10707
Deep Learning: Spring 2020

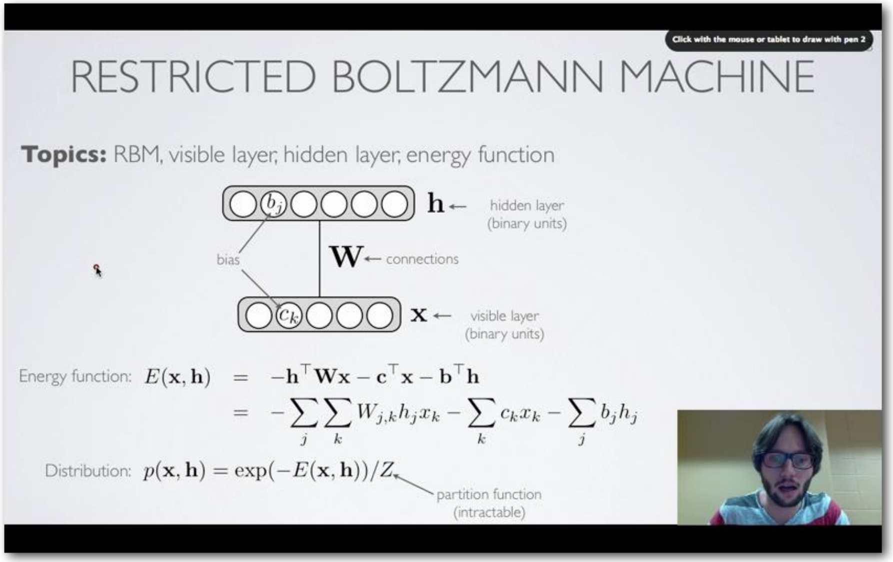
Andrej Risteski

Machine Learning Department

Lecture 13:
Learning using MCMC and variational methods: energy models, RBMs and DBNs

Disclaimer: Some of the material/slides for this lecture were borrowed from Hugo Larochelle's class on Neural Networks: https://sites.google.com/site/deeplearningsummerschool2016/

http://info.usherbrooke.ca/hlarochelle/neural_networks



RESTRICTED BOLTZMANN MACHINE

Topics: RBM, visible layer, hidden layer, energy function

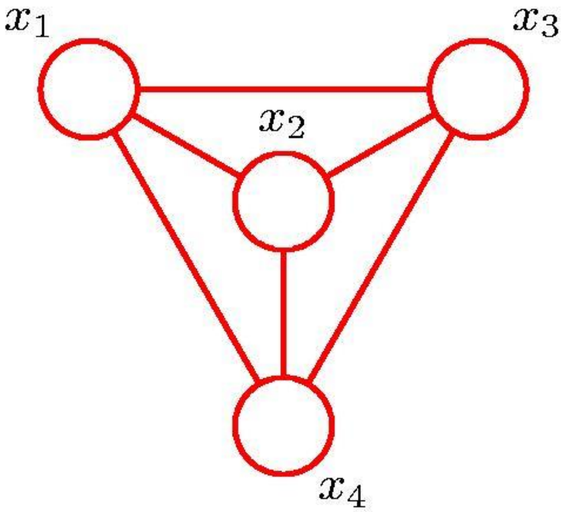
Energy function:
$$\begin{aligned} E(\mathbf{x},\mathbf{h}) &= -\mathbf{h}^\top \mathbf{W}\mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \\ &= -\sum_j \sum_k W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j \end{aligned}$$

Distribution: $p(\mathbf{x},\mathbf{h}) = \exp(-E(\mathbf{x},\mathbf{h}))/Z$ ← partition function (intractable)

Some are borrowed from Russ Salakhutdinov's offering of 10-707: https://deeplearning-cmu-10707.github.io/syllabus.html

Graphical Models

Recall: graph contains a set of nodes connected by edges.



In a probabilistic graphical model, each node represents a random variable, links represent "probabilistic dependencies" between random variables.

Graph specifies how joint distribution over all random variables decomposes into a **product** of factors, each factor depending on a subset of the variables.

Two types of graphical models:

- **Bayesian networks**, also known as Directed Graphical Models (the links have a particular directionality indicated by the arrows)
- **Markov Random Fields**, also known as Undirected Graphical Models (the links do not carry arrows and have no directional significance).

Algorithmic pros/cons of latent-variable models (so far)

RBM's

- Hard to draw samples ✗

(In fact, #P-hard provably, even in Ising models)

- Easy to sample posterior distribution over latents ✓

Directed models

- Easy to draw samples ✓
- Hard to sample posterior distribution over latents ✗

(In fact, #P-hard even in mixtures)

Canonical tasks with graphical models

Inference

Given values for the parameters θ of the model, *sample/calculate* marginals (e.g. sample $p_\theta(x_1), p_\theta(x_4, x_5), p_\theta(z|x)$, etc.)

Learning

Find values for the parameters θ of the model, that give a *high likelihood* for the observed data. (e.g. canonical way is solving maximum likelihood optimization

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p(x_i)$$

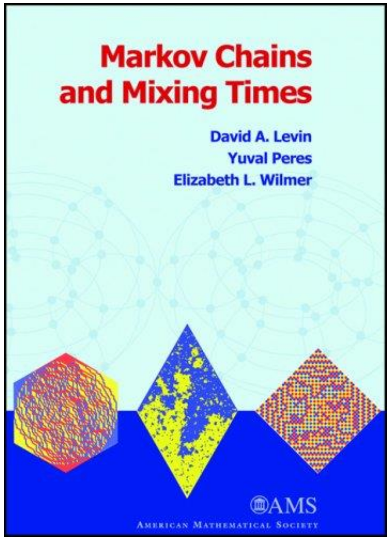
Other methods exist, e.g. method of moments (matching moments of model), but less used in deep learning practice.

Algorithmic approaches

When faced with a difficult to calculate probabilistic quantity (partition function, difficult posterior), there are two families of approaches:

MARKOV CHAIN MONTE CARLO

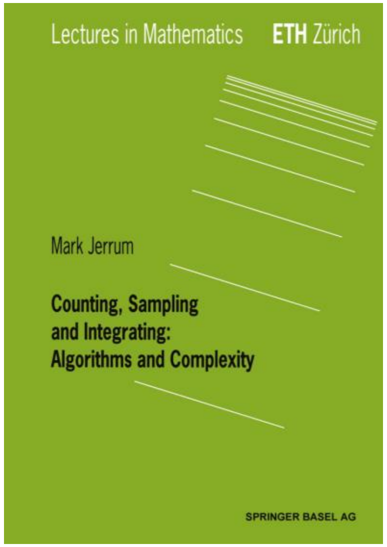
- Random walk w/ equilibrium distribution the one we are trying to sample from.
- Well studied in TCS.



Markov Chains and Mixing Times

David A. Levin
Yuval Peres
Elizabeth L. Wilmer

AMS
American Mathematical Society



Lectures in Mathematics ETH Zürich

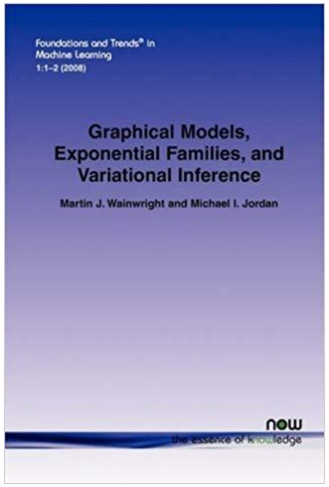
Mark Jerrum

Counting, Sampling and Integrating: Algorithms and Complexity

SPRINGER BASEL AG

VARIATIONAL METHODS

- Based on solving an optimization problem.
- Very popular in practice.
- Comparatively poorly understood



Foundations and Trends® in Machine Learning
1:1–2 (2008)

Graphical Models, Exponential Families, and Variational Inference

Martin J. Wainwright and Michael I. Jordan

now
the essence of knowledge

Part I: Learning completely observable energy models

Learning energy models

Goal: Sample from distribution given up to constant of proportionality:

$$p_\theta(x) \propto \exp(-E_\theta(x))$$

Recall our basic approach: maximum likelihood

Given data $x_1, x_2, \ldots, x_n$, solve the optimization problem

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

Expanding likelihoods: $\log\ p_\theta(x) = -E_\theta(x) - \log Z_\theta$

Our basic algorithm: gradient descent. Can we take gradients?

$\nabla_\theta E(\theta)$ is typically easy (e.g. $E(\theta)$ is a neural net, Ising model, etc.)

Learning energy models

Goal: Sample from distribution given up to constant of proportionality:

$$p_\theta(x) \propto \exp(-E_\theta(x))$$

Recall our basic approach: maximum likelihood

Given data $x_1, x_2, \ldots, x_n$, solve the optimization problem

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

$$\nabla_\theta \log Z_\theta = \frac{1}{Z_\theta} \nabla_\theta Z_\theta \;\; = \frac{1}{Z_\theta} \nabla_\theta \left(\int_x \exp(-E_\theta(x)) \right)$$

$$\frac{1}{Z_\theta} \int_x \exp(-E_\theta(x)) \nabla_\theta (-E_\theta(x)) = \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

Learning energy models

Goal: Sample from distribution given up to constant of proportionality:

$$p_\theta(x) \propto \exp(-E_\theta(x))$$

$$\nabla_\theta \left(\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(x_i) \right) = \frac{1}{n} \left(\sum_i -\nabla_\theta E_\theta(x_i) \right) - \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

$$\approx \underbrace{\mathbb{E}_{p_{data}}[-\nabla_\theta E_\theta(x)] - \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]}$$

Goal of the algorithm: *Try to make the expectation of the energy match*

Learning energy models

Let’s assume $x \in \mathbb{R}^d$. An obvious way to produce the estimates $\mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$: sample approximately from p_θ using Langevin dynamics.

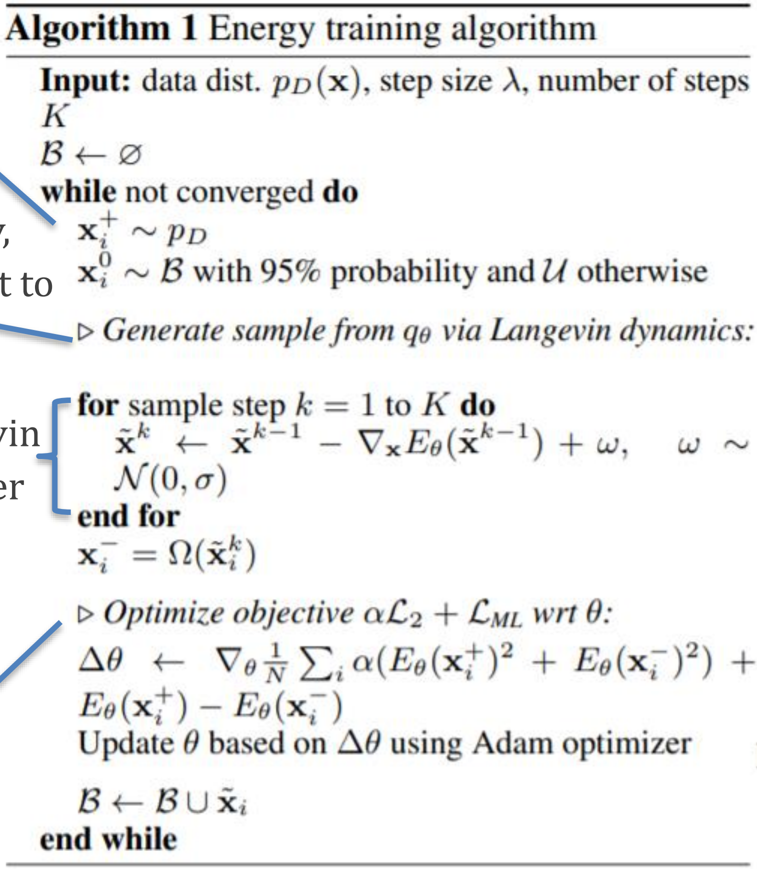
This was done recently: (Du, Mordatch ‘19), (Song, Ermon ‘19):

What’s the difficulty?

Data is multimodal: Langevin might take long to mix.

Learning energy models

The algorithm from (Du, Mordatch ‘19)



```
Algorithm 1 Energy training algorithm
Input: data dist. $p_D(\mathbf{x})$, step size $\lambda$, number of steps $K$
$\mathcal{B} \leftarrow \varnothing$
while not converged do
    $\mathbf{x}_i^+ \sim p_D$
    $\mathbf{x}_i^0 \sim \mathcal{B}$ with 95% probability and $\mathcal{U}$ otherwise

    ▷ Generate sample from $q_\theta$ via Langevin dynamics:
    for sample step $k = 1$ to $K$ do
        $\tilde{\mathbf{x}}^k \leftarrow \tilde{\mathbf{x}}^{k-1} - \nabla_{\mathbf{x}} E_\theta(\tilde{\mathbf{x}}^{k-1}) + \omega, \quad \omega \sim \mathcal{N}(0, \sigma)$
    end for
    $\mathbf{x}_i^- = \Omega(\tilde{\mathbf{x}}_i^k)$

    ▷ Optimize objective $\alpha\mathcal{L}_2 + \mathcal{L}_{ML}$ wrt $\theta$:
    $\Delta\theta \leftarrow \nabla_\theta \frac{1}{N} \sum_i \alpha(E_\theta(\mathbf{x}_i^+)^2 + E_\theta(\mathbf{x}_i^-)^2) + E_\theta(\mathbf{x}_i^+) - E_\theta(\mathbf{x}_i^-)$
    Update $\theta$ based on $\Delta\theta$ using Adam optimizer

    $\mathcal{B} \leftarrow \mathcal{B} \cup \tilde{\mathbf{x}}_i$
end while
```

Maintain buffer of previous samples to reduce mixing time

W/ some probability, start from random pt to encourage mode exploration

Langevin sampler

A bit of l2 regularization to ensure energy is somewhat smooth

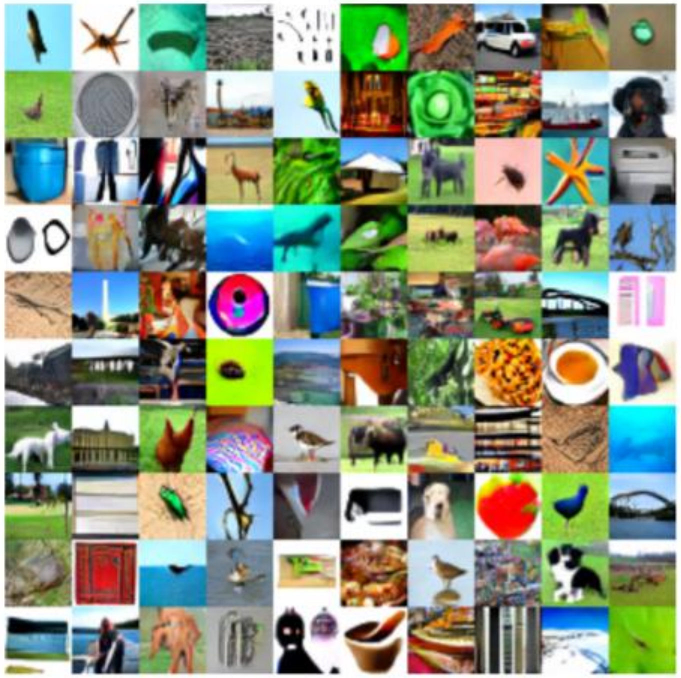


Figure 2: Conditional ImageNet32x32 EBM samples

Learning energy models

The algorithm from (Song, Ermon '19)

Not likelihood based, instead minimize:

$$\mathbb{E}_{p_{data}} ||\nabla_x \log p_{data}(x) - \left(-E_\theta(x)\right)||^2$$

(Turns out to be writeable in a form friendly for taking gradients)

To alleviate multimodality, they use a variant of ***simulated tempering,*** which we saw last time.

They also use ***smoothing by convolving*** with Gaussians to account for points with bad estimates of $E_\theta(x)$.

Learning energy models

The algorithm from (Song, Ermon '19)

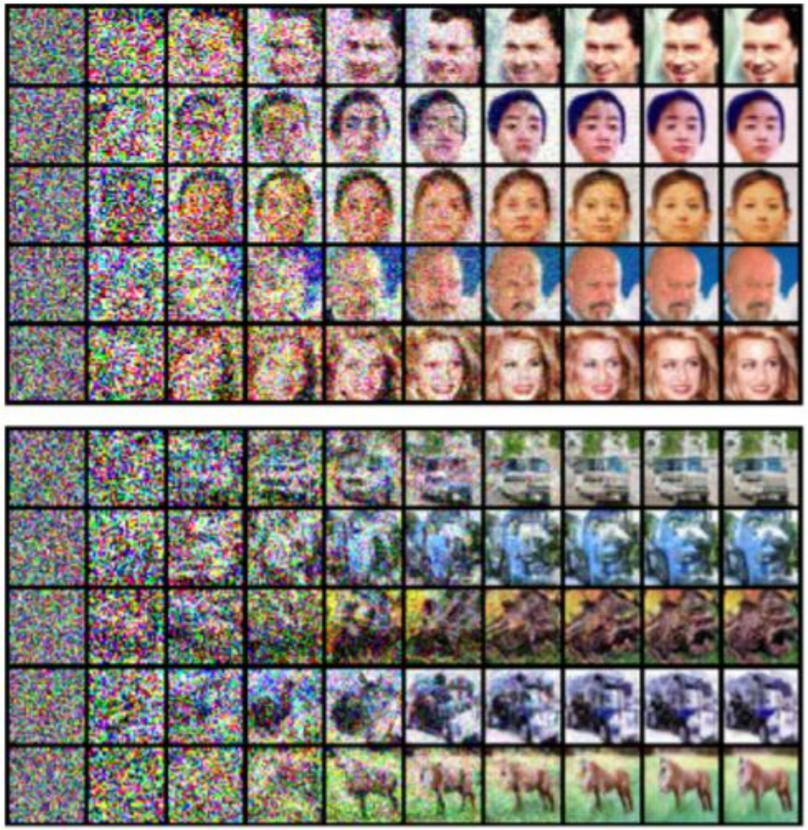
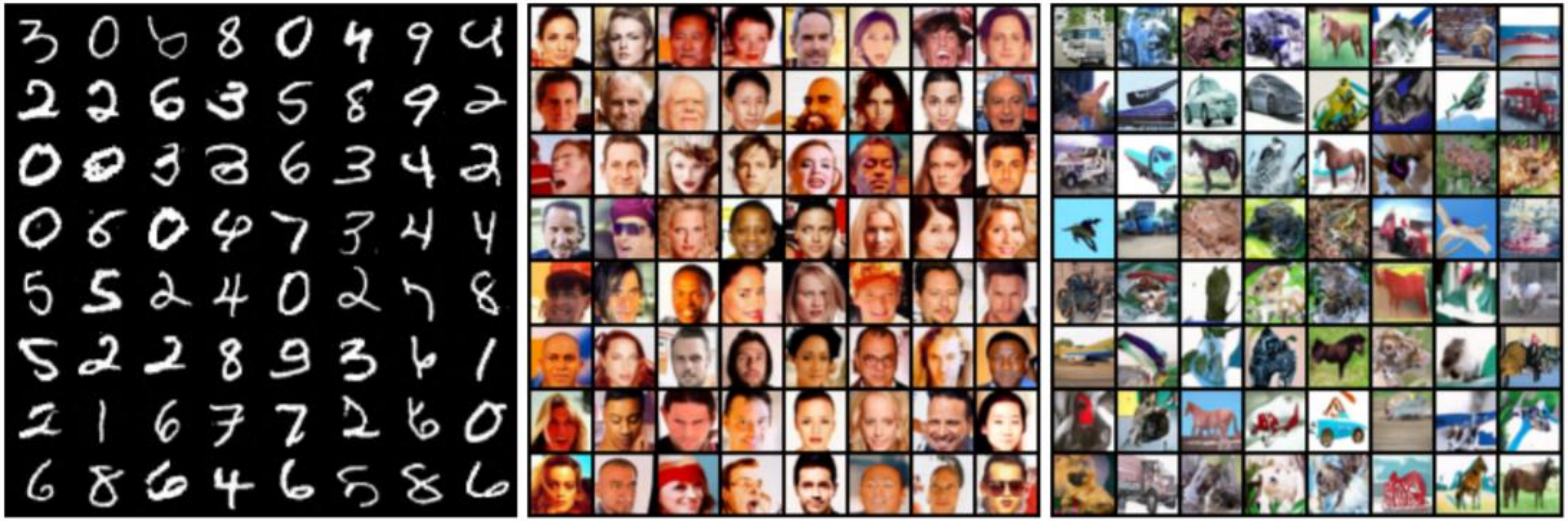


Figure 4: Intermediate samples of annealed Langevin dynamics.

Learning energy models

The algorithm from (Song, Ermon ‘19)



(a) MNIST

(b) CelebA

(c) CIFAR-10

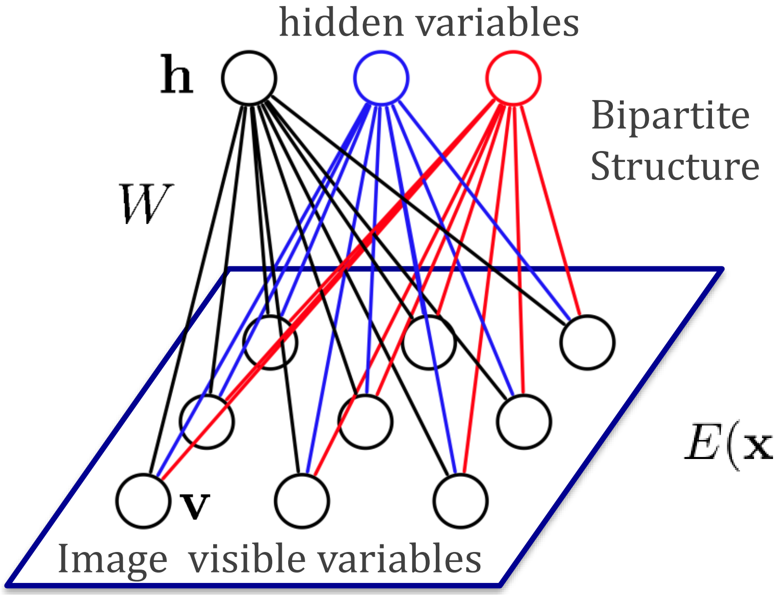
Figure 5: Uncurated samples on MNIST, CelebA, and CIFAR-10 datasets.

Part II: Learning Restricted Boltzmann Machines (RBMs)

Restricted Boltzmann Machines

An **undirected** latent-variable model

We denote visible and hidden variables with vectors **v, h** respectively:



Visible variables $\mathbf{x} \in \{\mathbf{0}, \mathbf{1}\}^{\mathbf{D}}$ are connected to hidden variables $\mathbf{h} \in \{0, 1\}^{F}$

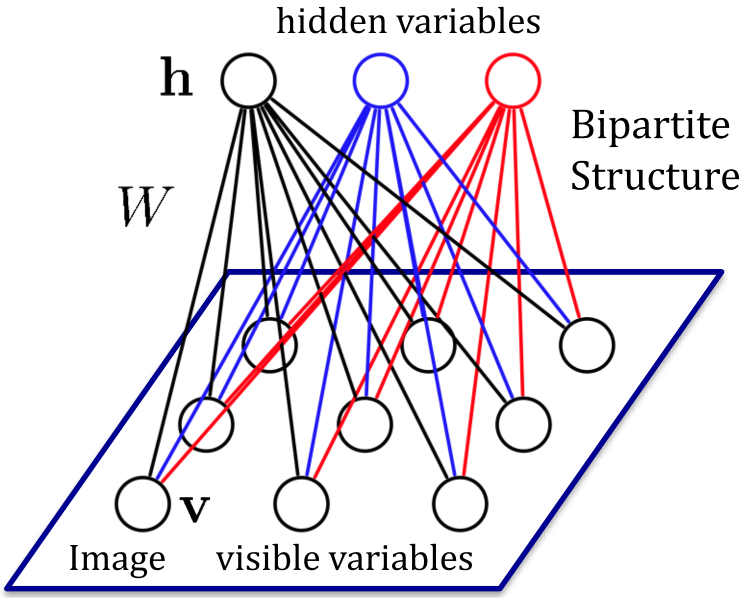
The energy of the joint configuration:

$$
\begin{aligned}
E(\mathbf{x}, \mathbf{h}) &= -\mathbf{h}^\top \mathbf{W} \mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \\
&= -\sum_j \sum_k W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j
\end{aligned}
$$

Probability of the joint configuration:

$$p(\mathbf{x}, \mathbf{h}) = \exp(-E(\mathbf{x}, \mathbf{h}))/Z$$

Restricted Boltzmann Machines



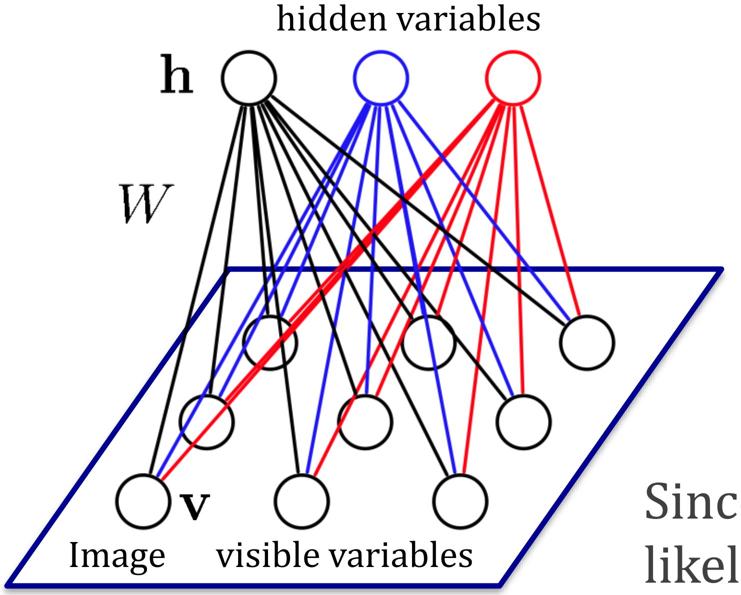
The **posterior** over the hidden variables is easy to sample from!
(Conditional independence!)

$$p(\mathbf{h}|\mathbf{x}) = \underbrace{\prod_j p(h_j|\mathbf{x})}_{\text{Factorizes}} \qquad p(h_j = 1|\mathbf{x}) = \frac{1}{1 + \exp(-(b_j + \mathbf{W}_{j}.\mathbf{x}))}$$

Similarly:

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h}) \qquad p(x_k = 1|\mathbf{h}) = \frac{1}{1 + \exp(-(c_k + \mathbf{h}^\top \mathbf{W}_{.k}))}$$

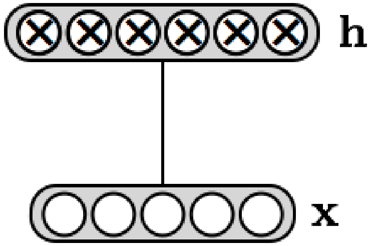
How to learn RBM's



Given data $x_1, x_2, \dots, x_n$, solve

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

Since we have latent variables, we need to express the likelihood when we marginalize out the latents:



How to learn RBM's

$$p(\mathbf{x}) = \sum_{\mathbf{h}\in\{0,1\}^H} \exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z$$

How to learn RBM’s

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\begin{aligned}
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&= \exp(\mathbf{c}^\top \mathbf{x}) \sum_{h_1\in\{0,1\}} \cdots \sum_{h_H\in\{0,1\}} \exp\left(\sum_j h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j\right)/Z
\end{aligned}
$$

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&= \exp(\mathbf{c}^\top \mathbf{x}) \left(\sum_{h_1\in\{0,1\}} \exp(h_1 \mathbf{W}_{1\cdot}\mathbf{x} + b_1 h_1)\right) \ldots \left(\sum_{h_H\in\{0,1\}} \exp(h_H \mathbf{W}_{H\cdot}\mathbf{x} + b_H h_H)\right)/Z
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&= \exp(\mathbf{c}^\top \mathbf{x}) \left(1 + \exp(b_1 + \mathbf{W}_{1\cdot}\mathbf{x})\right) \ldots \left(1 + \exp(b_H + \mathbf{W}_{H\cdot}\mathbf{x})\right) /Z
\end{aligned}
$$

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&= \exp(\mathbf{c}^\top \mathbf{x})\left(1 + \exp(b_1 + \mathbf{W}_{1\cdot}\mathbf{x})\right) \ldots \left(1 + \exp(b_H + \mathbf{W}_{H\cdot}\mathbf{x})\right)/Z \\
&= \exp(\mathbf{c}^\top \mathbf{x}) \exp(\log(1 + \exp(b_1 + \mathbf{W}_{1\cdot}\mathbf{x}))) \ldots \exp(\log(1 + \exp(b_H + \mathbf{W}_{H\cdot}\mathbf{x})))/Z
\end{aligned}
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How to learn RBM's

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&= \exp(\mathbf{c}^\top\mathbf{x})\,(1+\exp(b_1+\mathbf{W}_{1\cdot}\mathbf{x}))\ldots(1+\exp(b_H+\mathbf{W}_{H\cdot}\mathbf{x}))\,/Z \\
&= \exp(\mathbf{c}^\top\mathbf{x})\exp(\log(1+\exp(b_1+\mathbf{W}_{1\cdot}\mathbf{x})))\ldots\exp(\log(1+\exp(b_H+\mathbf{W}_{H\cdot}\mathbf{x})))/Z \\
&= \exp\left(\underbrace{\mathbf{c}^\top\mathbf{x} + \sum_{j=1}^{H}\log(1+\exp(b_j+\mathbf{W}_{j\cdot}\mathbf{x}))}_{=\,\mathrm{F}(\mathbf{x})}\right)/Z
\end{aligned}
$$

How to learn RBM’s

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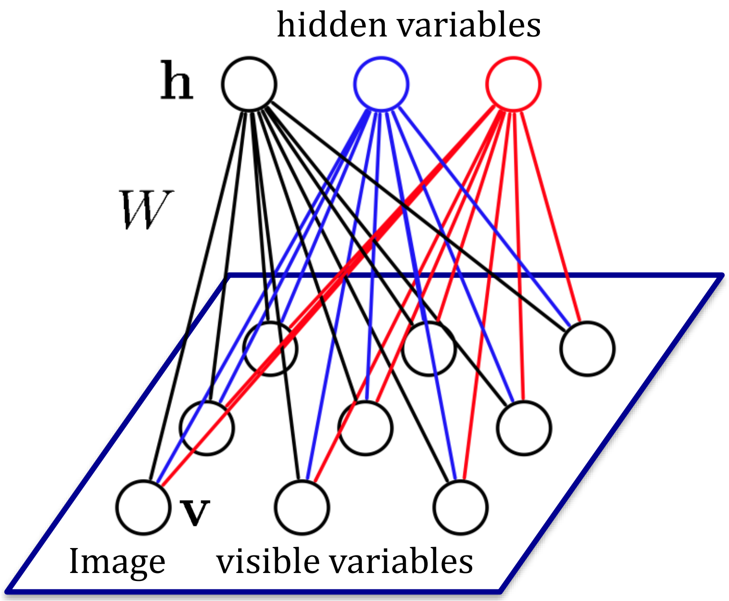
\end{aligned}
$$

$$= \exp\big(\mathrm{F}(\mathbf{x})\big)\,/\mathrm{Z}$$

How to learn RBM’s



Given data $x_1, x_2, \dots, x_n$, solve

$$\max_{\theta\in\Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

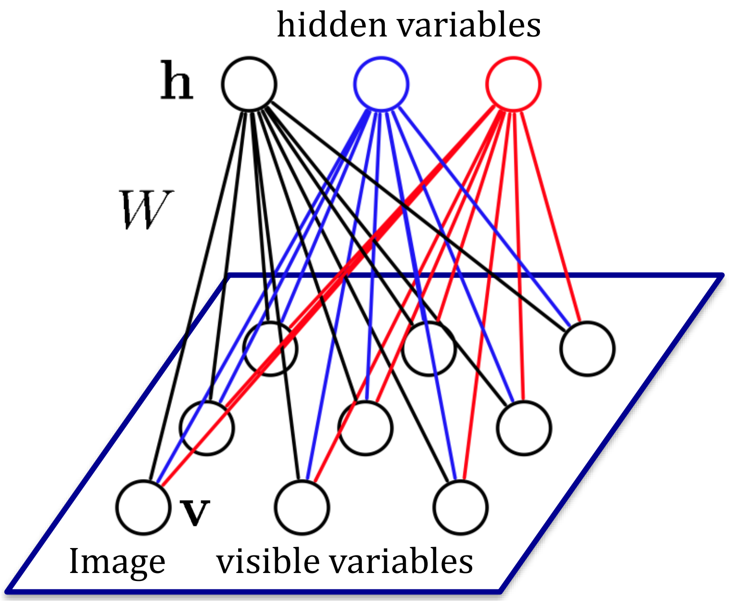
With this reduction, the undirected model calculations imply:

$$\nabla_\theta\left(\frac{1}{n}\sum_{i=1}^{n} \log p_\theta(x_i)\right) = \frac{1}{n}\left(\sum_i -\nabla_\theta F_\theta(x_i)\right) - \mathbb{E}_{p_\theta}[-\nabla_\theta F_\theta(x)]$$

$$\nabla_{\mathrm{W_{ij}}} \mathrm{F}_\theta(\mathbf{x}) = \nabla_{\mathrm{W_{ij}}}\left(\mathbf{c}^{\mathrm{T}}\mathbf{x} + \textstyle\sum_{\mathrm{j=1}}^{\mathrm{H}} \log\left(1+\exp\left(\mathrm{b_j} + \mathbf{W}_{\mathrm{j}}.\mathbf{x}\right)\right)\right) = \frac{\exp\left(\mathrm{b_j}+\mathbf{W}_{\mathrm{j}}.\mathbf{x}\right)}{1+\exp\left(\mathrm{b_j}+\mathbf{W}_{\mathrm{j}}.\mathbf{x}\right)}\mathbf{x}_{\mathrm{i}}$$

$$= \frac{1}{1+\exp\left(-\left(\mathrm{b_j}+\mathbf{W}_{\mathrm{j}}.\mathbf{x}\right)\right)}\mathbf{x}_{\mathrm{i}} = \mathrm{P}\left(\mathbf{h}_{\mathrm{j}} = 1\middle|\mathbf{x}\right)\mathbf{x}_{\mathrm{i}}$$

How to learn RBM’s



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$$\nabla_{\mathrm{W_{ij}}} \mathrm{F}_\theta(\mathbf{x}) = \mathrm{P}(\mathbf{h}_\mathrm{j} = 1|\mathbf{x})\, \mathbf{x}\_\mathrm{i} \quad \Rightarrow \quad \nabla_{\mathbf{W}} \mathrm{F}_\theta(\mathbf{x}) = \mathbf{h}(\mathbf{x})\, \mathbf{x}^\mathrm{T}$$

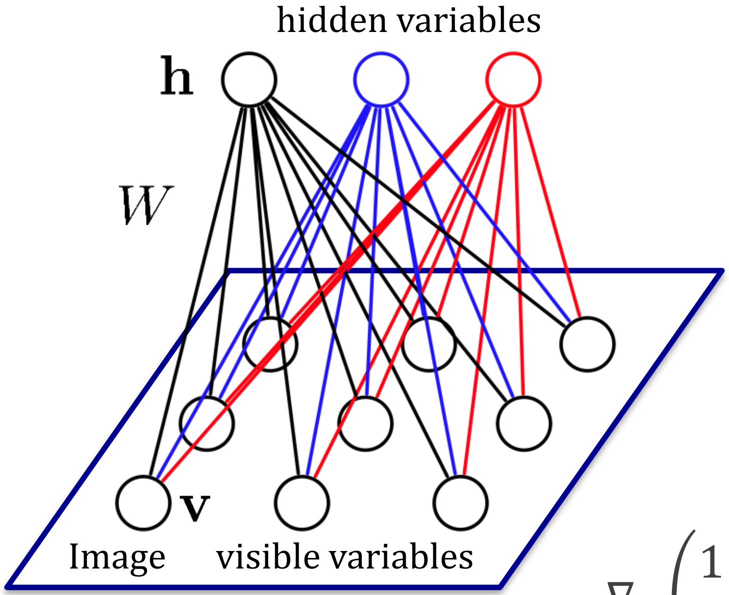
$$\nabla_{\boldsymbol{b}} \mathrm{F}_\theta(\mathbf{x}) = \mathbf{h}(\mathbf{x})$$

$$\nabla_{\mathrm{c}} \mathrm{F}_\theta(\mathbf{x}) = \mathbf{x}$$

$$\mathbf{h}(\mathbf{x}) \overset{\mathrm{def}}{=} \begin{pmatrix} p(h_1 = 1|\mathbf{x}) \\ \cdots \\ p(h_H = 1|\mathbf{x}) \end{pmatrix}$$

$$= \mathrm{sigm}(\mathbf{b} + \mathbf{W}\mathbf{x})$$

How to learn RBM's



Given data $x_1, x_2, \dots, x_n$, solve

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

$$\nabla_\theta \left(\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(x_i) \right) = \frac{1}{n} \left(\sum_i -\nabla_\theta F_\theta(x_i) \right) - \mathbb{E}_{p_\theta}[-\nabla_\theta F_\theta(x)]$$

The hard term is again: $\mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$ --- we need to draw samples from p_θ

We will draw samples using a Markov random walk: **Gibbs sampler**!

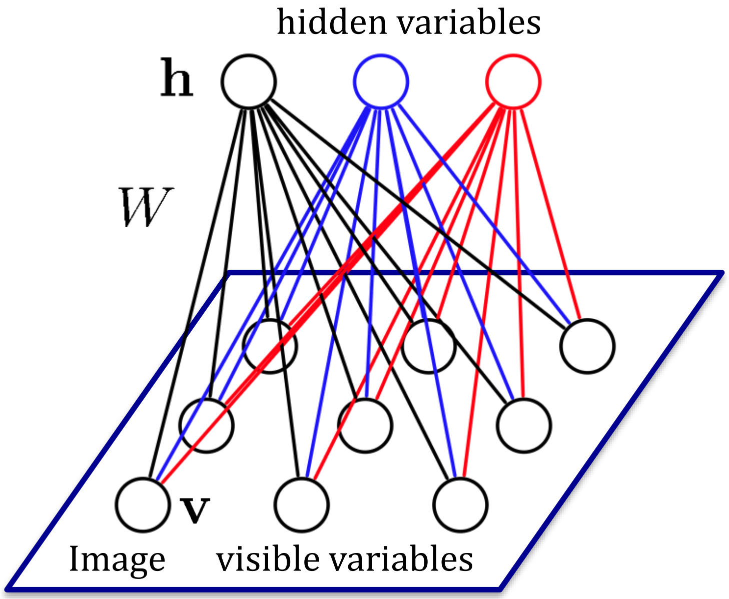
Gibbs sampling

Consider sampling a distribution over n variables $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$, s.t. each of the conditional distributions $P(x_i | \boldsymbol{x}_{-i})$ is easy to sample. :

A common way to do this is using **Gibbs sampling**:

```
Repeat:
    Let current state be $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$
    Pick $i \in [n]$ uniformly at random.
    Sample x $\sim P(X_i = x | \boldsymbol{x}_{-i})$
    Update state to $\boldsymbol{y} = (x_1, x_2, \dots, x_{i-1}, x, x_{i+1}, \dots, x_n)$
```

Gibbs sampling for RBM's

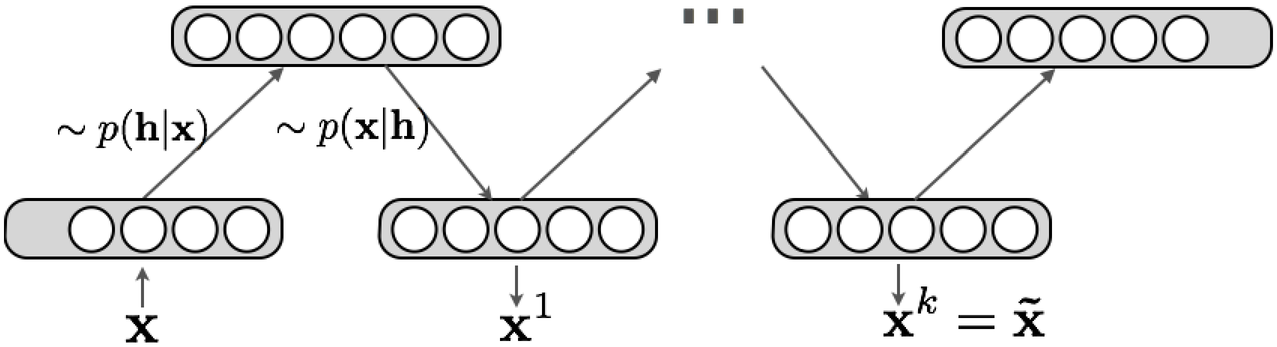


Repeat:

Sample $\mathbf{h} \sim P(\boldsymbol{h}|\boldsymbol{v})$

Sample $\mathbf{v} \sim P(\boldsymbol{v}|\boldsymbol{h})$

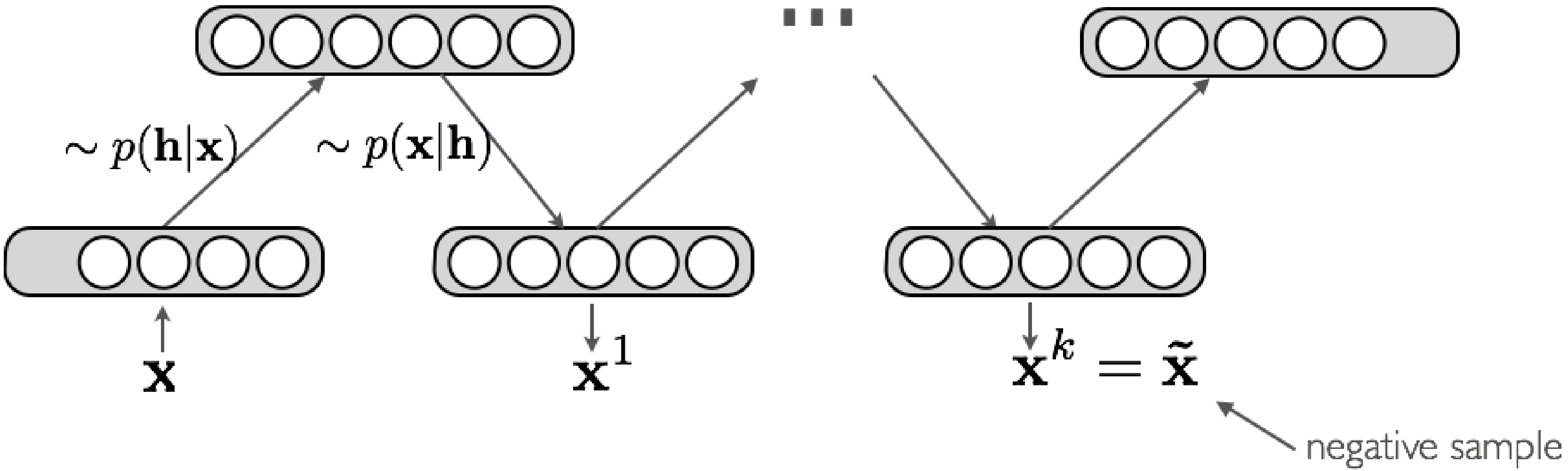
Pictorially:


$\sim p(\mathbf{h}|\mathbf{x})$
$\sim p(\mathbf{x}|\mathbf{h})$
...
$\mathbf{x}$
$\mathbf{x}^1$
$\mathbf{x}^k = \tilde{\mathbf{x}}$

Contrastive Divergence

Key idea behind Contrastive Divergence:

- Replace the expectation by a point estimate at $\tilde{\mathbf{x}}$
- Obtain the point $\tilde{\mathbf{x}}$ by Gibbs sampling
- Start sampling chain at $\mathbf{x}$



$\sim p(\mathbf{h}|\mathbf{x})$
$\sim p(\mathbf{x}|\mathbf{h})$
...
$\mathbf{x}$
$\mathbf{x}^1$
$\mathbf{x}^k = \tilde{\mathbf{x}}$
negative sample

k is often taken to be just 1.

Hinton, Neural Computation, 2002

CD-k Algorithm

For each training example $\mathbf{x}$

- Generate a negative sample $\tilde{\mathbf{x}}$ using k steps of Gibbs sampling, starting at the data point $\mathbf{x}$
- Update model parameters:

$$
\left.\begin{aligned}
\mathbf{W} &\Longleftarrow \mathbf{W} + \alpha\left(\mathbf{h}(\mathbf{x})\,\mathbf{x}^{\top} - \mathbf{h}(\tilde{\mathbf{x}})\,\tilde{\mathbf{x}}^{\top}\right)\\
\mathbf{b} &\Longleftarrow \mathbf{b} + \alpha\left(\mathbf{h}(\mathbf{x}) - \mathbf{h}(\tilde{\mathbf{x}})\right)\\
\mathbf{c} &\Longleftarrow \mathbf{c} + \alpha\left(\mathbf{x} - \tilde{\mathbf{x}}\right)
\end{aligned}\right\}
$$

Gradients we derived before

- Go back to 1 until stopping criteria

Step size

CD-k Algorithm

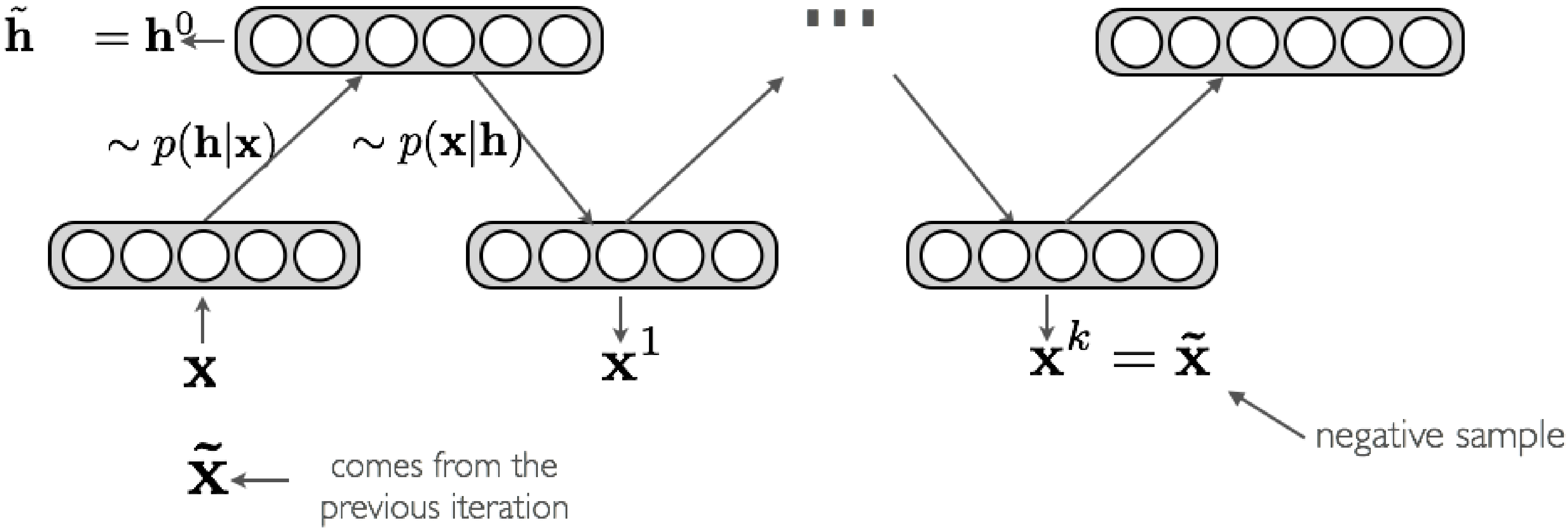
- CD-k: contrastive divergence with k iterations of Gibbs sampling

- In general, the bigger k is, the less biased the estimate of the gradient will be

- In practice, k=1 works well for learning good features and for pre-training

Persistent CD

Idea: instead of initializing the chain to $\mathbf{x}$, initialize the chain to the negative sample of the last iteration

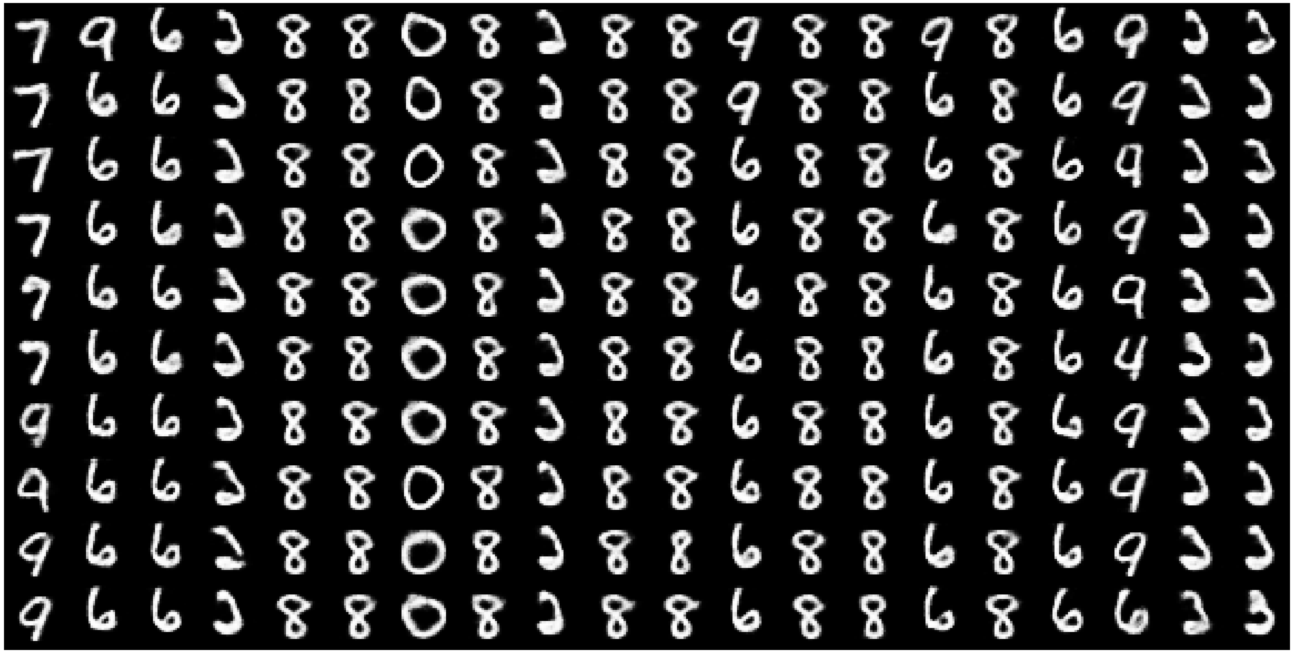


$\tilde{\mathbf{h}} = \mathbf{h}^0$
$\sim p(\mathbf{h}|\mathbf{x})$
$\sim p(\mathbf{x}|\mathbf{h})$
...
$\mathbf{x}$
$\mathbf{x}^1$
$\mathbf{x}^k = \tilde{\mathbf{x}}$
negative sample
$\tilde{\mathbf{x}}$
comes from the previous iteration

Tieleman, ICML, 2008

Example: MNIST

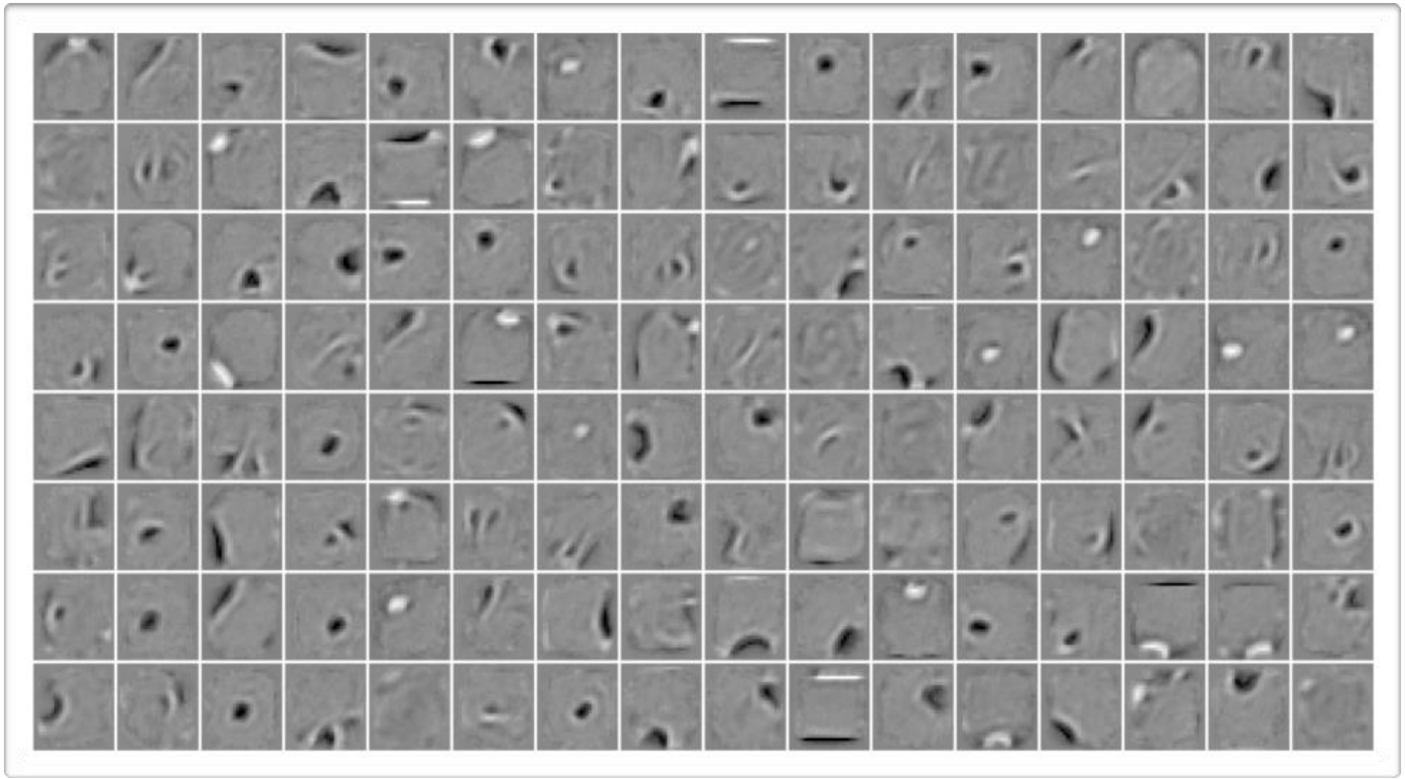
MNIST dataset:



Each row is small set of "initial points", after which next row is gotten by running 1000 Gibbs steps.

Learned Features

MNIST dataset:



(Larochelle et al., JMLR 2009)

Tricks and Debugging

Unfortunately, it is not easy to debug training RBMs (e.g. using gradient checks)

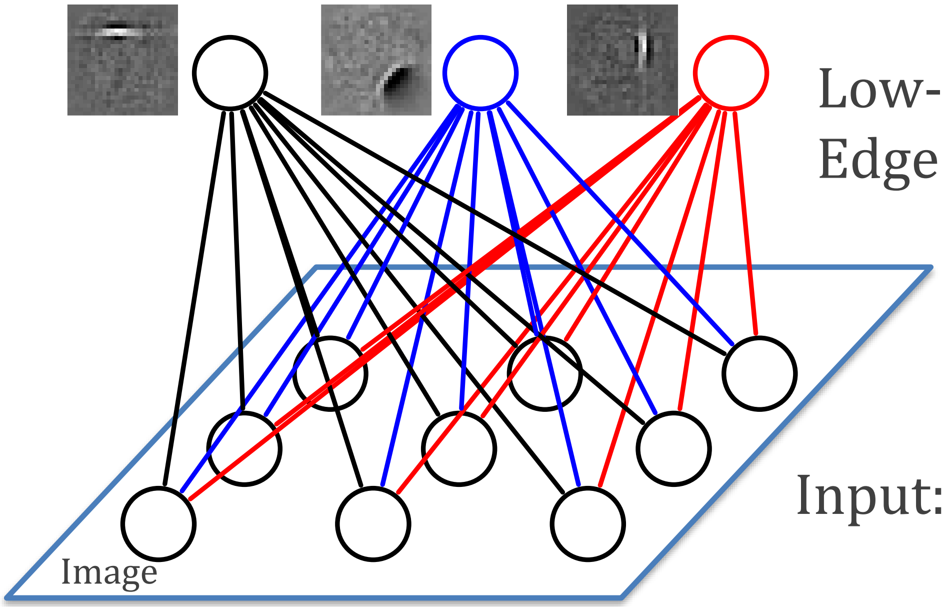
We instead rely on approximate "tricks"

- we plot the average stochastic reconstruction $||\mathbf{x}^{(t)} - \tilde{\mathbf{x}}||^2$ and see if it tends to decrease
- for inputs that correspond to image, we visualize the connection coming into each hidden unit as if it was an image
- gives an idea of the type of visual feature each hidden unit detects
- we can also try to approximate the partition function Z and see whether the (approximated) NLL decreases

(Salakhutdinov, Murray, ICML 2008)

Part II: Learning Deep Belief Networks (DBNs)

Deep Belief Network



Low-level features:
Edges

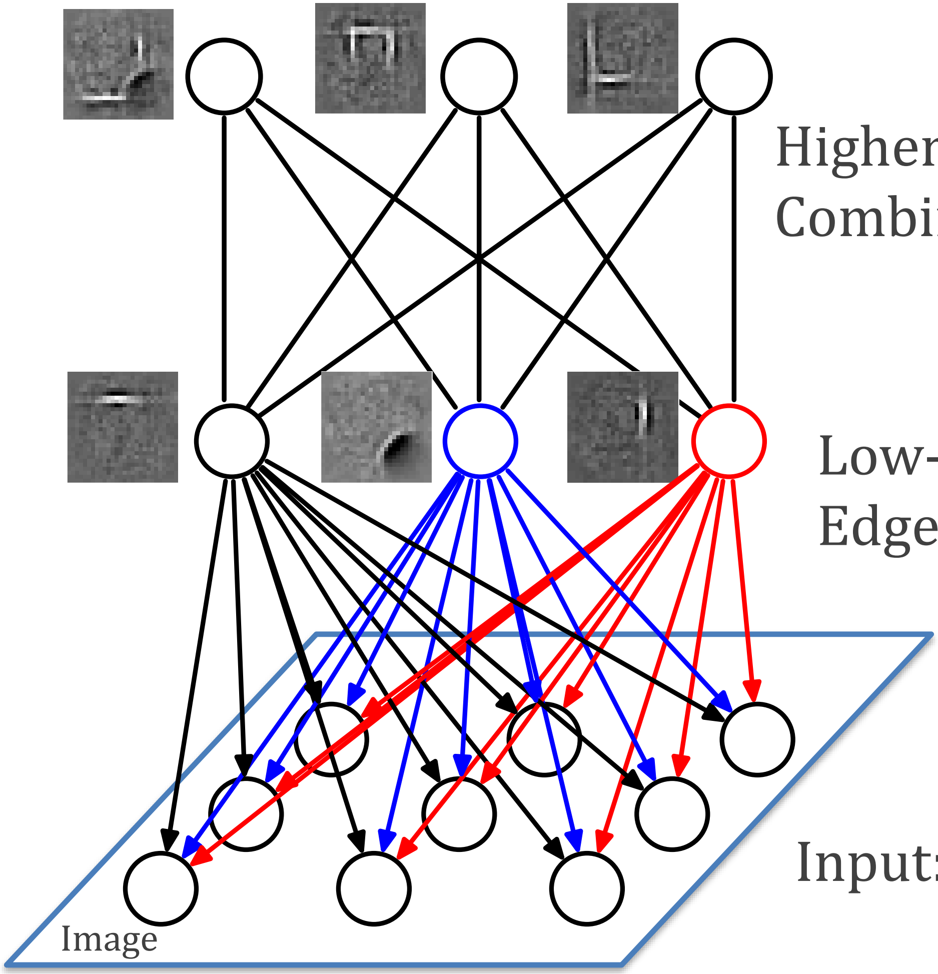
Built from **unlabeled** inputs.

Input: Pixels

(Hinton et.al. Neural Computation 2006)

Deep Belief Network

Internal representations capture higher-order statistical structure



Higher-level features:
Combination of edges

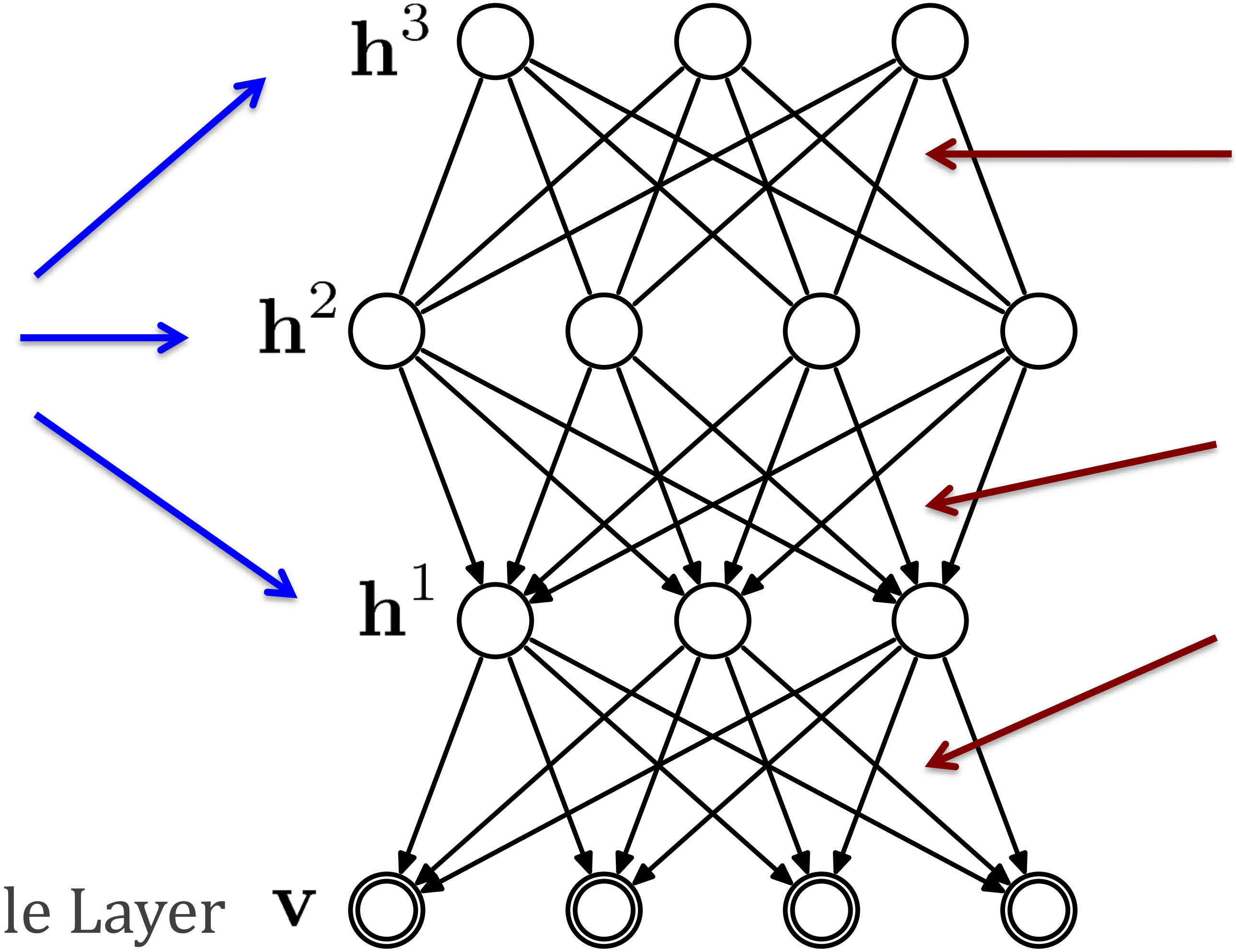
Low-level features:
Edges

Built from **unlabeled** inputs.

Input: Pixels

(Hinton et.al. Neural Computation 2006)

Deep Belief Network



Hidden Layers

RBM

Sigmoid Belief Network

Visible Layer

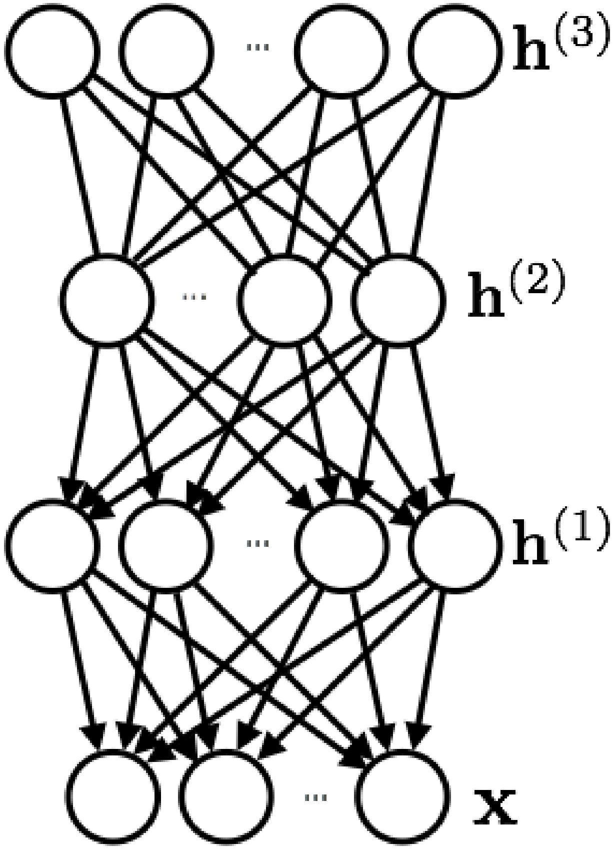
Deep Belief Network

Deep Belief Networks:

- it is a generative model that mixes undirected and directed connections between variables
- top 2 layers' distribution $p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)})$ is an RBM!
- other layers form a Bayesian network with conditional distributions:

$$p(h_j^{(1)} = 1|\mathbf{h}^{(2)}) = \mathrm{sigm}(\mathbf{b}^{(1)} + \mathbf{W}^{(2)}{}^\top \mathbf{h}^{(2)})$$

$$p(x_i = 1|\mathbf{h}^{(1)}) = \mathrm{sigm}(\mathbf{b}^{(0)} + \mathbf{W}^{(1)}{}^\top \mathbf{h}^{(1)})$$



Deep Belief Network

The joint distribution of a DBN is as follows

$$p(\mathbf{x}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)})\, p(\mathbf{h}^{(1)}|\mathbf{h}^{(2)})\, p(\mathbf{x}|\mathbf{h}^{(1)})$$

where

$$p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \exp\left(\mathbf{h}^{(2)}{}^{\top}\mathbf{W}^{(3)}\mathbf{h}^{(3)} + \mathbf{b}^{(2)}{}^{\top}\mathbf{h}^{(2)} + \mathbf{b}^{(3)}{}^{\top}\mathbf{h}^{(3)}\right)/Z$$

$$p(\mathbf{h}^{(1)}|\mathbf{h}^{(2)}) = \prod_j p(h_j^{(1)}|\mathbf{h}^{(2)})$$

$$p(\mathbf{x}|\mathbf{h}^{(1)}) = \prod_i p(x_i|\mathbf{h}^{(1)})$$

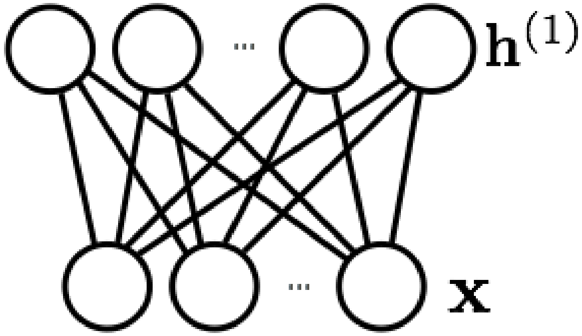
Why this odd parametrization?

Variational intuitions

Consider an RBM.

Let's write the marginal p(x) in terms of the Gibbs variational principle.

As $\mathrm{p(x)} = \sum_{\mathrm{h}^{(1)}} \mathrm{p(x, h^{(1)})}$ (i.e. a partition function of the model $\mathrm{p}\left(\mathrm{h}^{(1)}\right) \propto \mathrm{p(x, h^{(1)})}$), we have:



For every distribution $\mathrm{q}\left(\mathbf{h}^{(1)} \middle| \mathbf{x}\right)$:

$$\log p(\mathbf{x}) \geq \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{h}^{(1)}) - \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log q(\mathbf{h}^{(1)}|\mathbf{x})$$

Equality is attained if $\mathrm{q}\left(\mathbf{h}^{(1)} \middle| \mathbf{x}\right) = \mathrm{p}\left(\mathbf{h}^{(1)} \middle| \mathbf{x}\right)$.

In fact, LHS - RHS = $\mathrm{KL}(\mathrm{q}\left(\mathbf{h}^{(1)} \middle| \mathbf{x}\right) \middle| \middle| \mathrm{p}\left(\mathbf{h}^{(1)} \middle| \mathbf{x}\right)\big)$

Variational intuitions

Consider an RBM.

Let's write the marginal p(x) in terms of the Gibbs variational principle.

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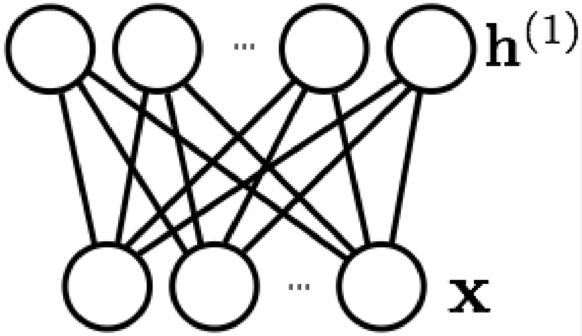


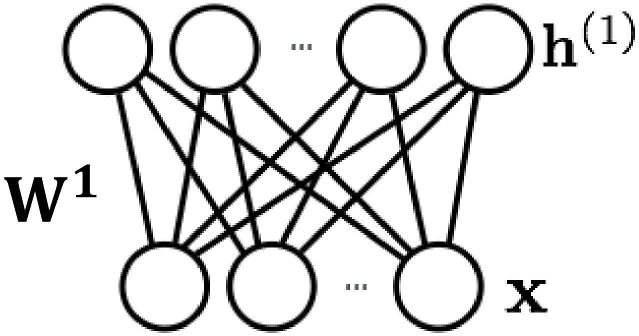
For every distribution $\mathrm{q}\left(\mathbf{h}^{(1)}\middle|\mathbf{x}\right)$:

$$\begin{aligned}\log p(\mathbf{x}) \quad &\geq \quad \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{h}^{(1)}) \\ &\quad - \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log q(\mathbf{h}^{(1)}|\mathbf{x})\end{aligned}$$

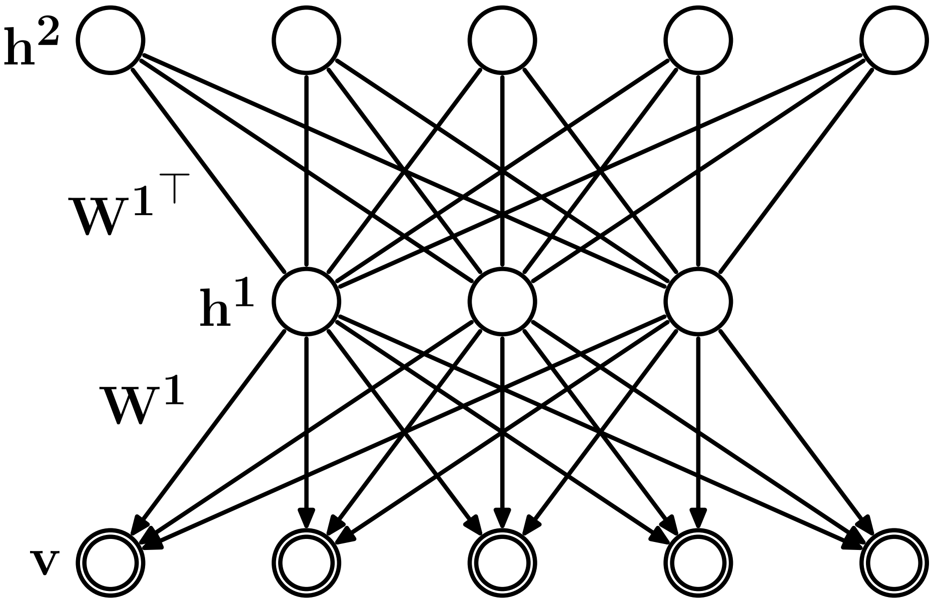
The idea will be to add layers, s.t. we improve the variational bound on the RHS.

Adding one layer

Observation: a two-layer DBN with appropriately tied weights is equivalent to an RBM:



$\Leftrightarrow$



$\mathbf{h}^{\mathbf{2}}$
$\mathbf{W}^{\mathbf{1}\top}$
$\mathbf{h}^{\mathbf{1}}$
$\mathbf{W}^{\mathbf{1}}$
$\mathbf{v}$

Formal proof is a little annoying. Intuition:

- Gibbs sampling converges to model distribution in first case.
- Gibbs sampling on top two layers, plus one last sample of x given $\mathrm{h}^{(1)}$ converges to model distribution in second.
- The steps in these two random walks are *exactly* the same.

Variational intuitions

adding 2nd layer means
untying the parameters

$$\begin{aligned}\log p(\mathbf{x}) \quad \geq \quad & \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \left(\log p(\mathbf{x}|\mathbf{h}^{(1)}) + \log p(\mathbf{h}^{(1)})\right) \\ & - \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log q(\mathbf{h}^{(1)}|\mathbf{x})\end{aligned}$$

- When adding a second layer, we model $p(\mathbf{h}^{(1)})$ using a separate set of parameters
  - ➢ they are the parameters of the RBM involving $\mathbf{h}^{(1)}$ and $\mathbf{h}^{(2)}$
  - ➢ $p(\mathbf{h}^{(1)})$ is now the marginalization of the second hidden layer

$$p(\mathbf{h}^{(1)}) = \sum_{\mathbf{h}^{(2)}} p(\mathbf{h}^{(1)}, \mathbf{h}^{(2)})$$

Variational intuitions

adding 2nd layer means
untying the parameters

$$\log p(\mathbf{x}) \geq \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \left(\log p(\mathbf{x}|\mathbf{h}^{(1)}) + \log p(\mathbf{h}^{(1)}) \right)$$
$$- \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log q(\mathbf{h}^{(1)}|\mathbf{x})$$

Layerwise training improves variational lower bound

- we can train the parameters o he
bound. This is equivalent to m .
terms are constant:

$$- \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log p(\mathbf{h}^{(1)})$$

- this is like training an RBM on data generated from $q(\mathbf{h}^{(1)}|\mathbf{x})$!

Variational intuitions

adding 2nd layer means
untying the parameters

$$\log p(\mathbf{x}) \geq \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \left(\log p(\mathbf{x}|\mathbf{h}^{(1)}) + \log p(\mathbf{h}^{(1)})\right)$$

$$- \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log q(\mathbf{h}^{(1)}|\mathbf{x})$$

- for $q(\mathbf{h}^{(1)}|\mathbf{x})$ we use **the posterior of the first layer RBM**. This is equivalent to a feed-forward (sigmoidal) layer, followed by sampling
- by initializing the weights of the second layer RBM as the transpose of the first layer weights, **the bound is initially tight!** (As we showed, a 2-layer DBN with tied weights is equivalent to a 1-layer RBM)
- Need not keep being tight:

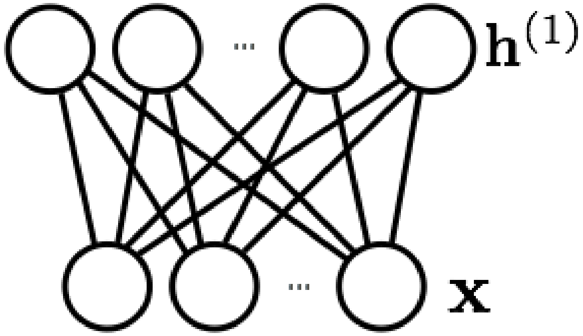
  as $p(\mathbf{h}^{(1)})$ changes, so does $\mathrm{p}(\mathbf{h}^{(1)}|\mathbf{x})$, and so does the KL to $\mathrm{q}(\mathbf{h}^{(1)}|\mathbf{x})$

Layer-wise Training

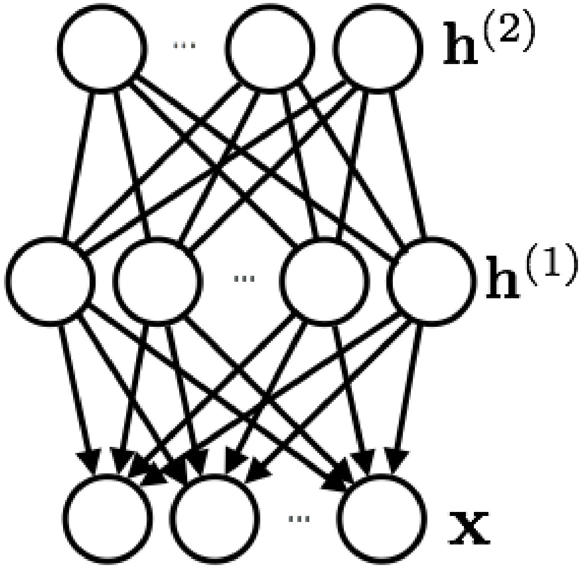
This is where the RBM stacking procedure comes from:

- **idea**: improve prior on last layer by adding another hidden layer

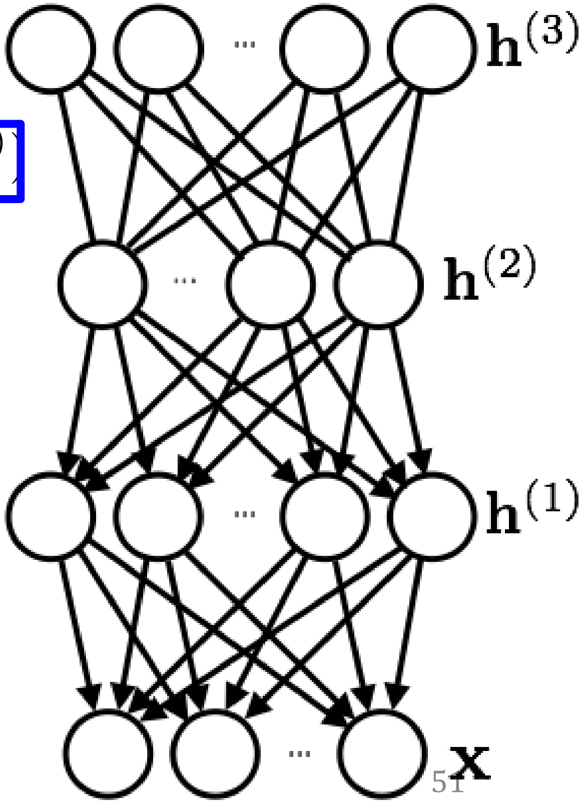
$$p(\mathbf{x}) = \sum_{\mathbf{h}^{(1)}} \boxed{p(\mathbf{x}, \mathbf{h}^{(1)})}$$



$$p(\mathbf{x}, \mathbf{h}^{(1)}) = p(\mathbf{x}|\mathbf{h}^{(1)}) \sum_{\mathbf{h}^{(2)}} \boxed{p(\mathbf{h}^{(1)}, \mathbf{h}^{(2)})}$$



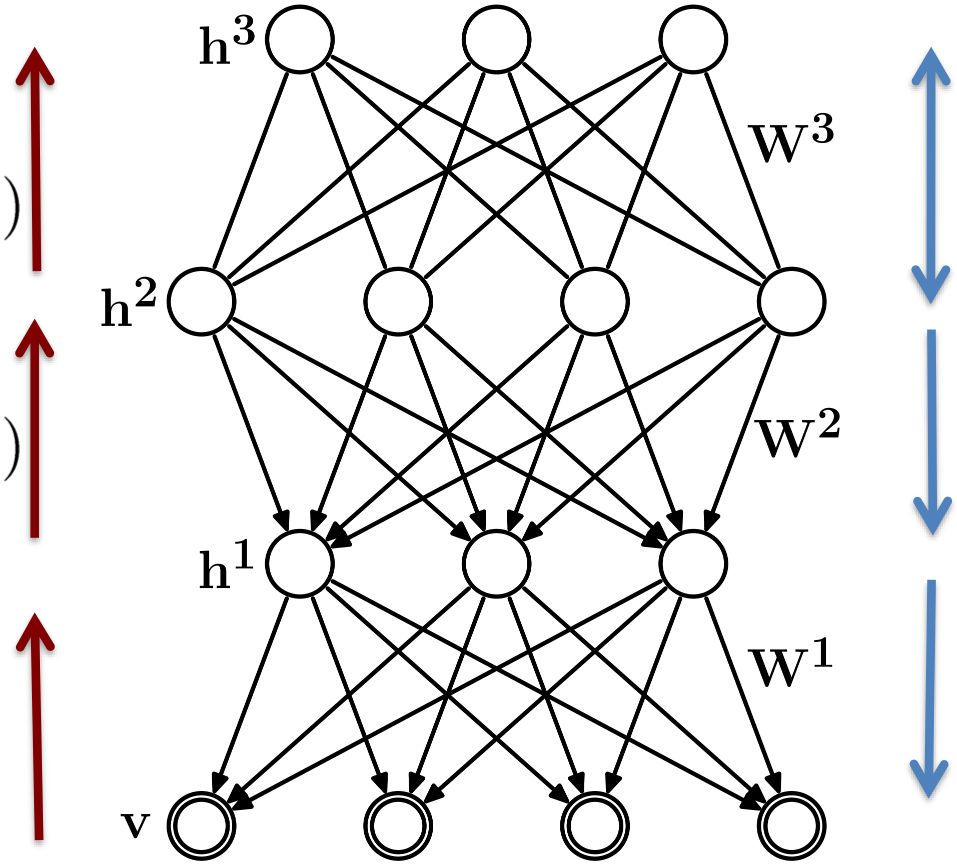
$$p(\mathbf{h}^{(1)}, \mathbf{h}^{(2)}) = p(\mathbf{h}^{(1)}|\mathbf{h}^{(2)}) \sum_{\mathbf{h}^{(3)}} p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)})$$



Deep Belief Network

Approximate Inference

Generative Process



$Q(\mathbf{h}^3|\mathbf{h}^2)$

$Q(\mathbf{h}^2|\mathbf{h}^1)$

$Q(\mathbf{h}^1|\mathbf{v})$

$P(\mathbf{h}^2, \mathbf{h}^3)$

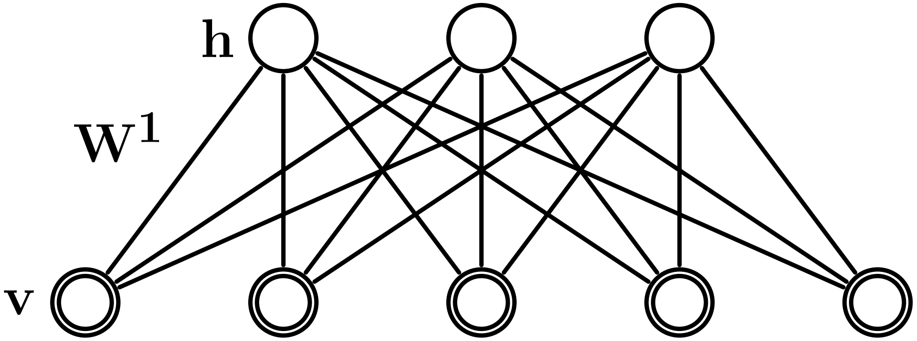
$P(\mathbf{h}^1|\mathbf{h}^2)$

$P(\mathbf{v}|\mathbf{h}^1)$

$$Q(\mathbf{h}^t|\mathbf{h}^{t-1}) = \prod_j \sigma\left(\sum_i W^t h_i^{t-1}\right) \qquad P(\mathbf{h}^{t-1}|\mathbf{h}^t) = \prod_j \sigma\left(\sum_i W^t h_i^t\right)$$

DBN Layer-wise Training

- Learn an RBM with an input layer v=x and a hidden layer h.

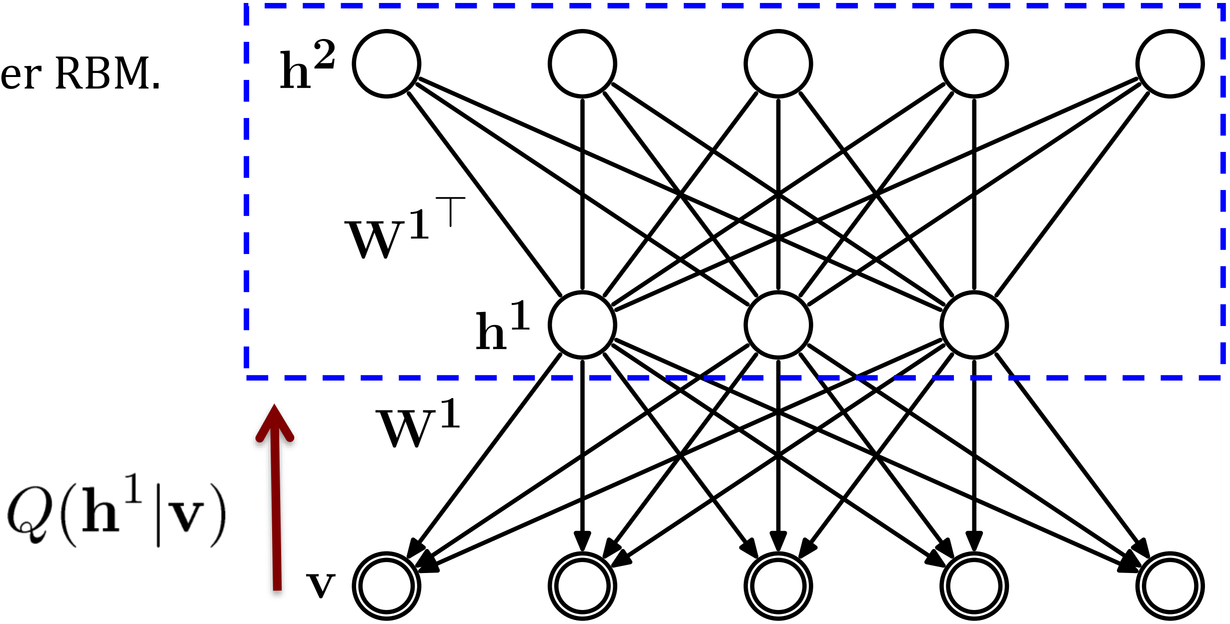


DBN Layer-wise Training

- Learn an RBM with an input layer v=x and a hidden layer h.

- Treat inferred values $Q(\mathbf{h}^1|\mathbf{v}) = P(\mathbf{h}^1|\mathbf{v})$ as the data for training 2nd-layer RBM.

- Learn and freeze 2nd layer RBM.



DBN Layer-wise Training

- Learn an RBM with an input layer v=x and a hidden layer h.

Unsupervised Feature Learning.

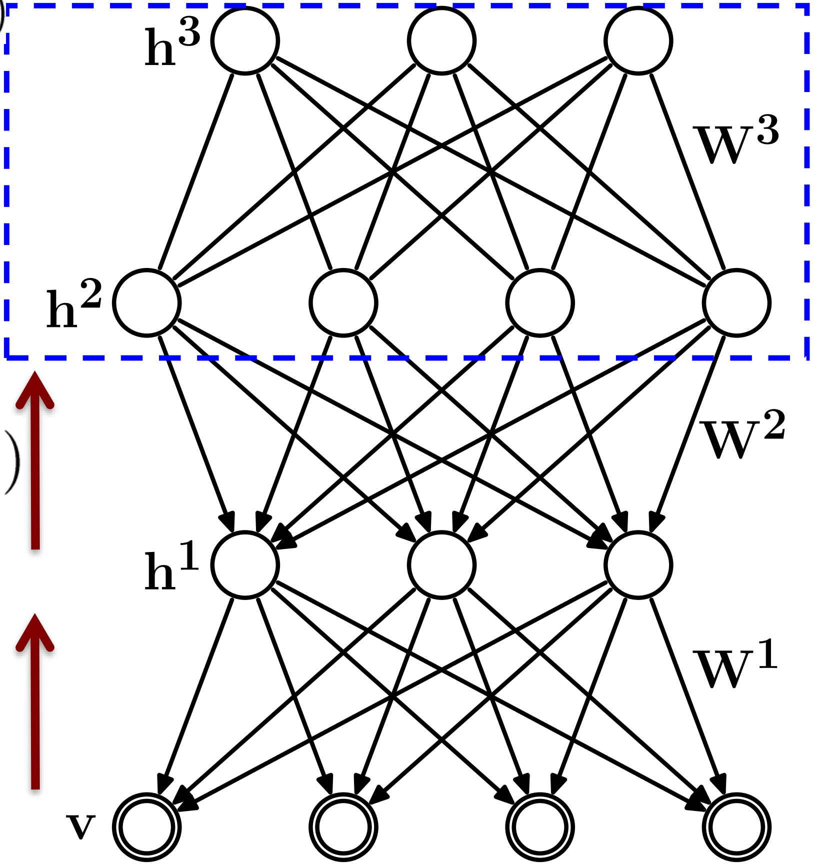
- Treat inferred values $Q(\mathbf{h}^1|\mathbf{v}) = P(\mathbf{h}^1|\mathbf{v})$ as the data for training 2nd-layer RBM.

- Learn and freeze 2nd layer RBM.

- Proceed to the next layer.

$Q(\mathbf{h}^2|\mathbf{h}^1)$

$Q(\mathbf{h}^1|\mathbf{v})$



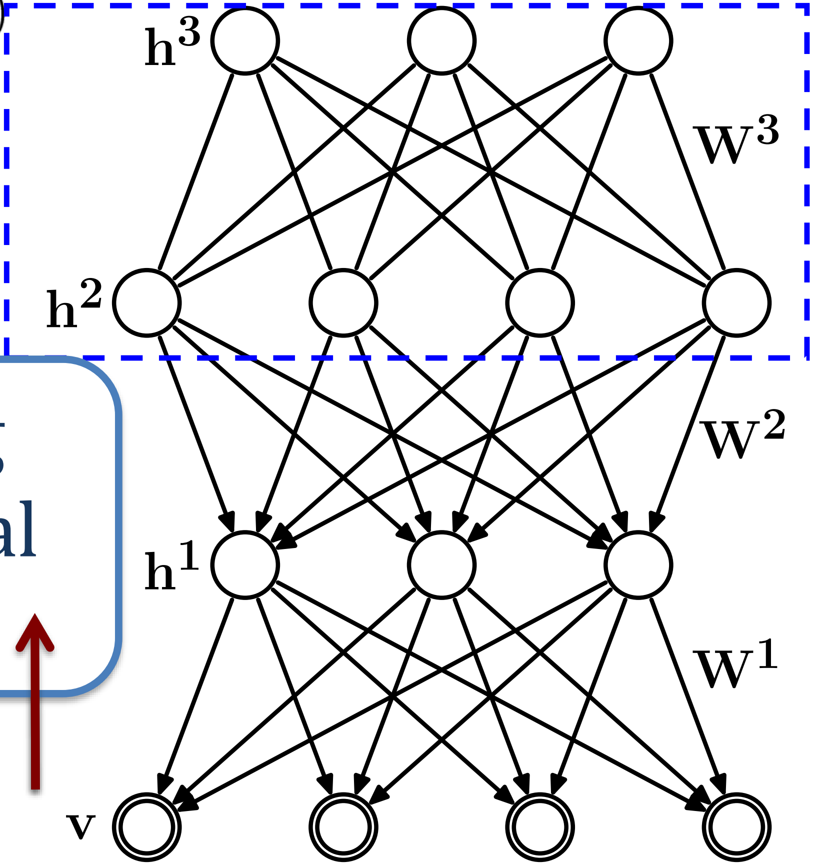
DBN Layer-wise Training

- Learn an RBM with an input layer v=x and a hidden layer h.

Unsupervised Feature Learning.

- Treat inferred values $Q(\mathbf{h}^1|\mathbf{v}) = P(\mathbf{h}^1|\mathbf{v})$ as the data for training 2nd-layer RBM.
- Learn and freeze 2nd layer RBM.
- Proce

Layerwise training improves variational lower bound



$Q(\mathbf{h}^1|\mathbf{v})$

Deep Belief Networks

This process of adding layers can be repeated recursively

- we obtain the greedy layer-wise pre-training procedure for neural networks

We now see that this procedure corresponds to maximizing a bound on the likelihood of the data in a DBN

- in theory, if our approximation $q(\mathbf{h}^{(1)}|\mathbf{x})$ is very far from the true posterior, the bound might be very loose
- this only means we might not be improving the true likelihood
- we might still be extracting better features!

Fine-tuning is done by the Up-Down algorithm

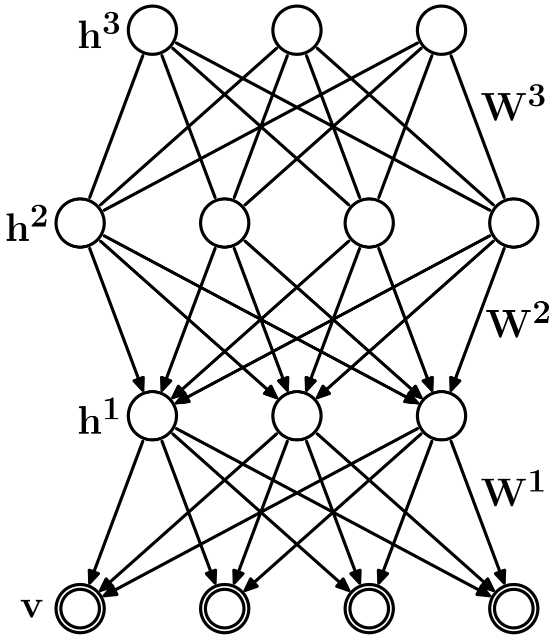
- A fast learning algorithm for deep belief nets. Hinton, Teh, Osindero, 2006.

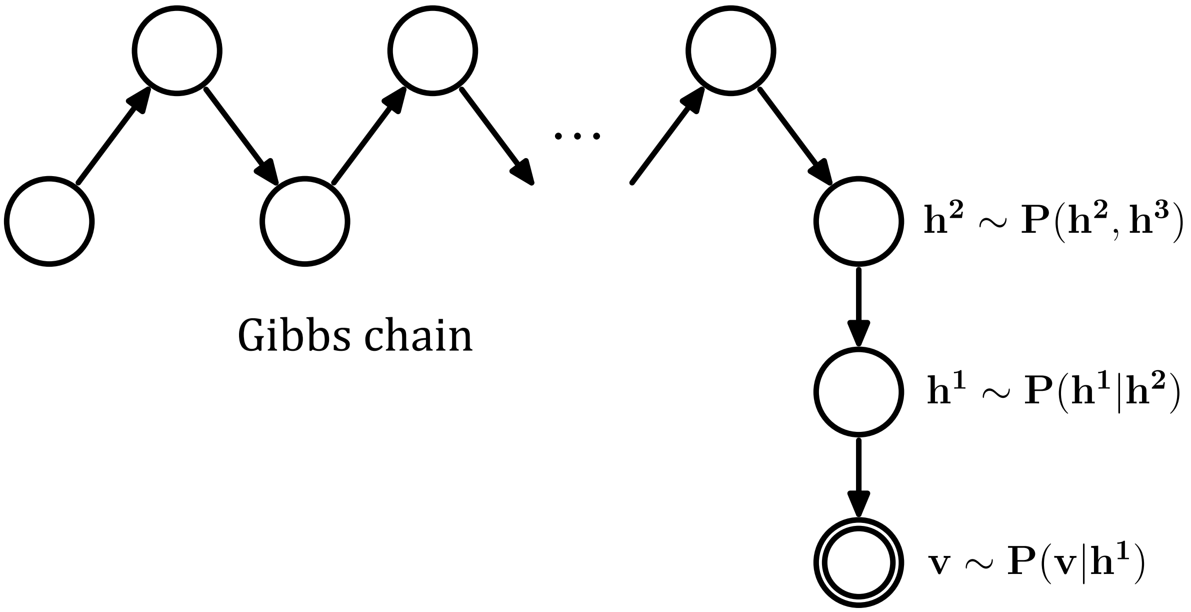
Sampling from DBNs

- To sample from the DBN model:

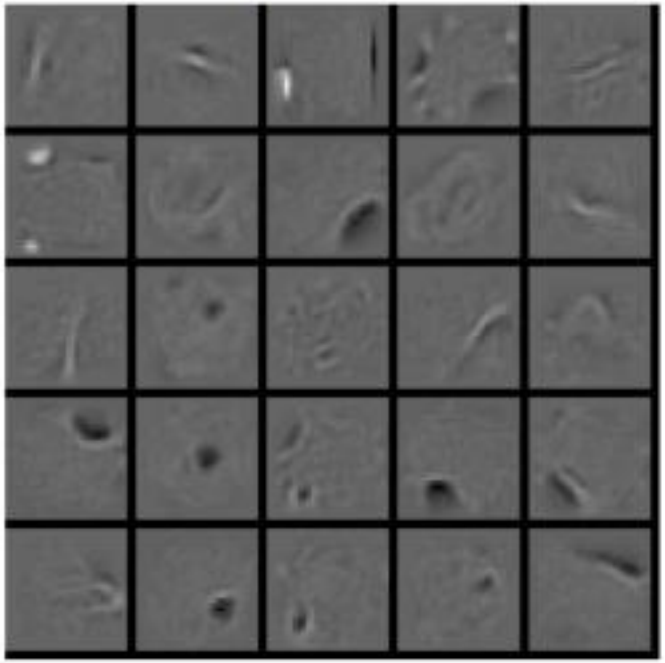
$$P(\mathbf{v}, \mathbf{h}^1, \mathbf{h}^2, \mathbf{h}^3) = P(\mathbf{v}|\mathbf{h}^1)P(\mathbf{h}^1|\mathbf{h}^2)P(\mathbf{h}^2, \mathbf{h}^3)$$

- Sample h^2 using alternating Gibbs sampling from RBM.
- Sample lower layers using sigmoid belief network.

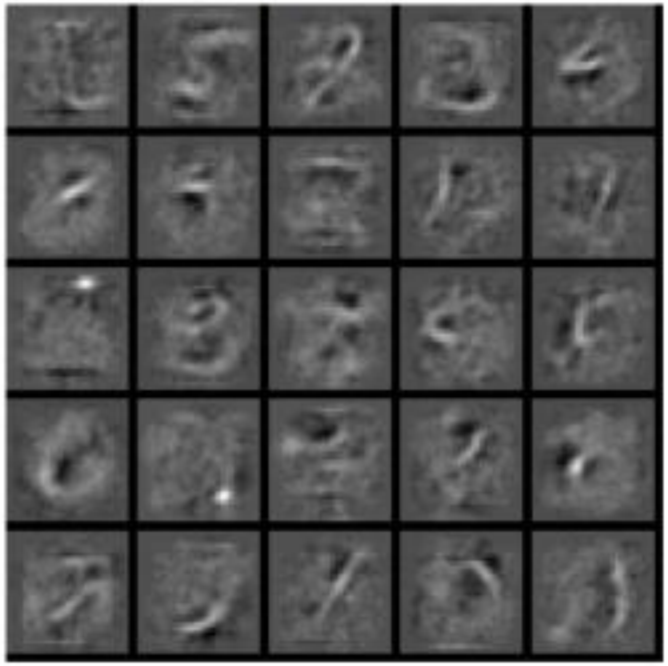



...
$\mathbf{h}^2 \sim \mathbf{P}(\mathbf{h}^2, \mathbf{h}^3)$
Gibbs chain
$\mathbf{h}^1 \sim \mathbf{P}(\mathbf{h}^1|\mathbf{h}^2)$
$\mathbf{v} \sim \mathbf{P}(\mathbf{v}|\mathbf{h}^1)$

Learned Features



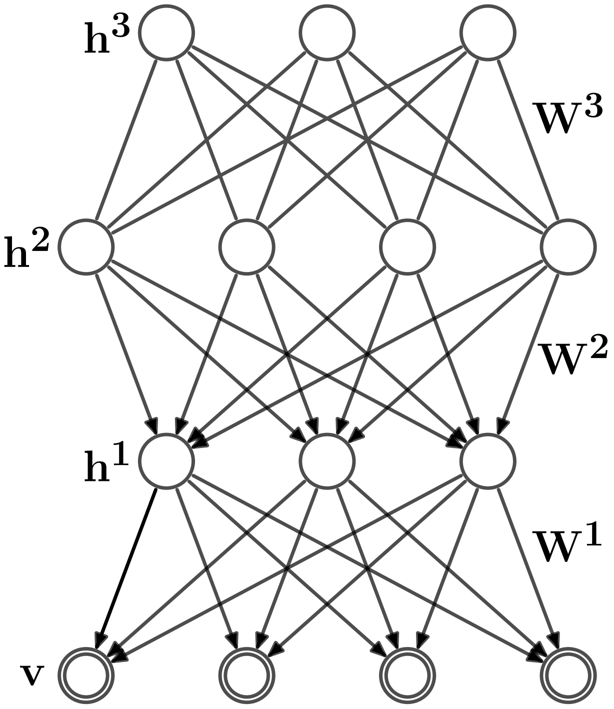
1^{st}-layer features



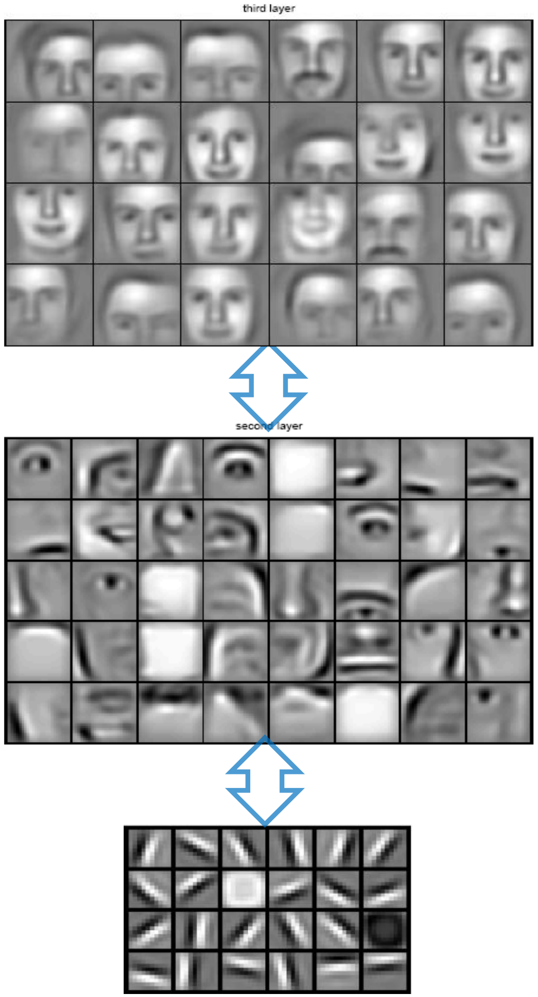
2^{nd}-layer features

Learning Part-based Representation

Convolutional DBN



Faces



Groups of parts.

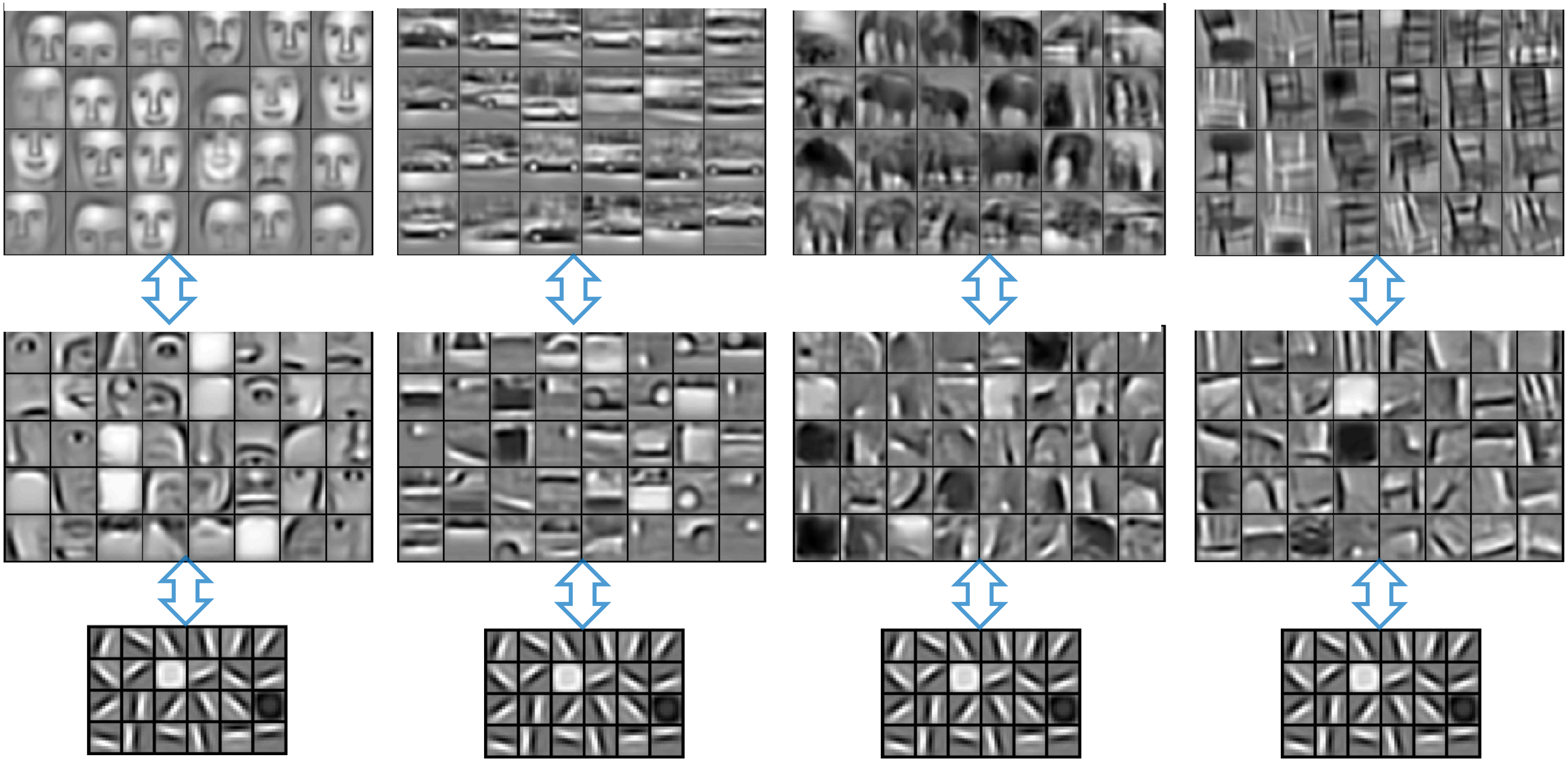
Object Parts

Trained on face images.

Lee et.al., ICML 2009

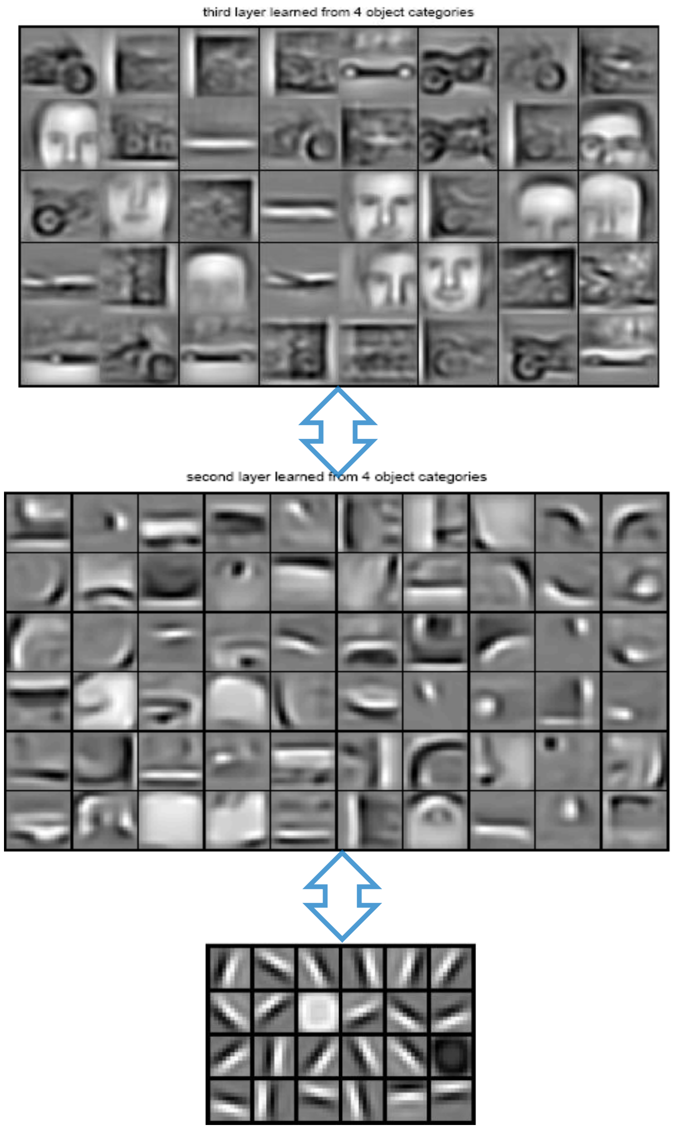
Learning Part-based Representation

Faces Cars Elephants Chairs



Lee et.al., ICML 2009

Learning Part-based Representation


third layer learned from 4 object categories
second layer learned from 4 object categories

Groups of parts.

Class-specific object parts

Trained from multiple classes (cars, faces, motorbikes, airplanes).

Lee et.al., ICML 2009