Restricted Boltzmann Machines

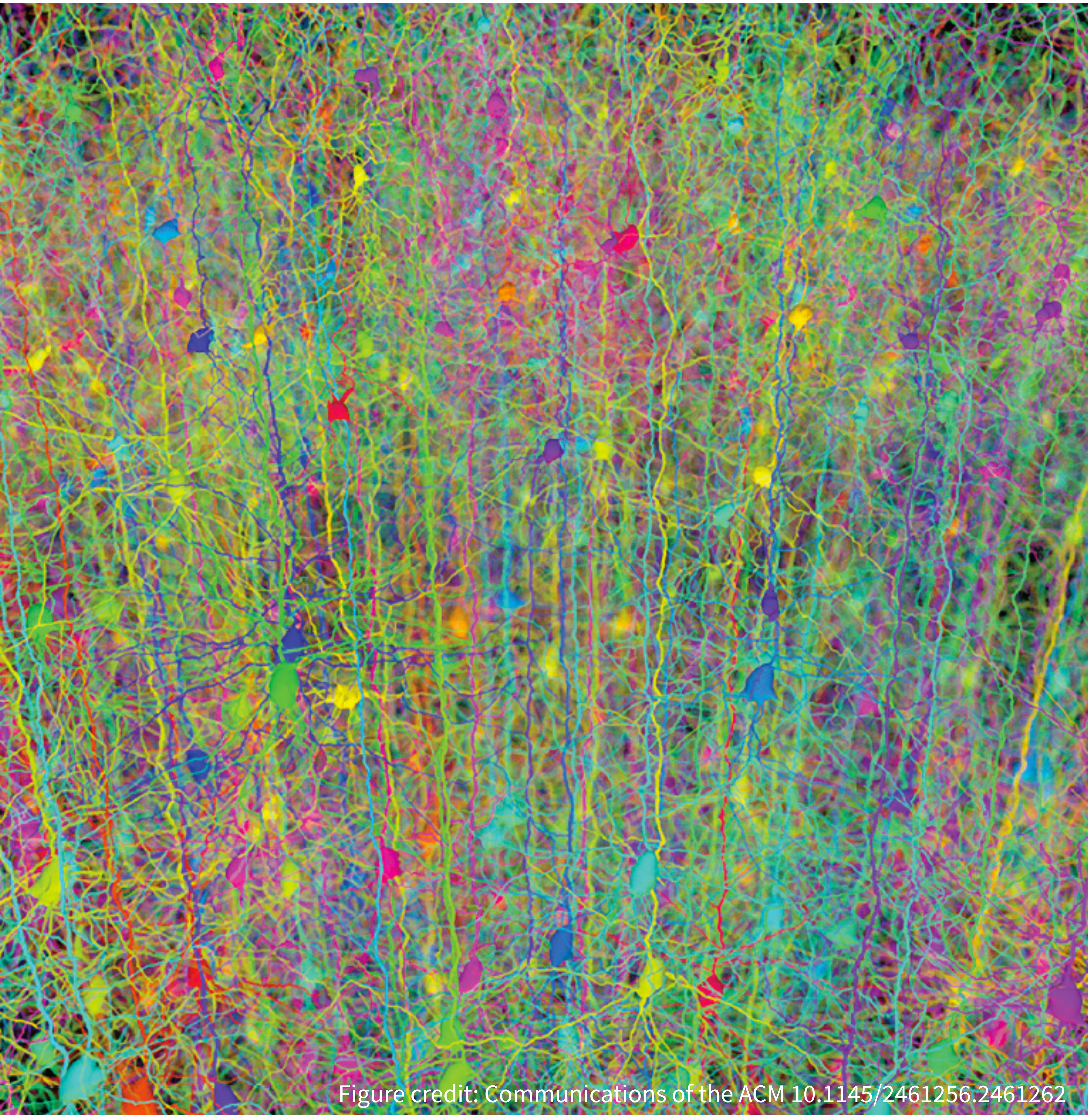

Figure credit: Communications of the ACM 10.1145/2461256.2461262

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Scaling ML to the Challenges of AI

Classification algorithms take an input from a high-dimensional distribution and summarize it with a category label

- During this process, the classifier discards most of the information in the input and produces a single output

It is possible to ask our ML models to do many other tasks

- Some of which require them to produce multiple outputs
- Most require a complete understanding of the entire structure of the input, with no option to ignore sections of it

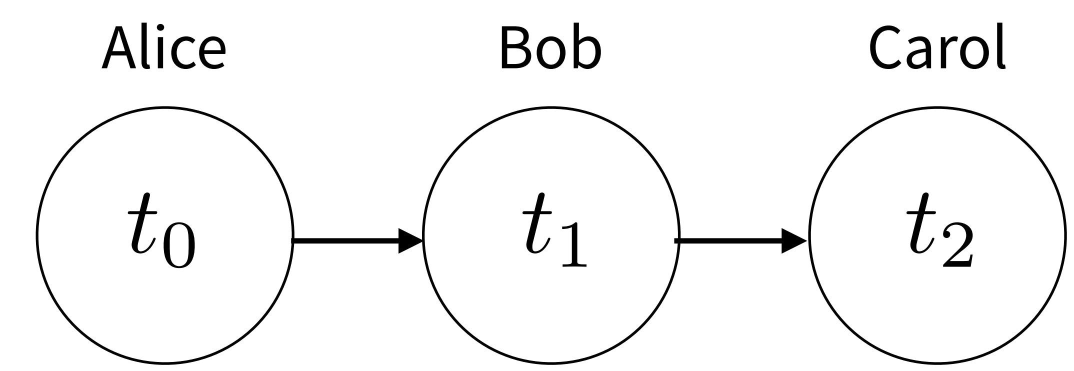
Structured Probabilistic Models for Machine Learning

Modeling a rich distribution over random variables is a challenging task, both computationally and statistically

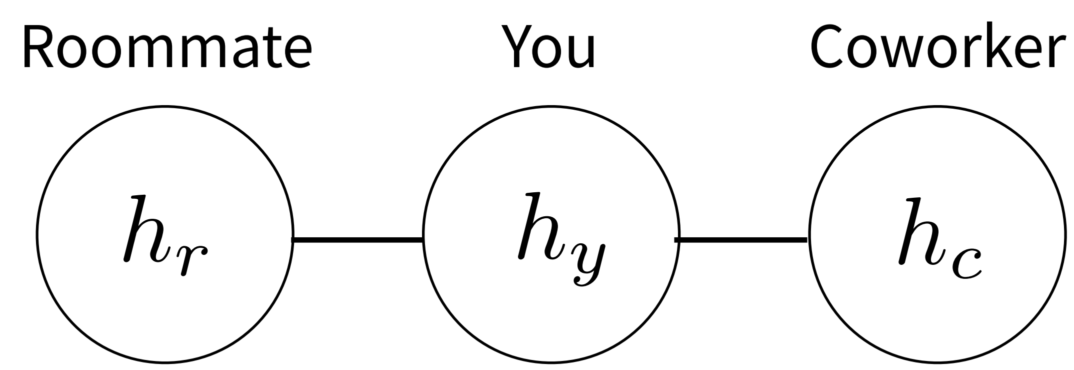
Structured probabilistic models (graphical models) provide a formal framework for modeling only direct interactions between random variables

- significantly fewer parameters
- estimated reliably from less data

directed graphical model



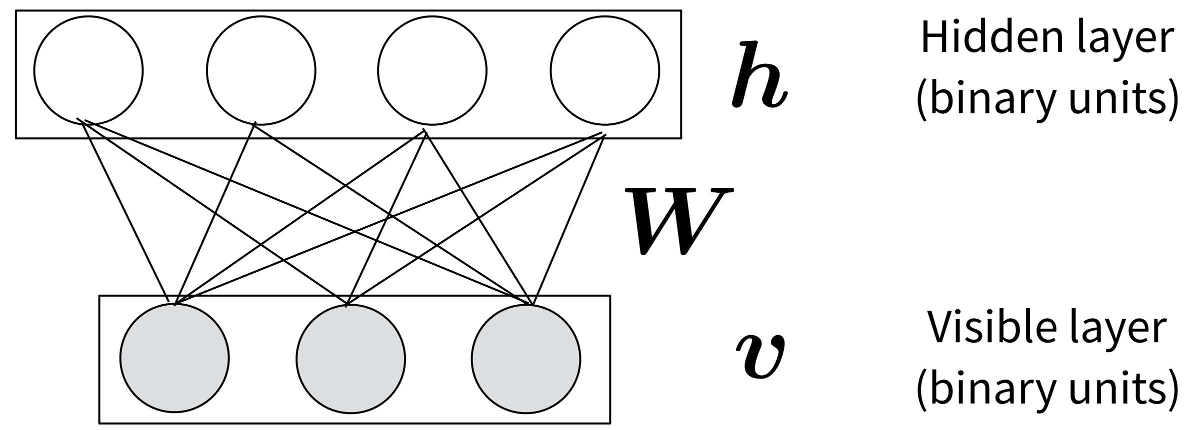
undirected graphical model



Reproduced from Goodfellow et al.

Restricted Boltzmann Machine

- Undirected graphical model with bipartite structure and restricted connectivity to make inference and learning easier



- Energy function:

$$E(\boldsymbol{v}, \boldsymbol{h}) = -\boldsymbol{b}^\top \boldsymbol{v} - \boldsymbol{c}^\top \boldsymbol{h} - \boldsymbol{v}^\top \boldsymbol{W} \boldsymbol{h}$$

- Distribution:

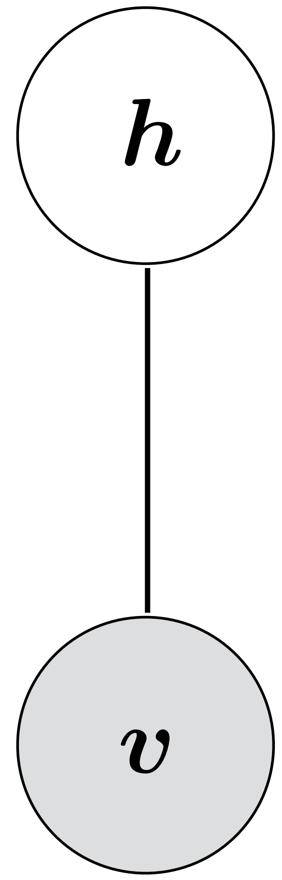
$$P(\mathbf{v} = \boldsymbol{v}, \mathbf{h} = \boldsymbol{h}) = \frac{1}{Z} \exp(-E(\boldsymbol{v}, \boldsymbol{h}))$$

$$Z = \sum_{\boldsymbol{v}} \sum_{\boldsymbol{h}} \exp\{-E(\boldsymbol{v}, \boldsymbol{h})\}$$

partition function
(intractable)

Markov Network View

Markov network with vector nodes:



$$
\begin{aligned}
P(\mathbf{v}=\boldsymbol{v},\mathbf{h}=\boldsymbol{h}) &= \exp(-E(\boldsymbol{v},\boldsymbol{h}))/Z \\
&= \exp(\boldsymbol{b}^\top\boldsymbol{v}+\boldsymbol{c}^\top\boldsymbol{h}+\boldsymbol{v}^\top\boldsymbol{W}\boldsymbol{h})/Z \\
&= \underbrace{\exp(\boldsymbol{b}^\top\boldsymbol{v})\exp(\boldsymbol{c}^\top\boldsymbol{h})\exp(\boldsymbol{v}^\top\boldsymbol{W}\boldsymbol{h})}_{\text{factors}}/Z
\end{aligned}
$$

The notation based on an energy function is simply an alternative to the representation as the product of factors

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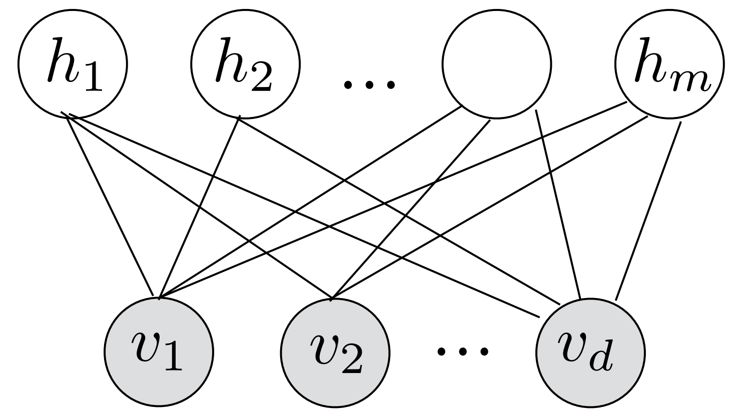
Markov Network View (2)

Markov network with scalar nodes:

$$P(\mathbf{v}=\boldsymbol{v},\mathbf{h}=\boldsymbol{h}) = \frac{1}{Z}\overbrace{\prod_j\prod_k \exp(W_{j,k}h_j v_k)}^{\text{pair-wise factors}} \left.\begin{array}{l}\displaystyle\prod_k \exp(b_k v_k)\\ \displaystyle\prod_j \exp(c_j h_j)\end{array}\right\}\text{unary factors}$$



This scalar visualization is more informative of the structure within the vectors

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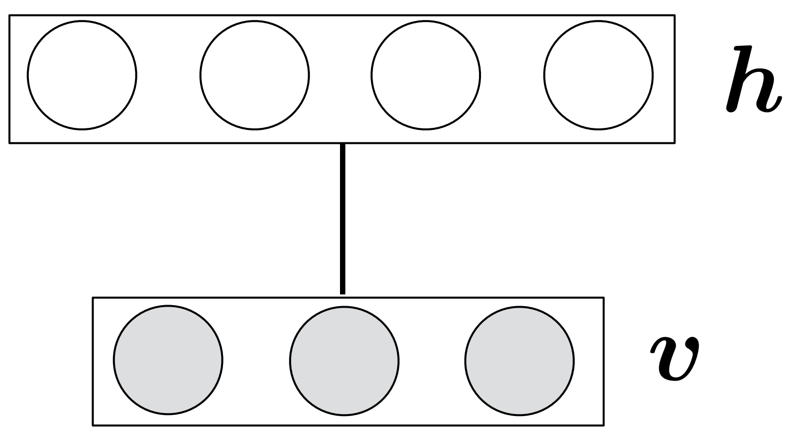
Inference in RBM

Though $P(\boldsymbol{v})$ is intractable, the bipartite graph structure of the RBM has the special property of its conditional distributions $P(\boldsymbol{h}|\boldsymbol{v})$ and $P(\boldsymbol{v}|\boldsymbol{h})$ being factorial and relatively simple to compute and sample:

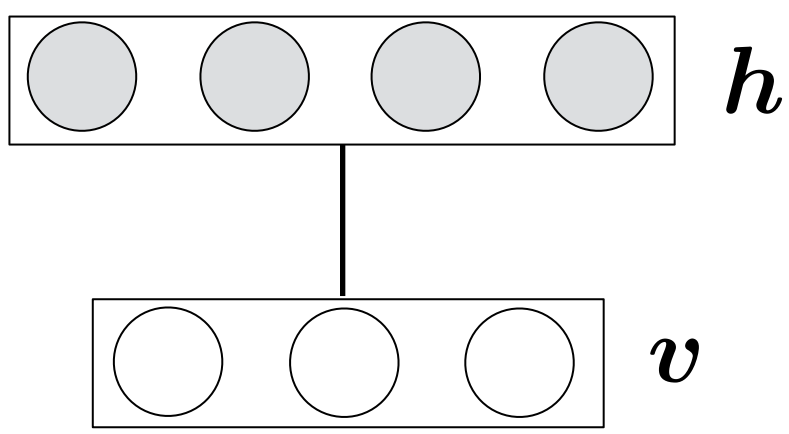


$$P(\boldsymbol{h}|\boldsymbol{v}) = \prod_j P(h_j = 1|\boldsymbol{v})$$

$$P(h_j = 1|\boldsymbol{v}) = \frac{1}{1 + \exp(-(c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:,j}))}$$

$$= \sigma(c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:,j})$$

jth column of $\boldsymbol{W}$



$$P(\boldsymbol{v}|\boldsymbol{h}) = \prod_k P(v_k = 1|\boldsymbol{h})$$

$$P(v_k = 1|\boldsymbol{h}) = \frac{1}{1 + \exp(-(b_k + \boldsymbol{W}_{k,:}\boldsymbol{h}))}$$

$$= \sigma(b_k + \boldsymbol{W}_{k,:}\boldsymbol{h})$$

kth row of $\boldsymbol{W}$

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Free Energy

- Many algorithms that operate on probabilistic models need to compute not $p_{\text{model}}(\boldsymbol{x})$ but only $\log \tilde{p}_{\text{model}}(\boldsymbol{x})$

- For energy-based models with latent variables $\boldsymbol{h}$, these algorithms are sometimes phrased in terms of the negative of this quantity, called the free energy:

$$\mathcal{F}(\boldsymbol{x}) = -\log \sum_{\boldsymbol{h}} \exp(-E(\boldsymbol{x}, \boldsymbol{h}))$$

- For the RBM:

$$\begin{aligned} P(\boldsymbol{v}) &= \sum_{\boldsymbol{h} \in \{0,1\}^m} P(\boldsymbol{v}, \boldsymbol{h}) = \sum_{\boldsymbol{h} \in \{0,1\}^m} \exp(-E(\boldsymbol{v}, \boldsymbol{h}))/Z \\ &= \exp\left(\boldsymbol{b}^\top \boldsymbol{v} + \sum_{j=1}^{m} \log\left(1 + \exp\left(c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:,j}\right)\right)\right)/Z \\ &= \exp\left(-\mathcal{F}(\boldsymbol{v})\right)/Z \end{aligned}$$