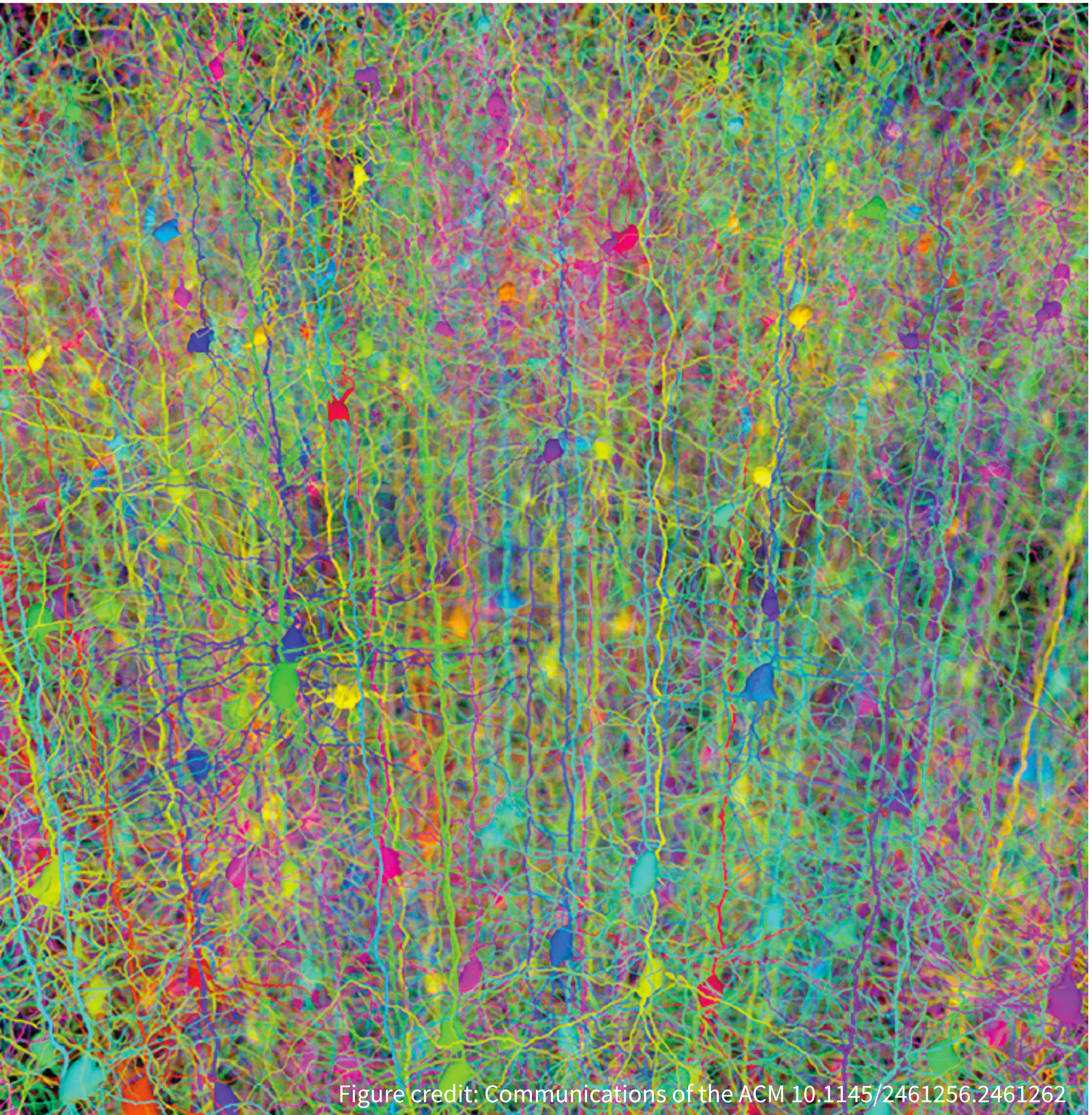
Training Restricted Boltzmann Machines



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Training RBMs

- To train an RBM, we would like to minimize the average negative log likelihood:

$$\frac{1}{n}\sum_{i=1}^{n} -\log P(\boldsymbol{v}^{(i)})$$

- We'd then like to proceed by stochastic gradient descent:

$$\frac{\partial -\log P(\boldsymbol{v}^{(i)})}{\partial \boldsymbol{\theta}} = \underbrace{\mathbb{E}_{\boldsymbol{h}}\left[\frac{\partial E(\boldsymbol{v}^{(i)},\boldsymbol{h})}{\partial \boldsymbol{\theta}}\,\middle|\,\boldsymbol{v}^{(i)}\right]}_{\text{positive phase}} - \underbrace{\mathbb{E}_{\boldsymbol{v},\boldsymbol{h}}\left[\frac{\partial E(\boldsymbol{v},\boldsymbol{h})}{\partial \boldsymbol{\theta}}\right]}_{\text{negative phase}}$$

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hard to compute!

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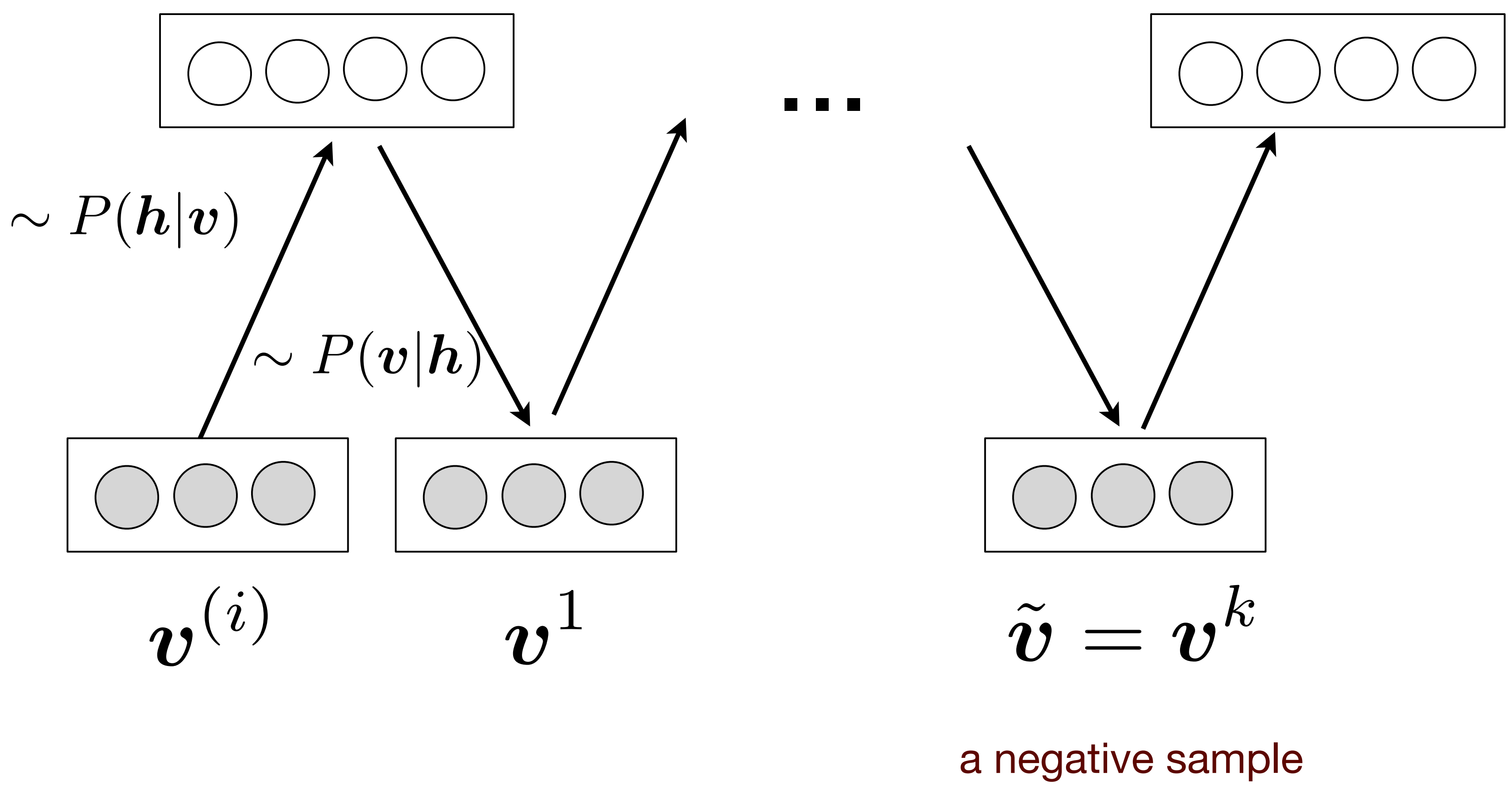
Contrastive Divergence (CD)

Idea:

- replace the expectation by a point estimate at $\tilde{\boldsymbol{v}}$
- obtain the point $\tilde{\boldsymbol{v}}$ by Gibbs sampling
- start sampling the chain at $\tilde{\boldsymbol{v}}^{(i)}$



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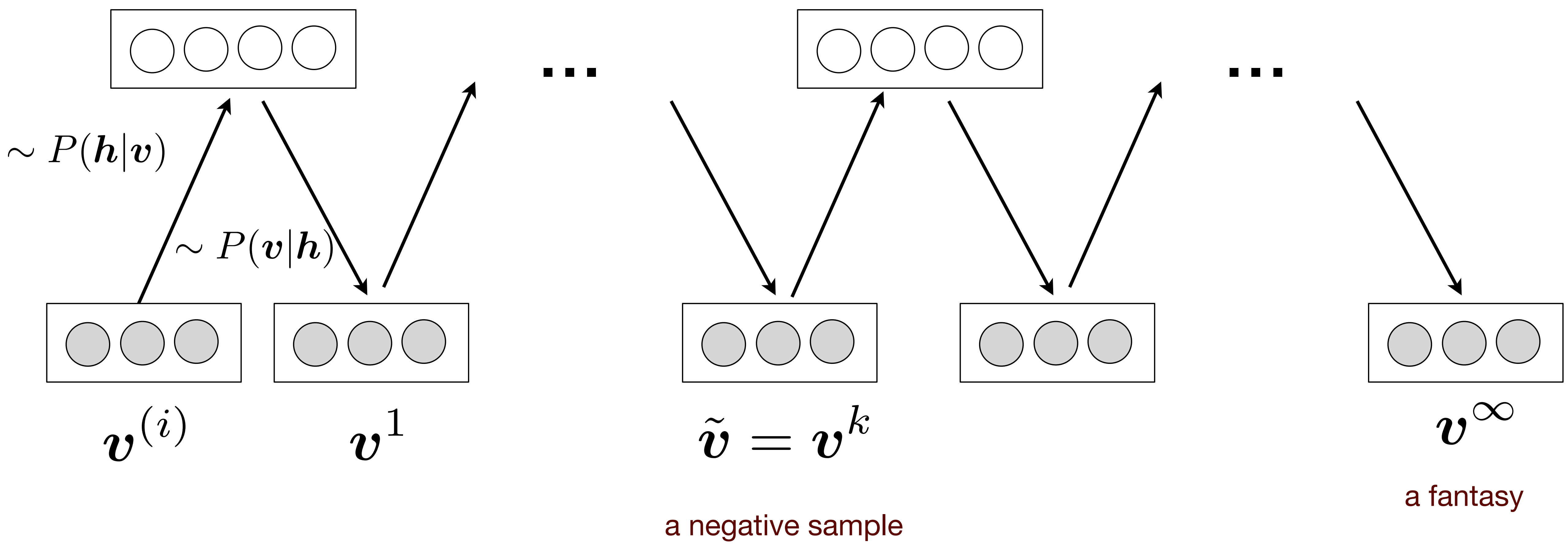

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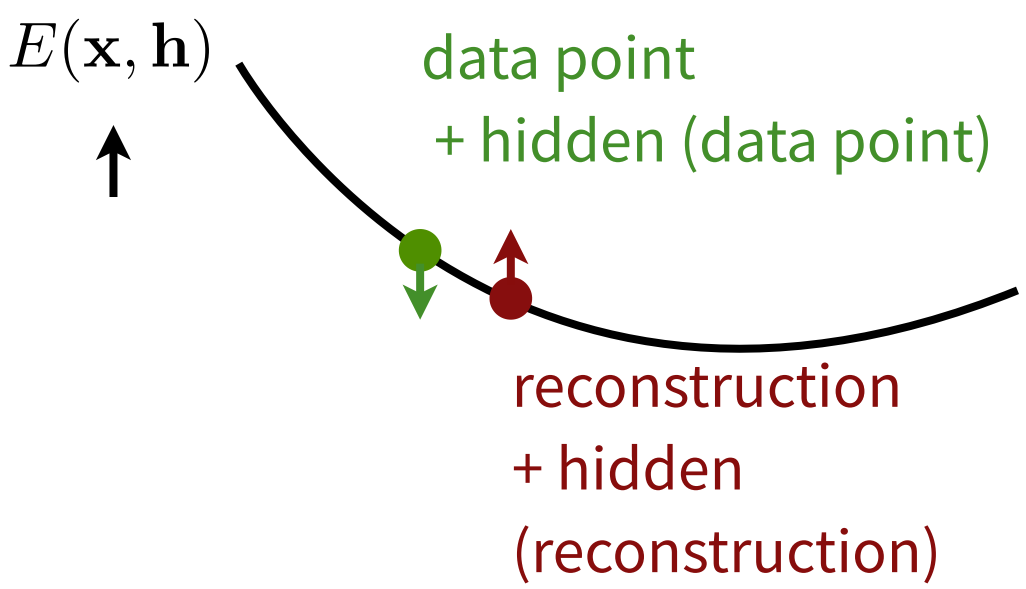
Contrastive Divergence (A picture)



$$\mathbb{E}_{\boldsymbol{h}}\left[\frac{\partial E(\boldsymbol{v}^{(i)}, \boldsymbol{h})}{\partial \boldsymbol{\theta}} \,\middle|\, \boldsymbol{v}^{(i)}\right] \approx \frac{\partial E(\boldsymbol{v}^{(i)}, \tilde{\boldsymbol{h}}^{(i)})}{\partial \boldsymbol{\theta}}$$

Change the weights to pull the energy down at the data point

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Change the weights to pull the energy up at the reconstruction

Credit: Geoff Hinton

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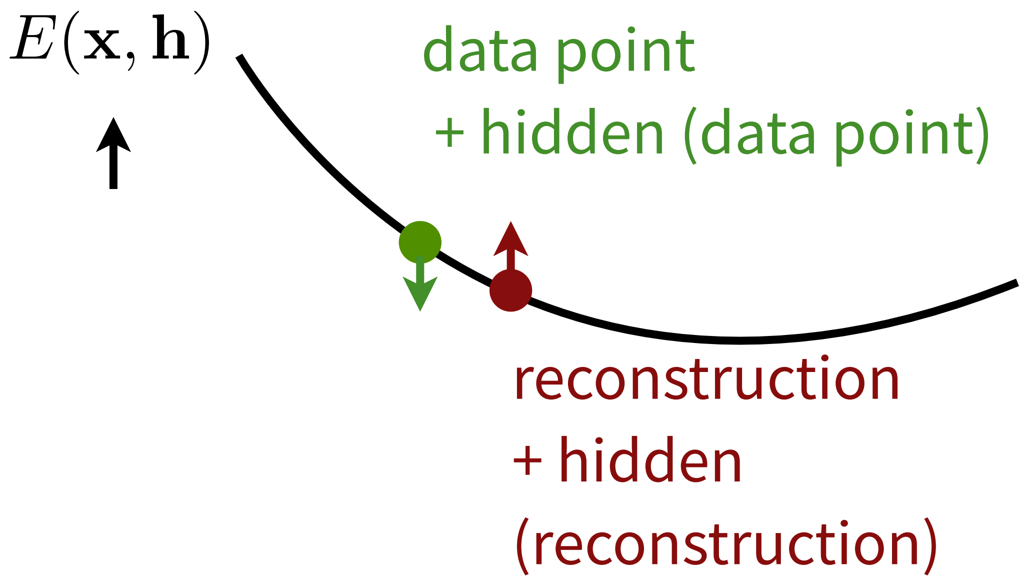

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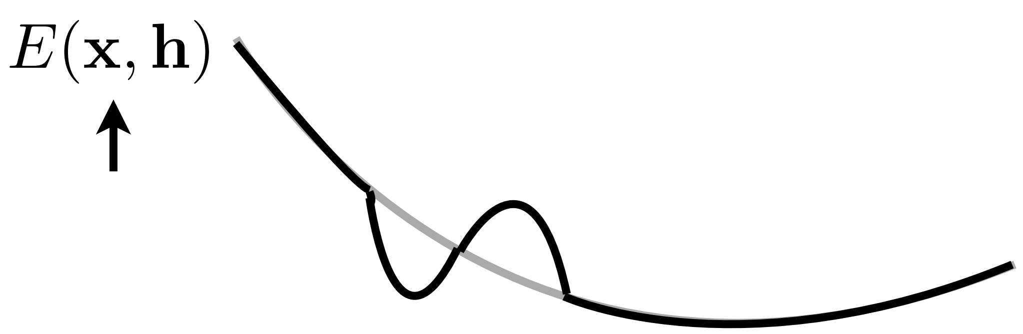

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Derivation of the Learning Rule

Given $\boldsymbol{v}^{(i)}$ and $\tilde{\boldsymbol{v}}$ the learning rule for $\boldsymbol{\theta} = \boldsymbol{W}$ becomes:

$$
\begin{aligned}
\boldsymbol{W} \Leftarrow \boldsymbol{W} &- \epsilon \left(\nabla_{\boldsymbol{W}} \left\{ -\log P(\boldsymbol{v}^{(i)}) \right\} \right) \\
= \boldsymbol{W} &- \epsilon \left(\mathbb{E}_{\boldsymbol{h}} \left[\nabla_{\boldsymbol{W}} E(\boldsymbol{v}^{(i)}, \boldsymbol{h}) \middle| \boldsymbol{v}^{(i)} \right] - \mathbb{E}_{\boldsymbol{v},\boldsymbol{h}} \left[\nabla_{\boldsymbol{W}} E(\boldsymbol{v}, \boldsymbol{h}) \right] \right) \\
\approx \boldsymbol{W} &- \epsilon \left(\mathbb{E}_{\boldsymbol{h}} \left[\nabla_{\boldsymbol{W}} E(\boldsymbol{v}^{(i)}, \boldsymbol{h}) \middle| \boldsymbol{v}^{(i)} \right] - \mathbb{E}_{\boldsymbol{h}} \left[\nabla_{\boldsymbol{W}} E(\tilde{\boldsymbol{v}}, \boldsymbol{h}) \left| \tilde{\boldsymbol{v}} \right. \right] \right) \\
= \boldsymbol{W} &+ \epsilon \left(\boldsymbol{h}(\boldsymbol{v}^{(i)}) \boldsymbol{v}^{(i)\top} - \boldsymbol{h}(\tilde{\boldsymbol{v}}) \tilde{\boldsymbol{v}}^{\top} \right)
\end{aligned}
$$

CD-k: Algorithm

1. For each training example $\boldsymbol{v}^{(i)}$

   i. generate a negative sample $\tilde{v}$ using k steps of Gibbs sampling, starting at $\boldsymbol{v}^{(i)}$

   ii. update parameters:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} + \epsilon \left(\boldsymbol{h}(\boldsymbol{v}^{(i)}) \boldsymbol{v}^{(i)\top} - \boldsymbol{h}(\tilde{\boldsymbol{v}}) \tilde{\boldsymbol{v}}^{\top} \right)$$

$$\boldsymbol{c} \leftarrow \boldsymbol{c} + \epsilon \left(\boldsymbol{h}(\boldsymbol{v}^{(i)}) - \boldsymbol{h}(\tilde{\boldsymbol{v}}) \right)$$

$$\boldsymbol{b} \leftarrow \boldsymbol{b} + \epsilon \left(\boldsymbol{v}^{(i)} - \tilde{\boldsymbol{v}} \right)$$

2. Go back to 1 until stopping criteria

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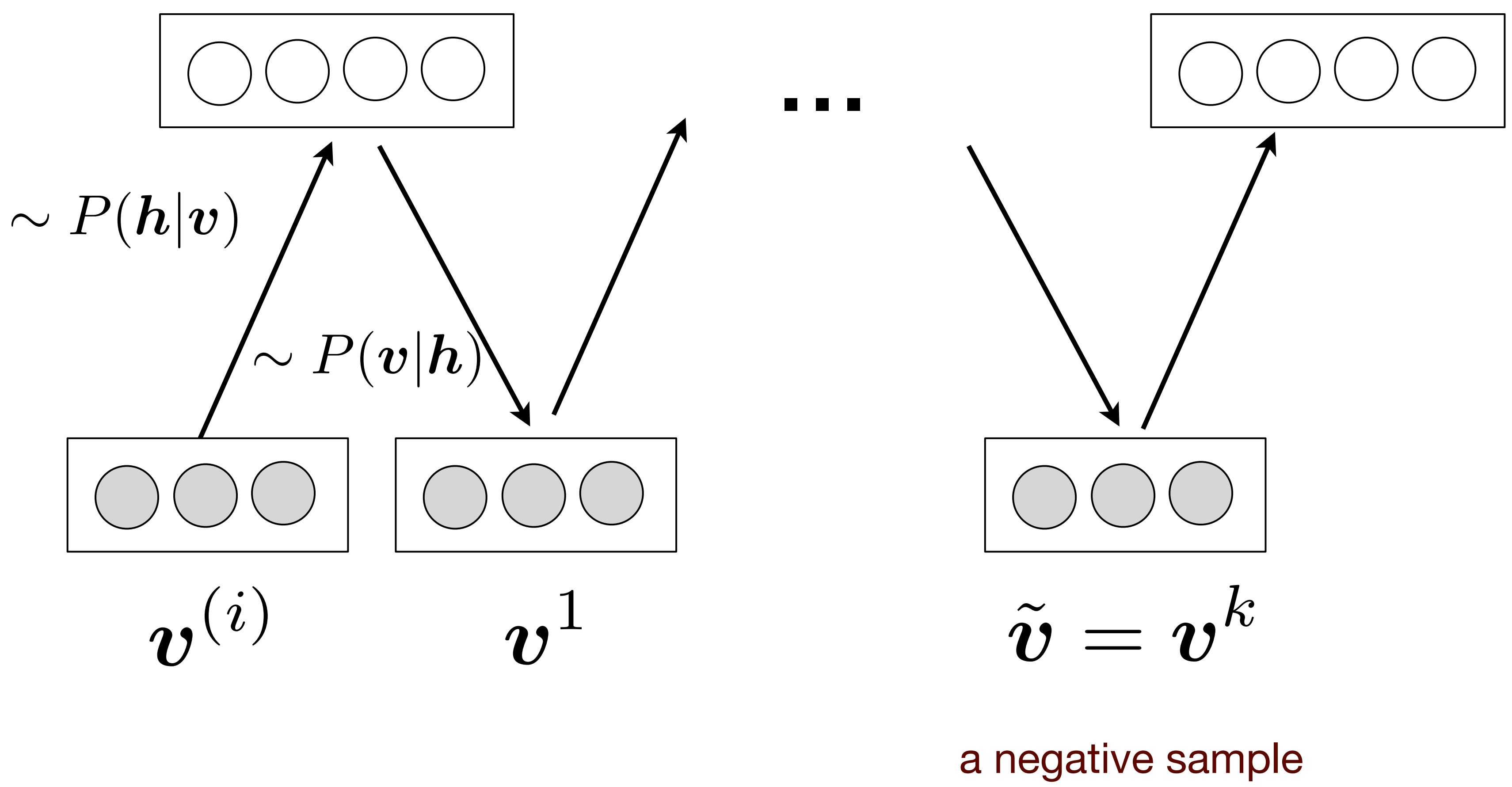
In general, the bigger k, the less biased the estimate of the gradient.
In practice, $k = 1$ works well for pre-training.

Persistent CD (PCD) (Tieleman 2008)

Idea:

- instead of initializing the chain to $\tilde{\boldsymbol{v}}^{(i)}$, initialize the chain to the negative sample of the last iteration



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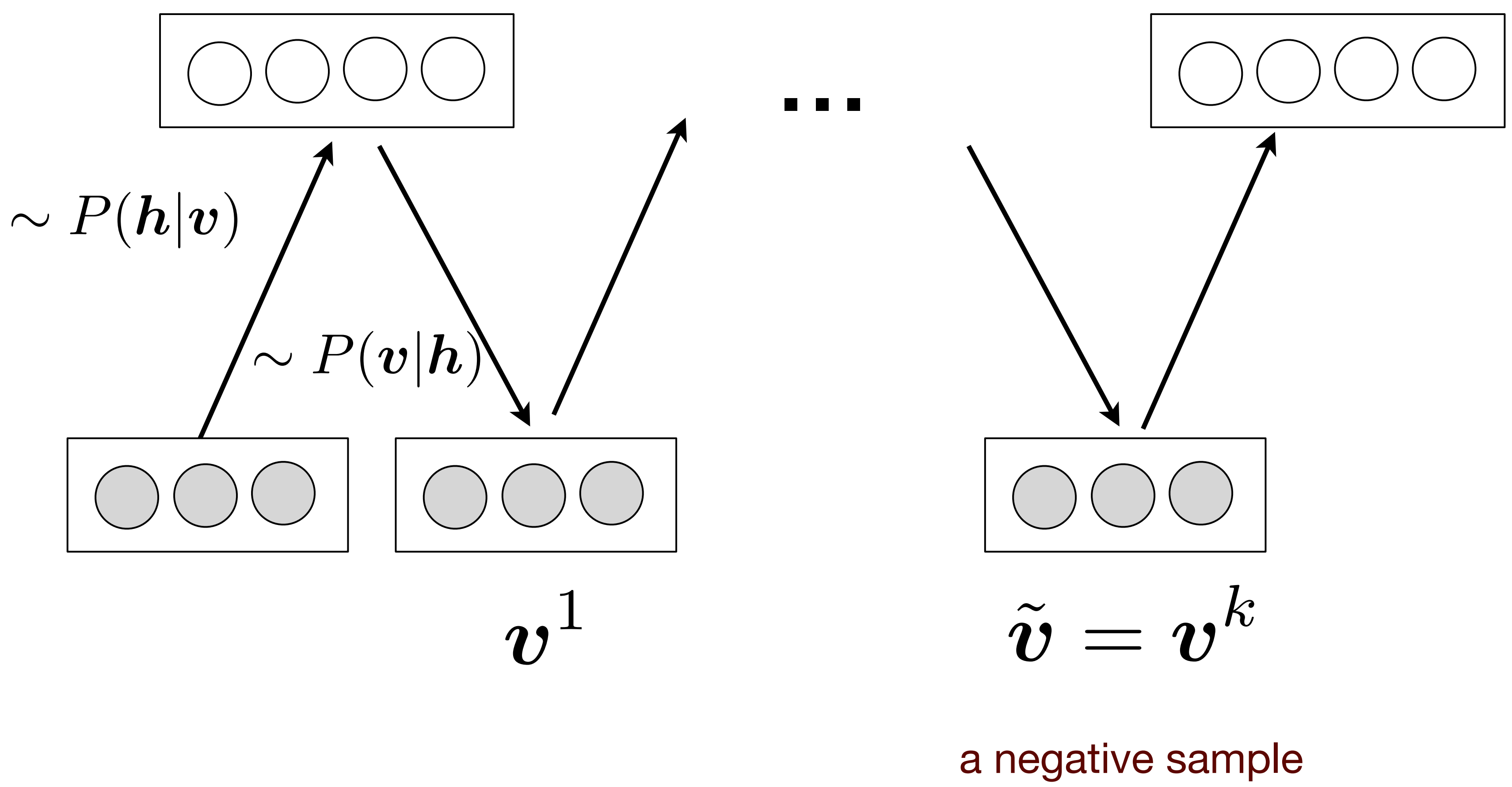

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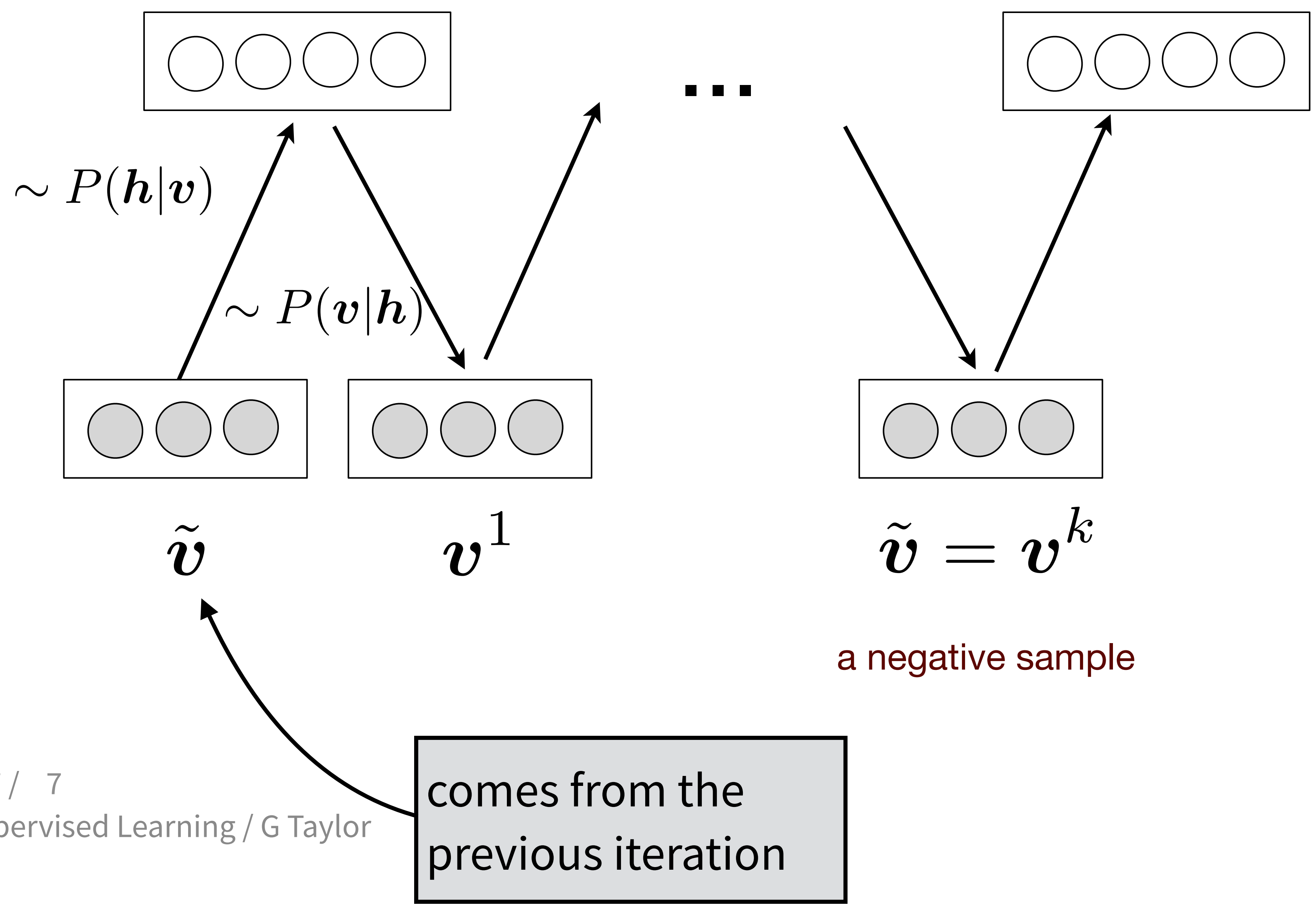

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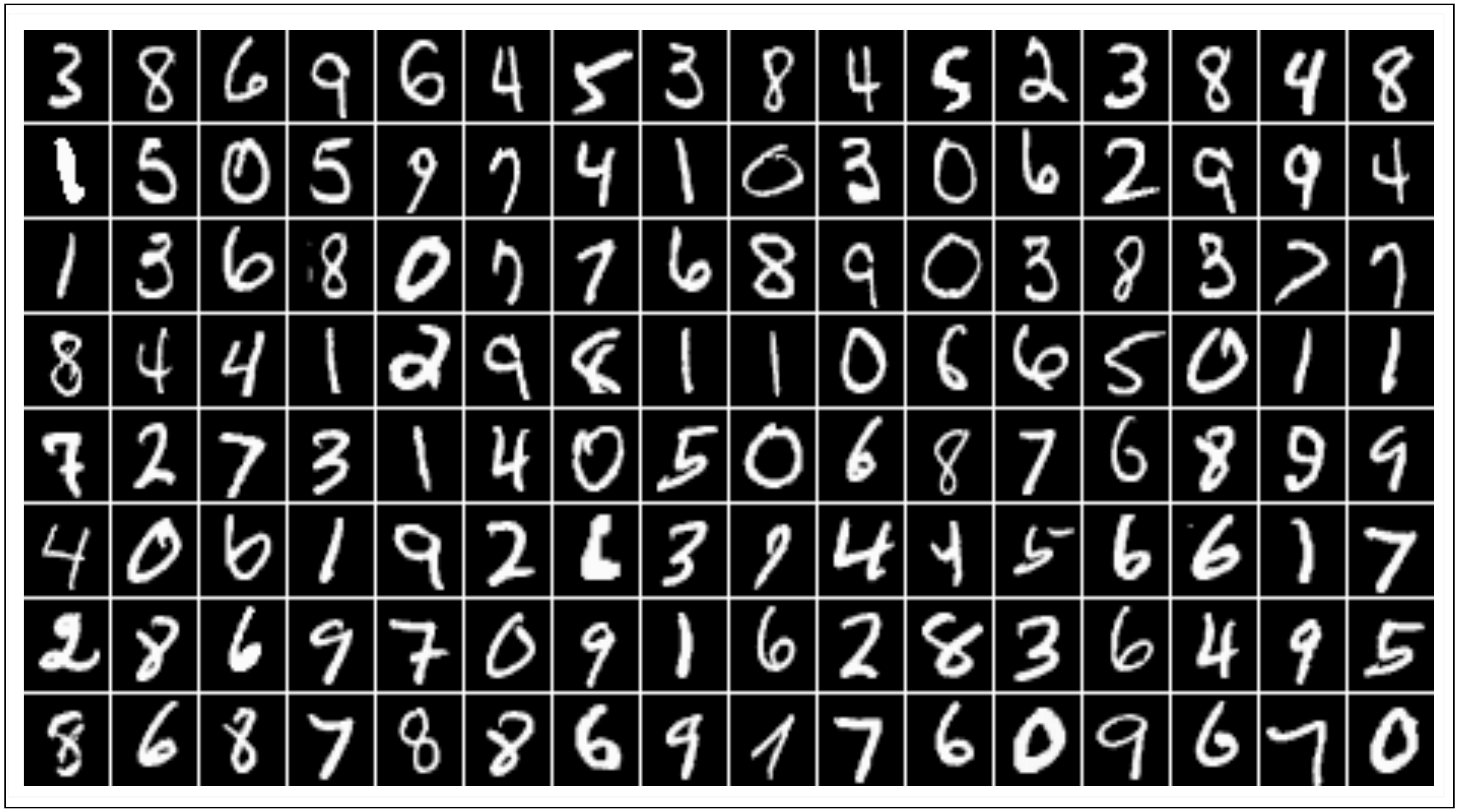
RBM: Example (MNIST)



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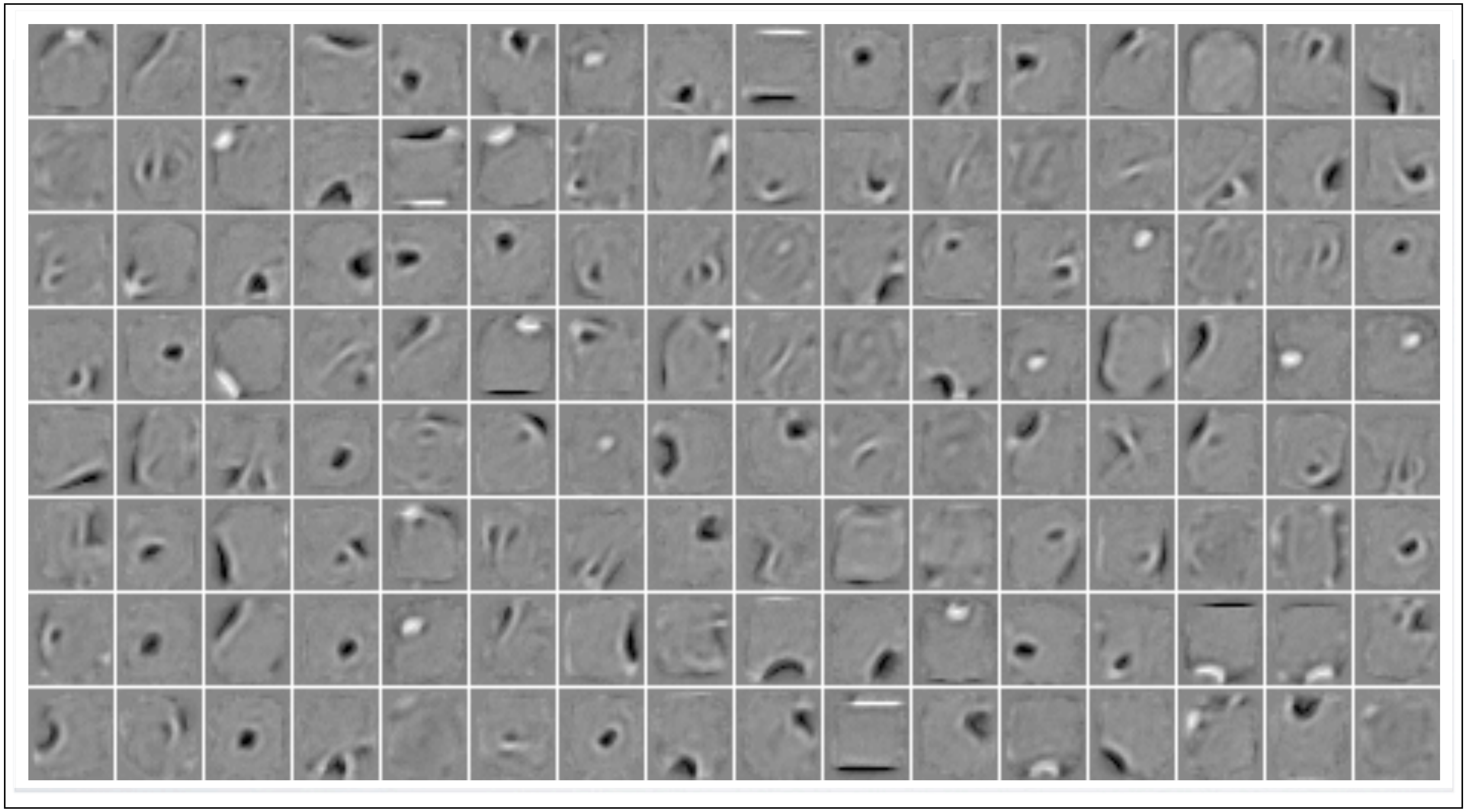
RBM: Example (Filters)



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RBMs: Debugging

- It's very difficult to monitor the training of RBMs because we do not have access to the log likelihood
- It's also not possible to check gradients with finite differences
- Can instead rely on some approximate "tricks":
  - plot average stochastic reconstruction $||\boldsymbol{v}^{(i)} - \tilde{\boldsymbol{v}}||^2$ and see if it tends to decrease
  - for inputs that correspond to images, visualize the connection coming into each hidden unit (the filters)
  - can also try to approximate the partition function Z and see whether the (approximated) NLL decreases

Gaussian-Bernoulli RBM

What if inputs are unbounded real values?

- Add a quadratic term to the energy function

$$E(\boldsymbol{v}, \boldsymbol{h}) = -\boldsymbol{b}^\top \boldsymbol{v} - \boldsymbol{c}^\top \boldsymbol{h} - \boldsymbol{v}^\top \boldsymbol{W} \boldsymbol{h} - \frac{1}{2}\boldsymbol{v}^\top \boldsymbol{v}$$

- Only thing that changes is that $P(\boldsymbol{v}|\boldsymbol{h})$ is now a Gaussian distribution with mean $\boldsymbol{\mu} = \boldsymbol{b} + \boldsymbol{W}^\top \boldsymbol{h}$ and identity covariance matrix

- Recommended to normalize the training set by
  - subtracting the mean of each input
  - dividing each input v_k by the training set standard deviation

- Should use a smaller learning rate than in a binary RBM