TECHNISCHE UNIVERSITÄT
CHEMNITZ

Neurocomputing

Restricted Boltzmann Machines

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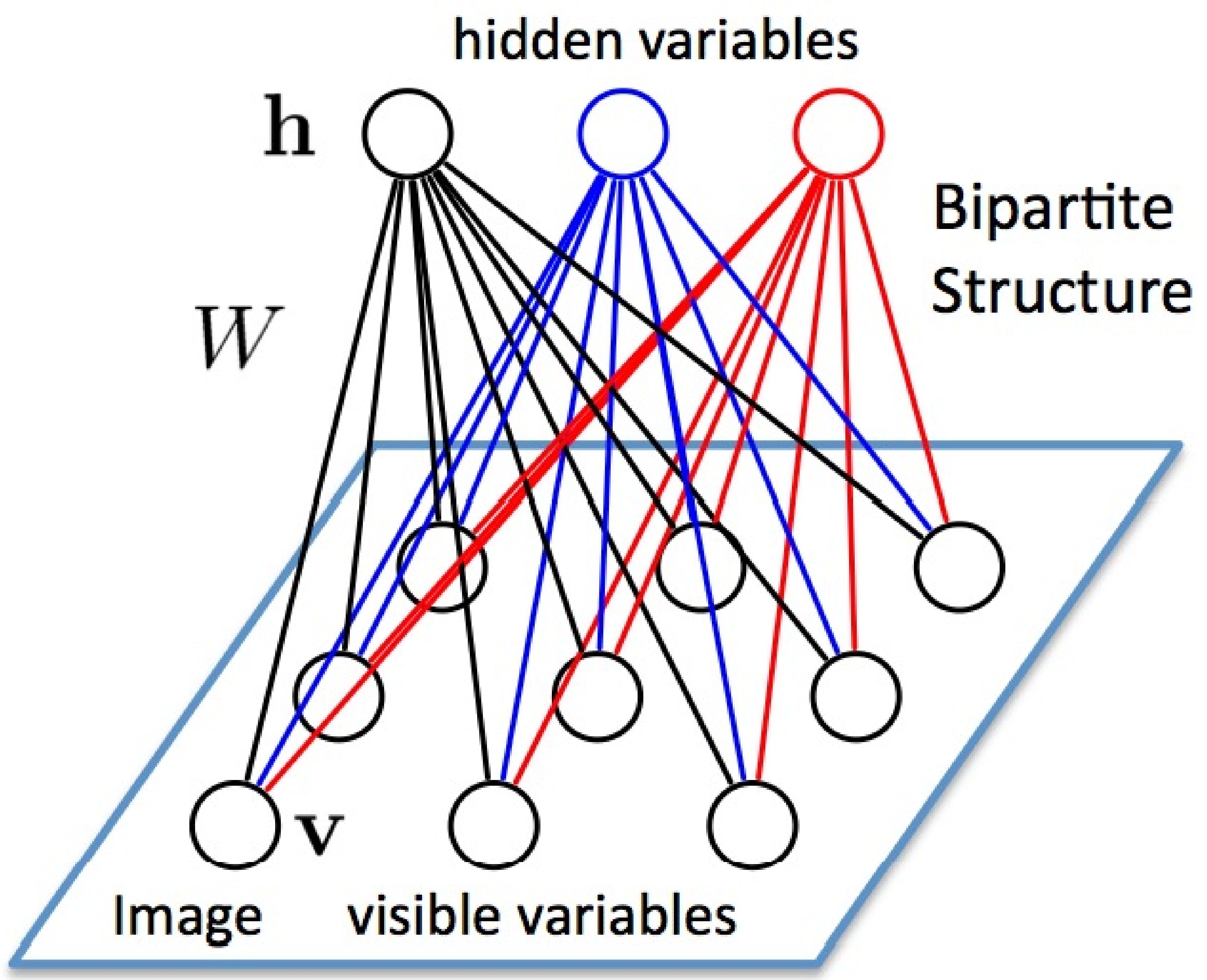
https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

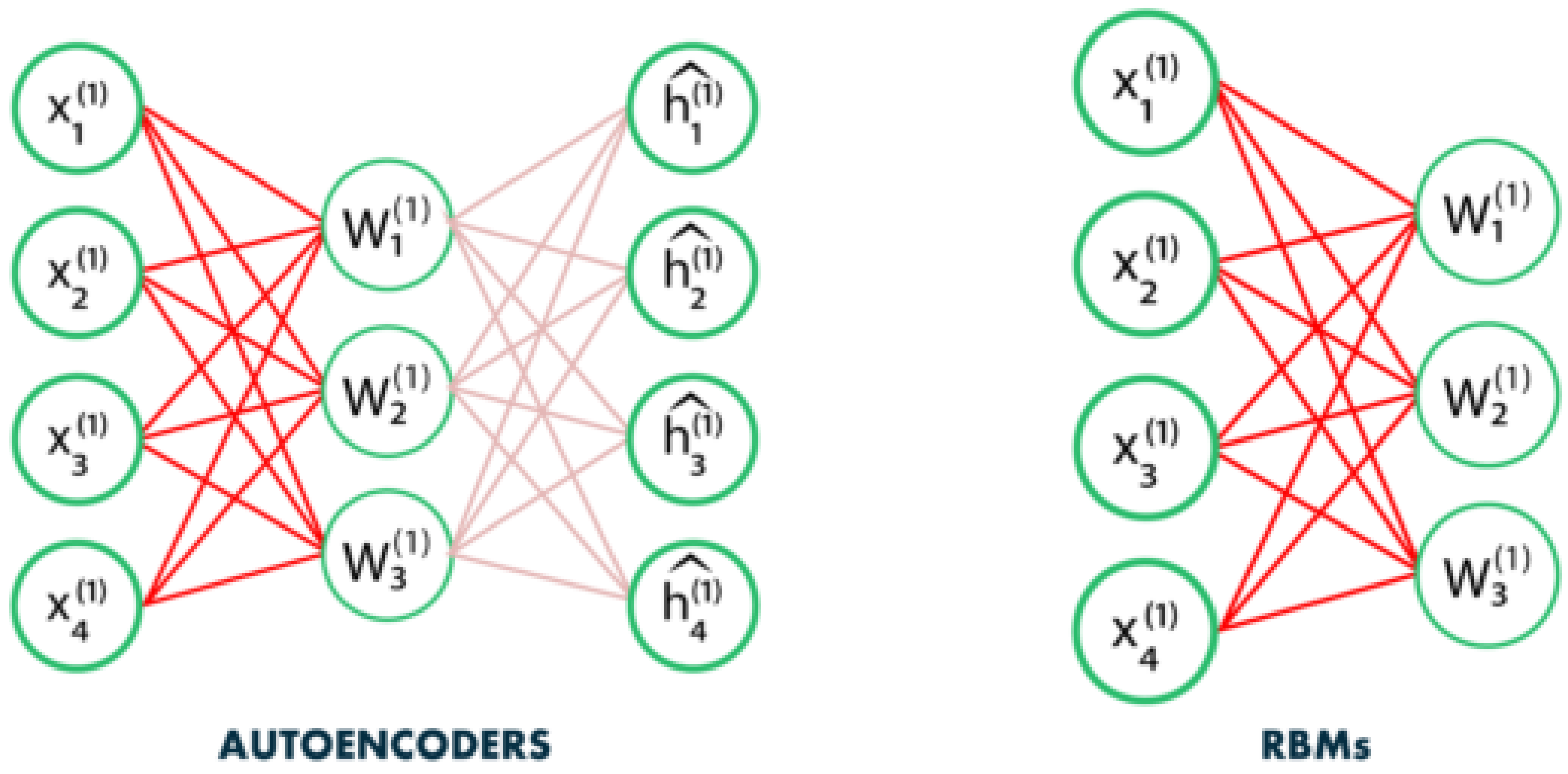
Restricted Boltzmann Machines

- Auto-encoders are not the only feature extractors that can be stacked.

- **Restricted Boltzmann Machines** (RBM) are generative stochastic artificial neural networks that can learn a probability distribution of their inputs.
- Their neurons form a bipartite graph with two groups of reciprocally connected units:
    - the **visible units** $\mathbf{v}$ (the inputs)
    - the **hidden units** $\mathbf{h}$ (the features or latent space).
- Connections are bidirectional between $\mathbf{v}$ and $\mathbf{h}$, but the neurons inside the two groups are independent from each other (*restricted*).
- The goal of learning is to find the weights allowing the network to **explain** best the input data.



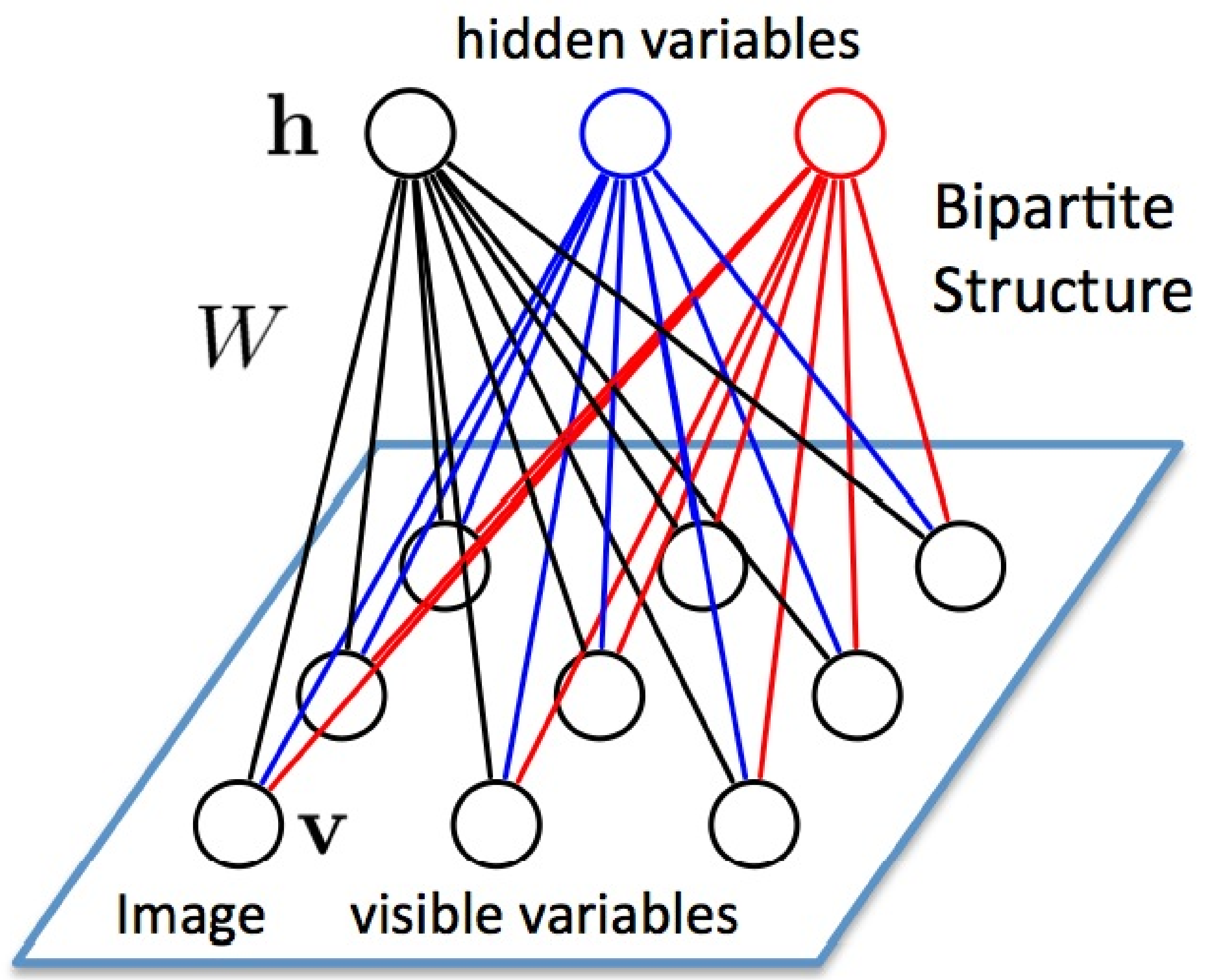
Restricted Boltzmann Machines



Source : https://www.edureka.co/blog/restricted-boltzmann-machine-tutorial/

- RBMs are a form of autoencoder where the input → feature weight matrix is the same as the feature → output matrix.
- There are two steps:
    - The **forward pass** $P(\mathbf{h}|\mathbf{x})$ propagates the visible units activation to the hidden units.
    - The **backward pass** $P(\mathbf{x}|\mathbf{h})$ reconstructs the visible units from the the hidden units.
- If the weight matrix is correctly chosen, the reconstructed input should “match” the original input: the data is explained.

Restricted Boltzmann Machines



- The visible and units are generally **binary units** (0 or 1), with a probability defined by the weights and biases and the logistic function:

$$P(h_j = 1|\mathbf{v}) = \sigma(\sum_i W_{ij} \, v_i + c_j)$$

$$P(v_i = 1|\mathbf{h}) = \sigma(\sum_i W_{ji} \, h_j + b_i)$$

- The weight matrix W and the biases $\mathbf{b}, \mathbf{c}$ are the parameters θ of a **probability distribution** over the activation of the visible and hidden units.

- The goal is to find the parameters which explain best the data (visible units), i.e. the ones maximizing the **log-likelihood** of the model for the data $(\mathbf{v}_1, \dots, \mathbf{v}_N)$.
- We use **maximum likelihood estimation** (MLE) to maximize the log-likelihood of the model:

$$\max_\theta \; \mathcal{L}(\theta) = \mathbb{E}_{\mathbf{v} \sim \mathcal{D}} [\log \, P_\theta(\mathbf{v})]$$

Restricted Boltzmann Machines

- In practice, MLE is not tractable in a RBM, as we cannot estimate the joint probability $P(\mathbf{v}, \mathbf{h})$ of $\mathbf{v}$ and $\mathbf{h}$ (too many combinations are possible).

$$P(\mathbf{v}) = \sum_{\mathbf{h}} P(\mathbf{v}, \mathbf{h})$$

- The main trick in **energy-based models** is to rewrite the probabilities using an energy function $E(\mathbf{v}, \mathbf{h})$:

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

where:

$$Z = \sum_{\mathbf{v},\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})} = \sum_{\mathbf{v}} P(\mathbf{v}) \sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}$$

is the **partition function** (a normalizing term).

- The probabilities come from a **Gibbs distribution** (or Boltzmann distribution) parameterized by the energy of the system.
- This is equivalent to a simple **softmax** over the energy…

Restricted Boltzmann Machines

- Having reformulated the probabilities in terms of energy:

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

we can introduce the **free energy** of the model for a sample $\mathbf{v}$ (how surprising is the input $\mathbf{v}$ for the model):

$$\mathcal{F}(\mathbf{v}) = - \log \sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}$$

- The log-likelihood of the model for a sample $\mathbf{v}$ of the training data $(\mathbf{v}_1, \dots, \mathbf{v}_N)$ becomes:

$$\log P(\mathbf{v}) = \log \frac{1}{Z} \sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})} = -\mathcal{F}(\mathbf{v}) + \log Z = -\mathcal{F}(\mathbf{v}) + \sum_{\mathbf{v}} P(\mathbf{v}) \, \mathcal{F}(\mathbf{v})$$

- Note that the second term sums over all possible inputs $\mathbf{v}$.
- Maximizing the log-likelihood of the model on the training data can be done using gradient ascent by following this gradient:

$$\nabla_\theta \mathcal{L}(\theta) = \mathbb{E}_{\mathbf{v}}[\nabla_\theta \log P(\mathbf{v}_i)] = \mathbb{E}_{\mathbf{v}}[-\nabla_\theta \mathcal{F}(\mathbf{v}) + \sum_{\mathbf{v}} P(\mathbf{v}) \nabla_\theta \mathcal{F}(\mathbf{v})]$$

Restricted Boltzmann Machines

- The free energy for a RBM with binary neurons is fortunately known analytically:

$$\mathcal{F}(\mathbf{v}) = - \sum_i b_i \, v_i - \sum_j \log(1 + \exp^{\sum_i W_{ij} \, v_i + c_j})$$

so finding the gradient w.r.t $\theta = (W, \mathbf{b}, \mathbf{c})$ of the first term on the r.h.s (the free energy of the sample) is easy:

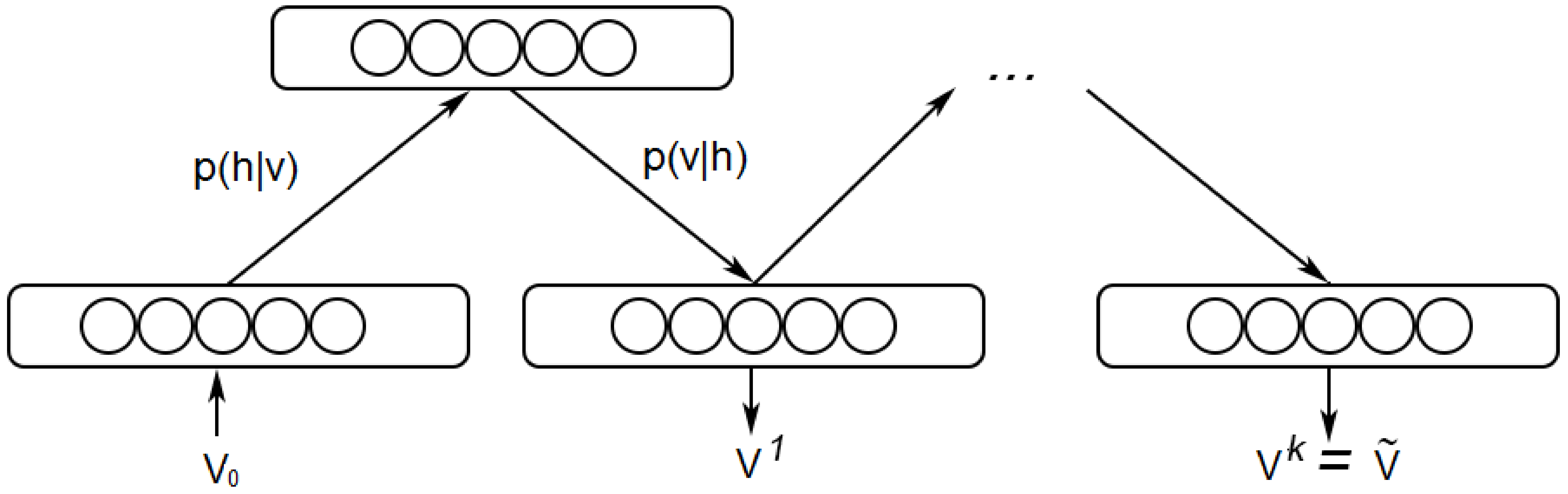
$$\nabla_\theta \log \, P(\mathbf{v}) = - \nabla_\theta \mathcal{F}(\mathbf{v}) + \sum_\mathbf{v} P(\mathbf{v}) \nabla_\theta \mathcal{F}(\mathbf{v})$$

- In particular, the gradient w.r.t the matrix W is the outer product between $\mathbf{v}$ and $P(\mathbf{h}|\mathbf{v})$:

$$\nabla_W \mathcal{F}(\mathbf{v}) = - \mathbf{v} \times P(\mathbf{h}|\mathbf{v})$$

- The problem is the second term: we would need to integrate over all possible values of the inputs $\mathbf{v}$, what is not tractable.
- We will therefore make an approximation using **Gibbs sampling** (a variant of **Monte-Carlo Markov Chain** sampling - MCMC) to estimate that second term.

Gibbs sampling



Source : https://towardsdatascience.com/deep-learning-meets-physics-restricted-boltzmann-machines-part-i-6df5c4918c15

- Gibbs sampling consists of repeatedly applying the encoder $P(\mathbf{h}|\mathbf{v})$ and the decoder $P(\mathbf{v}|\mathbf{h})$ on the input.
  - We start by setting $\mathbf{v}_0 = \mathbf{v}$ using a training sample.
  - We obtain $\mathbf{h}_0$ by computing $P(\mathbf{h}|\mathbf{v}_0)$ and sampling it.
  - We obtain $\mathbf{v}_1$ by computing $P(\mathbf{v}|\mathbf{h}_0)$ and sampling it.
  - ...
  - We obtain $\mathbf{v}_k$ by computing $P(\mathbf{v}|\mathbf{h}_{k-1})$ and sampling it.
- After enough iterations k, we should have a good estimate of $P(\mathbf{v}, \mathbf{h})$.
- The k iterations have generated enough **reconstructions** of $\mathbf{v}$ to cover the distribution of $\mathbf{v}$.

Contrastive divergence

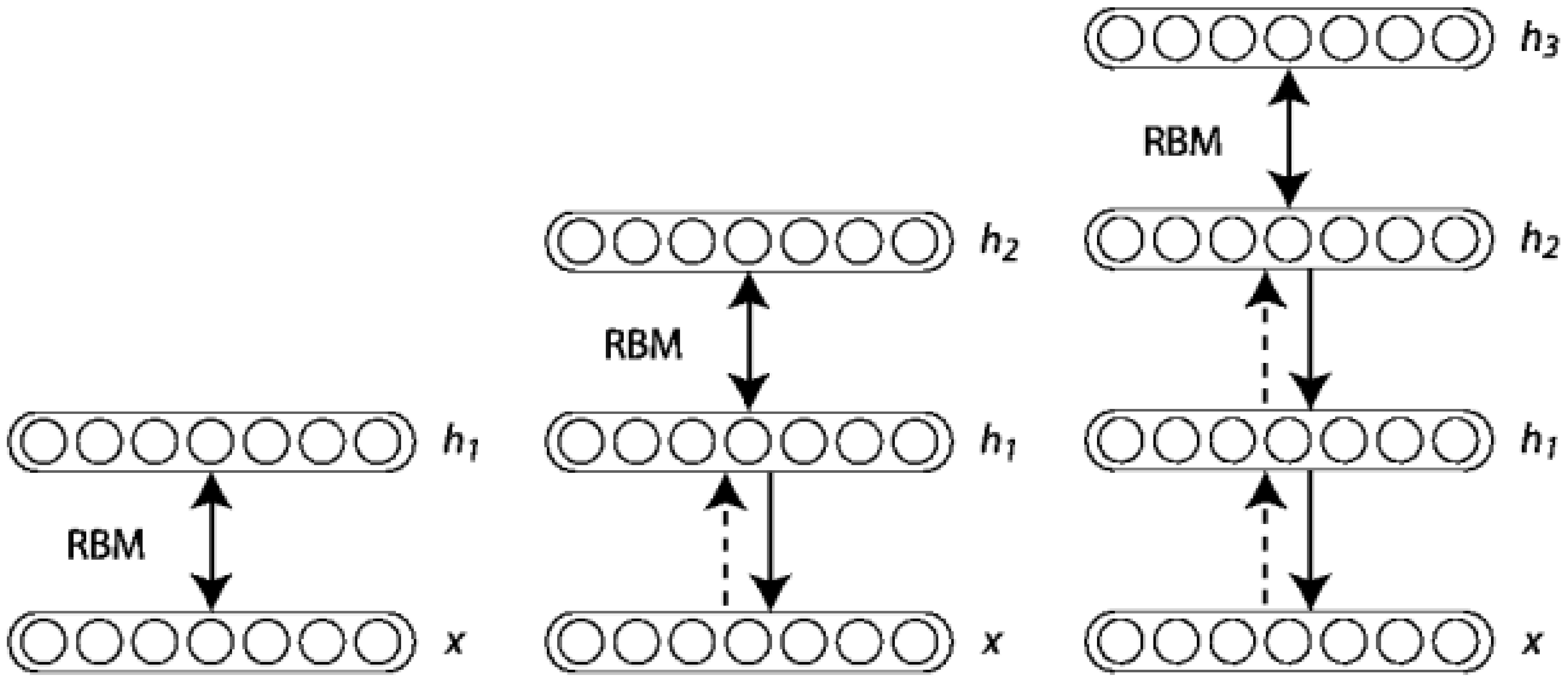
- We set $\mathbf{v}_0 = \mathbf{v}$ on a training sample and let Gibbs sampling iterate for k iterations until we obtain $\mathbf{v}_k = \mathbf{v}^*$.
- **Contrastive divergence** (CD-k) shows that the gradient of the log-likelihood can be approximated by:

$$\begin{aligned}\nabla_W \log\, P(\mathbf{v}) &= -\nabla_W \mathcal{F}(\mathbf{v}) + \sum_{\mathbf{v}} P(\mathbf{v}) \nabla_W \mathcal{F}(\mathbf{v}) \\ &\approx \mathbf{v} \times P(\mathbf{h}|\mathbf{v}) - \mathbf{v}^* \times P(\mathbf{h}|\mathbf{v}^*)\end{aligned}$$

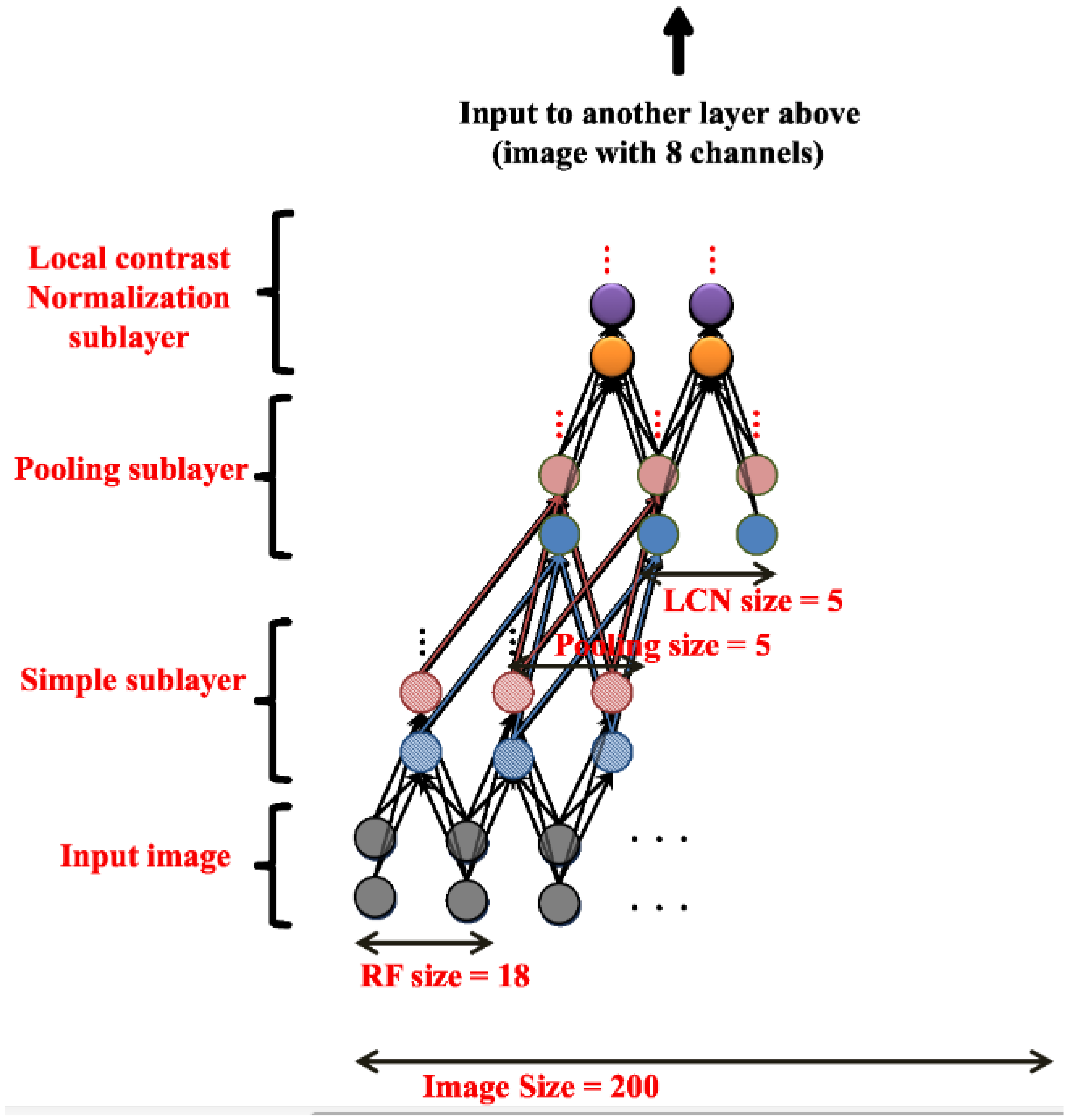
- The gradient of the log-likelihood is the difference between the initial explanation of $\mathbf{v}$ by the model, and its explanation after k iterations (relaxation).
- If the model is good, the reconstruction $\mathbf{v}^*$ is the same as the input $\mathbf{v}$, so the gradient is zero.
- An input $\mathbf{v}$ is likely under the RBM model if it is able to reconstruct it, i.e. when it is not surprising (the free energy is low).
- In practice, $k = 1$ gives surprisingly good results, but RBMs are very painful to train (hyperparameters)…

Deep Belief Networks = stacked RBMs

- A **Deep Belief Network** (DBM) is a simple stack of RBMS, trained using greedy layer-wise learning.
- The “bottom” parts of the DBM become unidirectional when learning the top part.

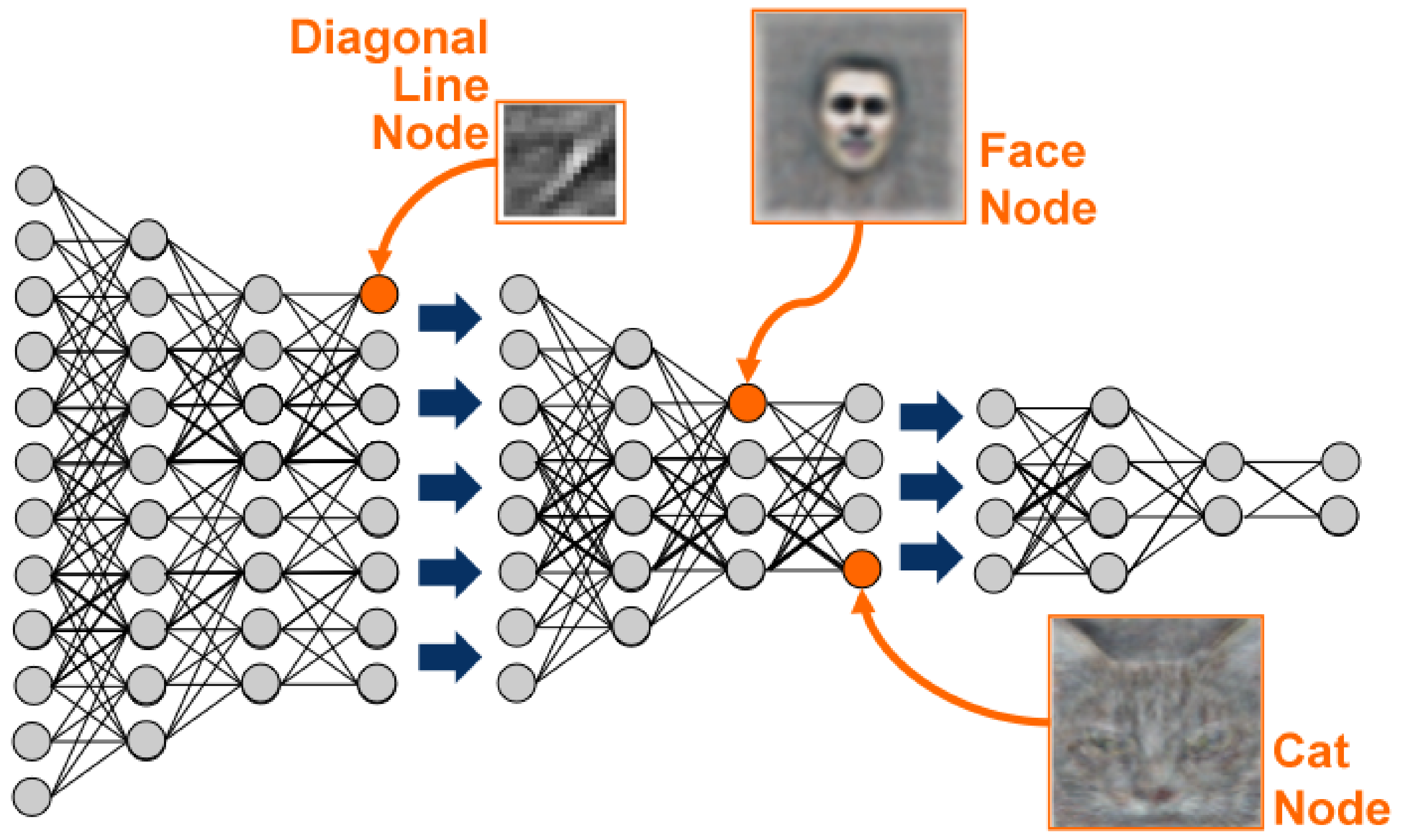


Application: Finding cats on the internet



- Andrew Ng and colleagues (Google, Stanford) used a similar technique to train a deep belief network on color images (200x200) taken from 10 million random unlabeled Youtube videos.
- Each layer was trained greedily. They used a particular form of autoencoder called **restricted Boltzmann machines** (RBM) and a couple of other tricks (receptive fields, contrast normalization).
- Training was distributed over 1000 machines (16.000 cores) and lasted for three days.
- There was absolutely no task: the network just had to watch youtube videos.
- After learning, they visualized what the neurons had learned.

Application: Finding cats on the internet



- After training, some neurons had learned to respond uniquely to faces, or to cats, without ever having been instructed to.
- The network can then be fine-tuned for classification tasks, improving the pre-AlexNet state-of-the-art on ImageNet by 70%.