence,

$$-\frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{b}^\top \mathbf{x} = -\frac{1}{2} \sum_{i<j} 2a_{ij} x_i x_j - \frac{1}{2} \sum_i a_{ii} x_i^2 - \sum_i b_i x_i \tag{S.6}$$

so that

$$\phi_{ij}(x_i, x_j) = \begin{cases} \exp\left(-a_{ij} x_i x_j\right) & \text{if } i < j \\ \exp\left(-\frac{1}{2} a_{ii} x_i^2 - b_i x_i\right) & \text{if } i = j \end{cases} \tag{S.7}$$

For $\mathbf{x} \in \mathbb{R}^d$, the distribution is a Gaussian with $\mathbf{A}$ equal to the inverse covariance matrix. For binary $\mathbf{x}$, the model is known as Ising model or Boltzmann machine. For $x_i \in \{-1, 1\}$,

$x_i^2 = 1$ for all i, so that the a_{ii} are constants that can be absorbed into the normalisation constant. This means that for $x_i \in \{-1, 1\}$, we can work with matrices $\mathbf{A}$ that have zeros on the diagonal.

(b) *For $p(x_1, \ldots, x_d) \propto \exp\left(-\frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{b}^\top \mathbf{x}\right)$, show that $x_i \perp\!\!\!\perp x_j \mid \{x_1, \ldots, x_d\} \setminus \{x_i, x_j\}$ if the (i,j)-th element of $\mathbf{A}$ is zero.*

Solution. The previous question showed that we can write $p(x_1, \ldots, x_d) \propto \prod_{i \leq j} \phi_{ij}(x_i, x_j)$ with potentials as in Equation (S.7). Consider two variables x_i and x_j for fixed (i, j). They only appear in the factorisation via the potential ϕ_{ij}. If $a_{ij} = 0$, the factor ϕ_{ij} becomes a constant, and no other factor contains x_i and x_j, which means that there is no edge between x_i and x_j if $a_{ij} = 0$. By the pairwise Markov property it then follows that $x_i \perp\!\!\!\perp x_j \mid \{x_1, \ldots, x_d\} \setminus \{x_i, x_j\}$.

Exercise 5. *Restricted Boltzmann machine (based on Barber Exercise 4.4)*

The restricted Boltzmann machine is an undirected graphical model for binary variables $\mathbf{v} = (v_1, \ldots, v_n)^\top$ and $\mathbf{h} = (h_1, \ldots, h_m)^\top$ with a probability mass function equal to

$$p(\mathbf{v}, \mathbf{h}) \propto \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{a}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h}\right), \tag{2}$$

where $\mathbf{W}$ is a $n \times m$ matrix. Both the v_i and h_i take values in $\{0, 1\}$. The v_i are called the "visibles" variables since they are assumed to be observed while the h_i are the hidden variables since it is assumed that we cannot measure them.

(a) *Use graph separation to show that the joint conditional $p(\mathbf{h}|\mathbf{v})$ factorises as*

$$p(\mathbf{h}|\mathbf{v}) = \prod_{i=1}^{m} p(h_i|\mathbf{v}).$$

Solution. Figure 1 on the left shows the undirected graph for $p(\mathbf{v}, \mathbf{h})$ with $n = 3, m = 2$. We note that the graph is bi-partite: there are only direct connections between the h_i and the v_i. Conditioning on $\mathbf{v}$ thus blocks all trails between the h_i (graph on the right). This means that the h_i are independent from each other given $\mathbf{v}$ so that

$$p(\mathbf{h}|\mathbf{v}) = \prod_{i=1}^{m} p(h_i|\mathbf{v}).$$

Figure 1: Left: Graph for $p(\mathbf{v}, \mathbf{h})$. Right: Graph for $p(\mathbf{h}|\mathbf{v})$

(b) Show that

$$p(h_i = 1|\mathbf{v}) = \frac{1}{1 + \exp\left(-b_i - \sum_j W_{ji} v_j\right)} \quad (3)$$

where W_{ji} is the (ji)-th element of $\mathbf{W}$, so that $\sum_j W_{ji} v_j$ is the inner product (scalar product) between the i-th column of $\mathbf{W}$ and $\mathbf{v}$.

Solution. For the conditional pmf $p(h_i|\mathbf{v})$ any quantity that does not depend on h_i can be considered to be part of the normalisation constant. A general strategy is to first work out $p(h_i|\mathbf{v})$ up to the normalisation constant and then to normalise it afterwards.

We begin with $p(\mathbf{h}|\mathbf{v})$:

$$\begin{aligned}
p(\mathbf{h}|\mathbf{v}) &= \frac{p(\mathbf{h}, \mathbf{v})}{p(\mathbf{v})} && \text{(S.8)}\\
&\propto p(\mathbf{h}, \mathbf{v}) && \text{(S.9)}\\
&\propto \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{a}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h}\right) && \text{(S.10)}\\
&\propto \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{b}^\top \mathbf{h}\right) && \text{(S.11)}\\
&\propto \exp\left(\sum_i \sum_j v_j W_{ji} h_i + \sum_i b_i h_i\right) && \text{(S.12)}
\end{aligned}$$

As we are interested in $p(h_i|\mathbf{v})$ for a fixed i, we can drop all the terms not depending on that h_i, so that

$$p(h_i|\mathbf{v}) \propto \exp\left(\sum_j v_j W_{ji} h_i + b_i h_i\right) \quad \text{(S.13)}$$

Since h_i only takes two values, 0 and 1, normalisation is here straightforward. Call the unnormalised pmf $\tilde{p}(h_i|\mathbf{v})$,

$$\tilde{p}(h_i|\mathbf{v}) = \exp\left(\sum_j v_j W_{ji} h_i + b_i h_i\right). \quad \text{(S.14)}$$

We then have

$$\begin{aligned}
p(h_i|\mathbf{v}) &= \frac{\tilde{p}(h_i|\mathbf{v})}{\tilde{p}(h_i = 0|\mathbf{v}) + \tilde{p}(h_i = 1|\mathbf{v})} && \text{(S.15)}\\
&= \frac{\tilde{p}(h_i|\mathbf{v})}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} && \text{(S.16)}\\
&= \frac{\exp\left(\sum_j v_j W_{ji} h_i + b_i h_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)}, && \text{(S.17)}
\end{aligned}$$

so that

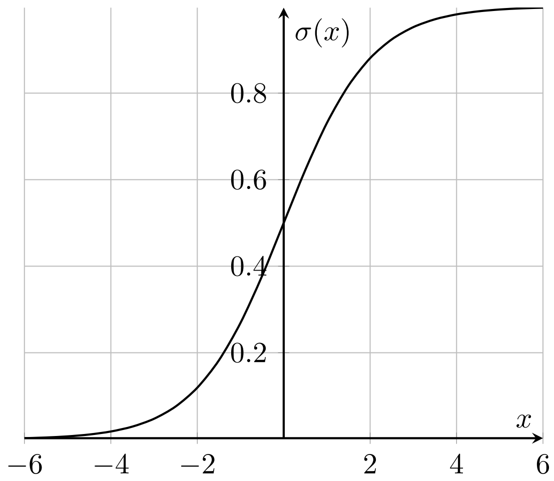
$$\begin{aligned}
p(h_i = 1|\mathbf{v}) &= \frac{\exp\left(\sum_j v_j W_{ji} + b_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} && \text{(S.18)}\\
&= \frac{1}{1 + \exp\left(-\sum_j v_j W_{ji} - b_i\right)}. && \text{(S.19)}
\end{aligned}$$

The probability $p(h = 0|\mathbf{v})$ equals $1 - p(h_i = 1|\mathbf{v})$, which is

$$p(h_i = 0|\mathbf{v}) = \frac{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} - \frac{\exp\left(\sum_j v_j W_{ji} + b_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} \tag{S.20}$$

$$= \frac{1}{1 + \exp\left(\sum_j W_{ji} v_j + b_i\right)} \tag{S.21}$$

The function $x \mapsto 1/(1 + \exp(-x))$ is called the logistic function. It is a sigmoid function and is thus sometimes denoted by $\sigma(x)$. For other versions of the sigmoid function, see https://en.wikipedia.org/wiki/Sigmoid_function.



With that notation, we have

$$p(h_i = 1|\mathbf{v}) = \sigma\left(\sum_j W_{ji} v_j + b_i\right).$$

(c) Use a symmetry argument to show that

$$p(\mathbf{v}|\mathbf{h}) = \prod_i p(v_i|\mathbf{h}) \quad \textit{and} \quad p(v_i = 1|\mathbf{h}) = \frac{1}{1 + \exp\left(-a_i - \sum_j W_{ij} h_j\right)}$$

Solution. Since $\mathbf{v}^\top \mathbf{W} \mathbf{h}$ is a scalar we have $(\mathbf{v}^\top \mathbf{W} \mathbf{h})^\top = \mathbf{h}^\top \mathbf{W}^\top \mathbf{v} = \mathbf{v}^\top \mathbf{W} \mathbf{h}$, so that

$$p(\mathbf{v}, \mathbf{h}) \propto \exp\left(\mathbf{v}^\top \mathbf{W} \mathbf{h} + \mathbf{a}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h}\right) \tag{S.22}$$

$$\propto \exp\left(\mathbf{h}^\top \mathbf{W}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h} + \mathbf{a}^\top \mathbf{v}\right). \tag{S.23}$$

To derive the result, we note that $\mathbf{v}$ and a now take the place of $\mathbf{h}$ and $\mathbf{b}$ from before, and that we now have $\mathbf{W}^\top$ rather than $\mathbf{W}$. In Equation (3), we thus replace h_i with v_i, b_i with a_i, and W_{ji} with W_{ij} to obtain $p(v_i = 1|\mathbf{h})$. In terms of the sigmoid function, we have

$$p(v_i = 1|\mathbf{h}) = \sigma\left(\sum_j W_{ij} h_j + a_i\right).$$

Note that while $p(\mathbf{v}|\mathbf{h})$ factorises, the marginal $p(\mathbf{v})$ does generally not. The marginal $p(\mathbf{v})$ can here be obtained in closed form up to its normalisation constant.

$$
\begin{aligned}
p(\mathbf{v}) &= \sum_{\mathbf{h}\in\{0,1\}^m} p(\mathbf{v},\mathbf{h}) && \text{(S.24)}\\
&= \frac{1}{Z}\sum_{\mathbf{h}\in\{0,1\}^m} \exp\left(\mathbf{v}^\top\mathbf{W}\mathbf{h} + \mathbf{a}^\top\mathbf{v} + \mathbf{b}^\top\mathbf{h}\right) && \text{(S.25)}\\
&= \frac{1}{Z}\sum_{\mathbf{h}\in\{0,1\}^m} \exp\left(\sum_{ij} v_i h_j W_{ij} + \sum_i a_i v_i + \sum_j b_j h_j\right) && \text{(S.26)}\\
&= \frac{1}{Z}\sum_{\mathbf{h}\in\{0,1\}^m} \exp\left(\sum_{j=1}^m h_j \left[\sum_i v_i W_{ij} + b_j\right] + \sum_i a_i v_i\right) && \text{(S.27)}\\
&= \frac{1}{Z}\sum_{\mathbf{h}\in\{0,1\}^m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) \exp\left(\sum_i a_i v_i\right) && \text{(S.28)}\\
&= \frac{1}{Z}\exp\left(\sum_i a_i v_i\right) \sum_{\mathbf{h}\in\{0,1\}^m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) && \text{(S.29)}\\
&= \frac{1}{Z}\exp\left(\sum_i a_i v_i\right) \sum_{h_1,\ldots,h_m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) && \text{(S.30)}
\end{aligned}
$$

Importantly, each term in the product only depends on a single h_j, so that by sequentially applying the distributive law, we have

$$
\begin{aligned}
\sum_{h_1,\ldots,h_m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) &= \left[\sum_{h_1,\ldots,h_{m-1}} \prod_{j=1}^{m-1} \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right)\right] \cdot \\
&\quad \sum_{h_m} \exp\left(h_m \left[\sum_i v_i W_{im} + b_m\right]\right) && \text{(S.31)}\\
&= \ldots \\
&= \prod_{j=1}^m \left[\sum_{h_j} \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right)\right] && \text{(S.32)}
\end{aligned}
$$

Since $h_j \in \{0,1\}$, we obtain

$$
\sum_{h_j} \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) = 1 + \exp\left(\sum_i v_i W_{ij} + b_j\right) \qquad \text{(S.33)}
$$

and thus

$$
p(\mathbf{v}) = \frac{1}{Z}\exp\left(\sum_i a_i v_i\right) \prod_{j=1}^m \left[1 + \exp\left(\sum_i v_i W_{ij} + b_j\right)\right]. \qquad \text{(S.34)}
$$

Note that in the derivation of $p(\mathbf{v})$ we have not used the assumption that the visibles v_i are binary. The same expression would thus obtained if the visibles were defined in another space, e.g. the real numbers.

While $p(\mathbf{v})$ is written as a product, $p(\mathbf{v})$ does not factorise into terms that depend on subsets of the v_i. On the contrary, all v_i are present in all factors. Since $p(\mathbf{v})$ does not factorise, computing the normalising Z is expensive. For binary visibles $v_i \in \{0, 1\}$, Z equals

$$Z = \sum_{\mathbf{v}\in\{0,1\}^n} \exp\left(\sum_i a_i v_i\right) \prod_{j=1}^m \left[1 + \exp\left(\sum_i v_i W_{ij} + b_j\right)\right] \tag{S.35}$$

where we have to sum over all 2^n configurations of the visibles $\mathbf{v}$. This is computationally expensive, or even prohibitive if n is large ($2^{20} = 1048576$, $2^{30} > 10^9$). Note that different values of a_i, b_i, W_{ij} yield different values of Z. (This is a reason why Z is called the partition *function* when the a_i, b_i, W_{ij} are free parameters.)

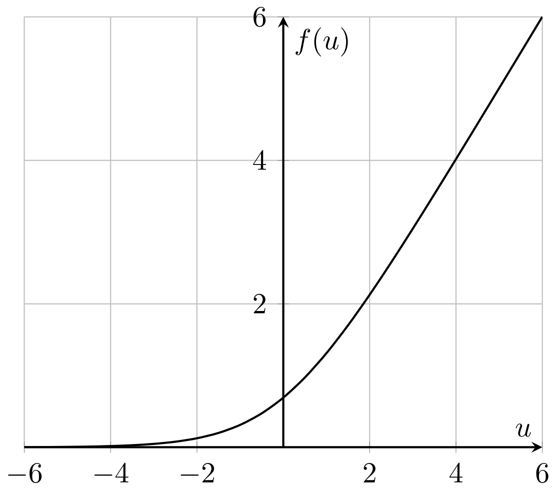
It is instructive to write $p(\mathbf{v})$ in the log-domain,

$$\log p(\mathbf{v}) = \log Z + \sum_{i=1}^n a_i v_i + \sum_{j=1}^m \log\left[1 + \exp\left(\sum_i v_i W_{ij} + b_j\right)\right], \tag{S.36}$$

and to introduce the nonlinearity $f(u)$,

$$f(u) = \log\left[1 + \exp(u)\right], \tag{S.37}$$

which is called the softplus function and plotted below. The softplus function is a smooth approximation of $\max(0, u)$, see e.g. https://en.wikipedia.org/wiki/Rectifier_(neural_networks)



With the softplus function $f(u)$, we can write $\log p(\mathbf{v})$ as

$$\log p(\mathbf{v}) = \log Z + \sum_{i=1}^n a_i v_i + \sum_{j=1}^m f\left(\sum_i v_i W_{ij} + b_j\right). \tag{S.38}$$

The parameter b_j plays the role of a threshold as shown in the figure below. The terms $f\left(\sum_i v_i W_{ij} + b_j\right)$ can be interpreted in terms of feature detection. The sum $\sum_i v_i W_{ij}$ is the inner product between $\mathbf{v}$ and the j-th column of $\mathbf{W}$, and the inner product is largest if $\mathbf{v}$ equals the j-th column. We can thus consider the columns of $\mathbf{W}$ to be feature-templates, and the $f\left(\sum_i v_i W_{ij} + b_j\right)$ a way to measure how much of each feature is present in $\mathbf{v}$.

Further, $\sum_i v_i W_{ij} + b_j$ is also the input to the sigmoid function when computing $p(h_j = 1|\mathbf{v})$. Thus, the conditional probability for h_j to be one, i.e. "active", can be considered to be an indicator of the presence of the j-th feature (j-th column of $\mathbf{W}$) in the input $\mathbf{v}$. If v is such that $\sum_i v_i W_{ij} + b_j$ is large for many j, i.e. if many features are detected, then $f\left(\sum_i v_i W_{ij} + b_j\right)$ will be non-zero for many j, and $\log p(\mathbf{v})$ will be large.