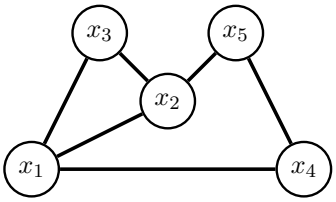
**Exercise 1.** ***Visualising and analysing Gibbs distributions via undirected graphs***

*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 $\text{ne}_3$.)

*(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 $\text{ne}_3$, 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***

*We here consider the graph in Figure 1.*

*(a) What is the set of Gibbs distributions that are induced by the graph?*

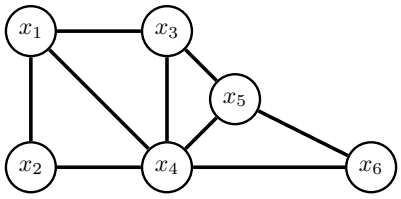



Figure 1: Graph for Exercise 2

**Solution.** The graph in Figure 1 has four maximal cliques:

$$(x_1, x_2, x_4) \quad (x_1, x_3, x_4) \quad (x_3, x_4, x_5) \quad (x_4, x_5, x_6)$$

The Gibbs distributions are thus

$$p(x_1, \ldots, x_6) \propto \phi_1(x_1, x_2, x_4)\phi_2(x_1, x_3, x_4)\phi_3(x_3, x_4, x_5)\phi_4(x_4, x_5, x_6)$$

*(b) Let $p$ be a pdf that factorises according to the graph. Can we expect that $p(x_3|x_2, x_4) = p(x_3|x_4)$?*

**Solution.** $p(x_3|x_2, x_4) = p(x_3|x_4)$ means that $x_3 \perp\!\!\!\perp x_2 \mid x_4$. We can use the graph to check whether this generally holds for pdfs that factorise according to the graph. There are multiple trails from $x_3$ to $x_2$, including the trail $(x_3, x_1, x_2)$, which is not blocked by $x_4$. From the graph, we thus cannot conclude that $x_3 \perp\!\!\!\perp x_2 \mid x_4$, and $p(x_3|x_2, x_4) = p(x_3|x_2)$ will generally not hold (the relation may hold for some carefully defined factors $\phi_i$).

*(c) Explain why $x_2 \perp\!\!\!\perp x_5 \mid x_1, x_3, x_4, x_6$ holds.*

**Solution.** The distribution that factorises according to the graph satisfies the pairwise Markov property. Since $x_2$ and $x_5$ are not neighbours, and $x_1, x_3, x_4, x_6$ are the remaining nodes in the graph, the independence relation follows from the pairwise Markov property.

*(d) Assume you would like to approximate $\mathbb{E}(x_1x_2x_5 \mid x_3, x_4)$, i.e. the expected value of the product of $x_1$, $x_2$, and $x_5$ given $x_3$ and $x_4$, with a sample average. Do you need to have joint observations for all five variables, i.e. of the tuples $(x_1, x_2, x_3, x_4, x_5)$?*

**Solution.** In the graph, all trails from $\{x_1, x_2\}$ to $x_5$ are blocked by $\{x_3, x_4\}$, so that $x_1, x_2 \perp\!\!\!\perp x_5 \mid x_3, x_4$. We thus have

$$\mathbb{E}(x_1x_2x_5 \mid x_3, x_4) = \mathbb{E}(x_1x_2 \mid x_3, x_4)\mathbb{E}(x_5 \mid x_3, x_4).$$

Hence, we only need joint observations of $(x_1, x_2, x_3, x_4)$ and $(x_3, x_4, x_5)$. Variables $(x_1, x_2)$ and $x_5$ do not need to be jointly measured.

### Exercise 3. *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*

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

*These models are typically 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 $\phi_{ij}$ for $i \leq j$?*

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

$$\mathbf{x}^\top \mathbf{A}\mathbf{x} = \sum_{ij} a_{ij} x_i x_j \tag{S.1}$$

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

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

$$-\frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{b}^\top \mathbf{x} = -\frac{1}{2}\sum_{i<j} 2a_{ij} x_i x_j - \frac{1}{2}\sum_i a_{ii} x_i^2 - \sum_i b_i x_i \tag{S.3}$$

so that

$$\phi_{ij}(x_i, x_j) = \begin{cases} \exp\left(-a_{ij} x_i x_j\right) & \text{if } i \neq j \\ \exp\left(-\frac{1}{2} a_{ii} x_i^2 - b_i x_i\right) & \text{if } i = j \end{cases} \tag{S.4}$$

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.4). Consider two variables $x_i$ and $x_j$ for fixed $(i, j)$. They only appear in the factorisation via the potential $\phi_{ij}$. If $a_{ij} = 0$, the factor $\phi_{ij}$ 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 4. *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*

$$p(\mathbf{v}, \mathbf{h}) \propto \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{a}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h}\right), \tag{1}$$

*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 2 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 2: Left: Graph for $p(\mathbf{v}, \mathbf{h})$. Right: Graph for $p(\mathbf{h}|\mathbf{v})$

*(b) Show that*

$$p(h_i = 1|\mathbf{v}) = \frac{1}{1 + \exp\left(-b_i - \sum_j W_{ji} v_j\right)} \tag{2}$$

*where $W_{ji}$ is the $(ji)$-th element of $\mathbf{W}$, so that $\sum_j W_{ji} v_j$ is the inner 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 $p(\mathbf{h}|\mathbf{v})$:

$$\begin{aligned}
p(\mathbf{h}|\mathbf{v}) &= \frac{p(\mathbf{h}, \mathbf{v})}{p(\mathbf{v})} && \text{(S.5)}\\
&\propto p(\mathbf{h}, \mathbf{v}) && \text{(S.6)}\\
&\propto \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{a}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h}\right) && \text{(S.7)}\\
&\propto \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{b}^\top \mathbf{h}\right) && \text{(S.8)}\\
&\propto \exp\left(\sum_i \sum_j v_j W_{ji} h_i + \sum_i b_i h_i\right) && \text{(S.9)}
\end{aligned}$$

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

$$p(h_i|\mathbf{v}) \propto \exp\left(\sum_j v_j W_{ji} h_i + b_i h_i\right) \tag{S.10}$$

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

$$\tilde{p}(h_i|\mathbf{v}) = \exp\left(\sum_j v_j W_{ji} h_i + b_i h_i\right). \tag{S.11}$$

We then have

$$p(h_i|\mathbf{v}) = \frac{\tilde{p}(h_i|\mathbf{v})}{\tilde{p}(h_i = 0|\mathbf{v}) + \tilde{p}(h_i = 1|\mathbf{v})} \tag{S.12}$$

$$= \frac{\tilde{p}(h_i|\mathbf{v})}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} \tag{S.13}$$

$$= \frac{\exp\left(\sum_j v_j W_{ji} h_i + b_i h_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)}, \tag{S.14}$$

so that

$$p(h_i = 1|\mathbf{v}) = \frac{\exp\left(\sum_j v_j W_{ji} + b_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} \tag{S.15}$$

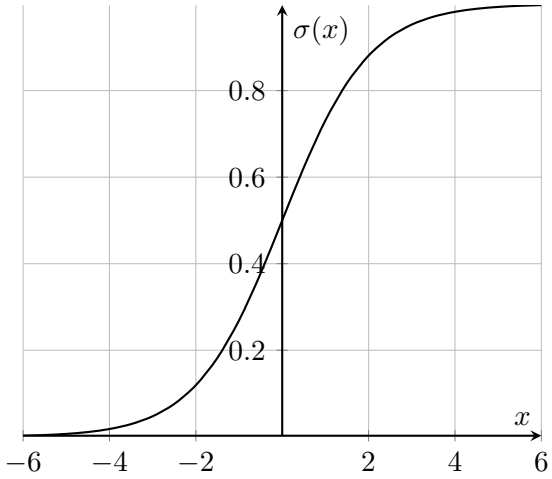
$$= \frac{1}{1 + \exp\left(-\sum_j v_j W_{ji} - b_i\right)}. \tag{S.16}$$

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

$$p(h_i = 0|\mathbf{v}) = \frac{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} - \frac{\exp\left(\sum_j v_j W_{ji} + b_i\right)}{1 + \exp\left(\sum_j v_j W_{ji} + b_i\right)} \tag{S.17}$$

$$= \frac{1}{1 + \exp\left(\sum_j W_{ji} v_j + b_i\right)} \tag{S.18}$$

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

$$p(\mathbf{v}, \mathbf{h}) \propto \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{a}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h}\right) \tag{S.19}$$

$$\propto \exp\left(\mathbf{h}^\top \mathbf{W}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h} + \mathbf{a}^\top \mathbf{v}\right). \tag{S.20}$$

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 (2), 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.

$$p(\mathbf{v}) = \frac{1}{Z} \sum_{\mathbf{h} \in \{0,1\}^m} \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{a}^\top \mathbf{v} + \mathbf{b}^\top \mathbf{h}\right) \tag{S.21}$$

$$= \frac{1}{Z} \sum_{\mathbf{h} \in \{0,1\}^m} \exp\left(\sum_{ij} v_i h_j W_{ij} + \sum_i a_i v_i + \sum_j b_j h_j\right) \tag{S.22}$$

$$= \frac{1}{Z} \sum_{\mathbf{h} \in \{0,1\}^m} \exp\left(\sum_{j=1}^m h_j \left[\sum_i v_i W_{ij} + b_j\right] + \sum_i a_i v_i\right) \tag{S.23}$$

$$= \frac{1}{Z} \sum_{\mathbf{h} \in \{0,1\}^m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) \exp\left(\sum_i a_i v_i\right) \tag{S.24}$$

$$= \frac{1}{Z} \exp\left(\sum_i a_i v_i\right) \sum_{\mathbf{h} \in \{0,1\}^m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) \tag{S.25}$$

$$= \frac{1}{Z} \exp\left(\sum_i a_i v_i\right) \sum_{h_1, \ldots, h_m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) \tag{S.26}$$

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

$$\sum_{h_1, \ldots, h_m} \prod_{j=1}^m \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) = \left[\sum_{h_1, \ldots, h_{m-1}} \prod_{j=1}^{m-1} \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right)\right] \cdot \sum_{h_m} \exp\left(h_m \left[\sum_i v_i W_{im} + b_m\right]\right) \tag{S.27}$$

$$= \ldots$$

$$= \prod_{j=1}^m \left[\sum_{h_j} \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right)\right] \tag{S.28}$$

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

$$\sum_{h_j} \exp\left(h_j \left[\sum_i v_i W_{ij} + b_j\right]\right) = 1 + \exp\left(\sum_i v_i W_{ij} + b_j\right) \tag{S.29}$$

and thus

$$p(\mathbf{v}) = \frac{1}{Z} \exp\left(\sum_i a_i v_i\right) \prod_{j=1}^{m} \left[1 + \exp\left(\sum_i v_i W_{ij} + b_j\right)\right]. \tag{S.30}$$

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

$$Z = \sum_{\mathbf{v} \in \{0,1\}^n} \exp\left(\sum_i a_i v_i\right) \prod_{j=1}^{m} \left[1 + \exp\left(\sum_i v_i W_{ij} + b_j\right)\right] \tag{S.31}$$

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.)

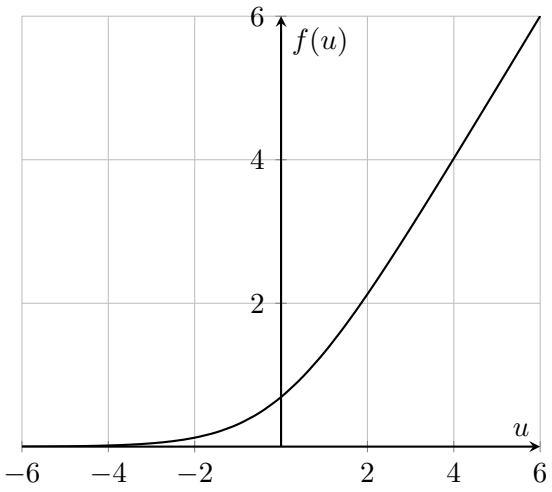
It is instructive to write $p(\mathbf{v})$ in the log-domain,

$$\log p(\mathbf{v}) = \log Z + \sum_{i=1}^{n} a_i v_i + \sum_{j=1}^{m} \log\left[1 + \exp\left(\sum_i v_i W_{ij} + b_j\right)\right], \tag{S.32}$$

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

$$f(u) = \log\left[1 + \exp(u)\right], \tag{S.33}$$

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

$$\log p(\mathbf{v}) = \log Z + \sum_{i=1}^{n} a_i v_i + \sum_{j=1}^{m} f\left(\sum_i v_i W_{ij} + b_j\right). \tag{S.34}$$

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 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.