

10417-617
Deep Learning: Fall 2020

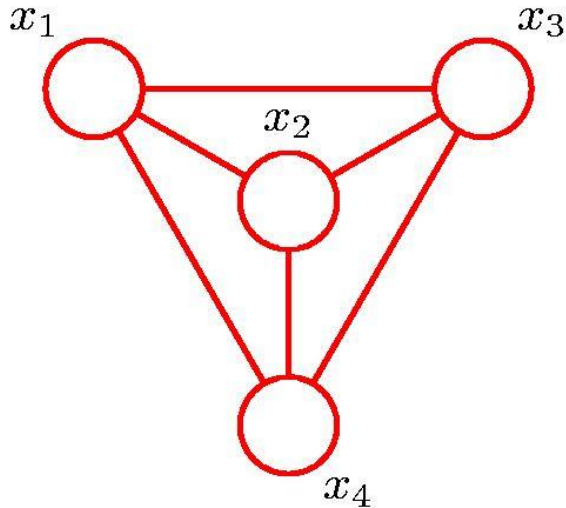
Andrej Risteski

Machine Learning Department

Lecture 13:
Variational methods, applications to
learning latent-variable
directed models

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

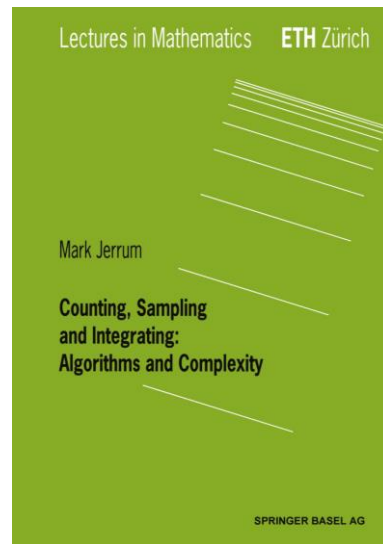
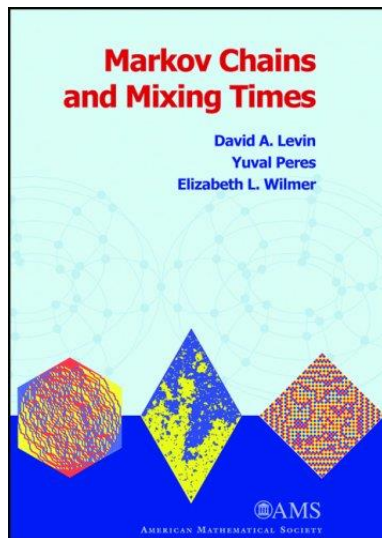
- ⌘ Easy to draw samples 
- ⌘ Hard to sample posterior distribution over latents 
(In fact, #P-hard even in mixtures)

Algorithmic approaches

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

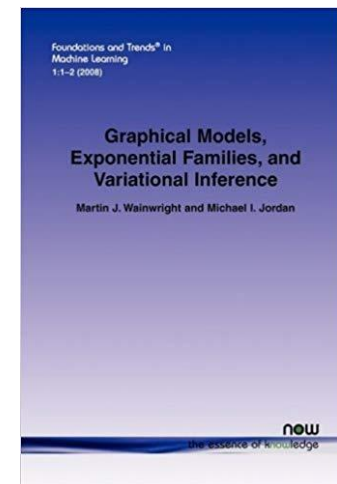
MARKOV CHAIN MONTE CARLO

❖ **Random walk** w/ equilibrium distribution the one we are trying to sample from.



VARIATIONAL METHODS

❖ Based on solving an **optimization** problem.



Part I: approximating posteriors via variational methods

Sampling posteriors in latent-variable directed models

Recall, sampling from the **posterior distribution** $P(z|x)$ is **hard**:



Up to
normalizing
const, simple...

Complicated partition function:

$$\sum_{\text{Diseases}} P(\text{Diseases}, \text{Symptoms})$$

Again, can be #P-hard to sample from!!

Variational methods for approximating posteriors

Gibbs variational principle: Let $p(z, x)$ be a joint distribution over latent variables and observables. Then,

$$p(z|x) = \operatorname{argmax}_{q(z|x): \text{distribution over } Z} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x) \}$$
$$-H(q(z|x)) \quad - \quad \mathbb{E}_{z \sim q} [\log p(z, x)]$$

In fact, for every $q(z|x)$, we have

$$\log p(x) = -(-H(q(z|x)) - \mathbb{E}_{z \sim q} [\log p(z, x)]) + KL(q(z|x) || p(z|x))$$

Variational methods for partition functions

Gibbs variational principle: Let $p(z, x)$ be a joint distribution over latent variables and observables. Then,

$$p(z|x) = \underset{q(z|x): \text{distribution over } Z}{\operatorname{argmax}} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$

In fact, for every $q(z|x)$, we have

$$\log p(x) = KL(q(z|x) || p(z|x)) - (-H(q(z|x)) - \mathbb{E}_{z \sim q}[\log p(z, x)])$$

Why:

$$\begin{aligned} 0 \leq KL(q(z|x) || p(z|x)) &= \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z|x) \\ &= -H(q(z|x)) - \mathbb{E}_{q(z|x)} \log \frac{p(z, x)}{p(x)} \\ &= -H(q(z|x)) - \mathbb{E}_{q(z|x)} \log p(z, x) + \log p(x) \end{aligned}$$

Equality is attained if and only if $KL(q(z|x) || p(z|x))=0$ i. e. $q(z|x) = p(z|x)$

Variational methods for approximating posteriors

Gibbs variational principle: Let $p(z, x)$ be a joint distribution over latent variables and observables. Then,

$$p(z|x) = \operatorname{argmax}_{q(z|x): \text{distribution over } Z} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$
$$\log p(x) = -(-H(q(z|x)) - \mathbb{E}_{z \sim q}[\log p(z, x)]) + KL(q(z|x) || p(z|x))$$

Why is this useful?

(1) Instead of finding the argmax over **all** distributions over Z , we can maximize over some **simpler** parametric family \mathcal{Q} , i.e. we can solve

$$\max_{q(z|x) \in \mathcal{Q}} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$

The argmax of the above distribution solves $\min_{q(z|x) \in \mathcal{Q}} KL(q(z|x) || p(z|x))$.

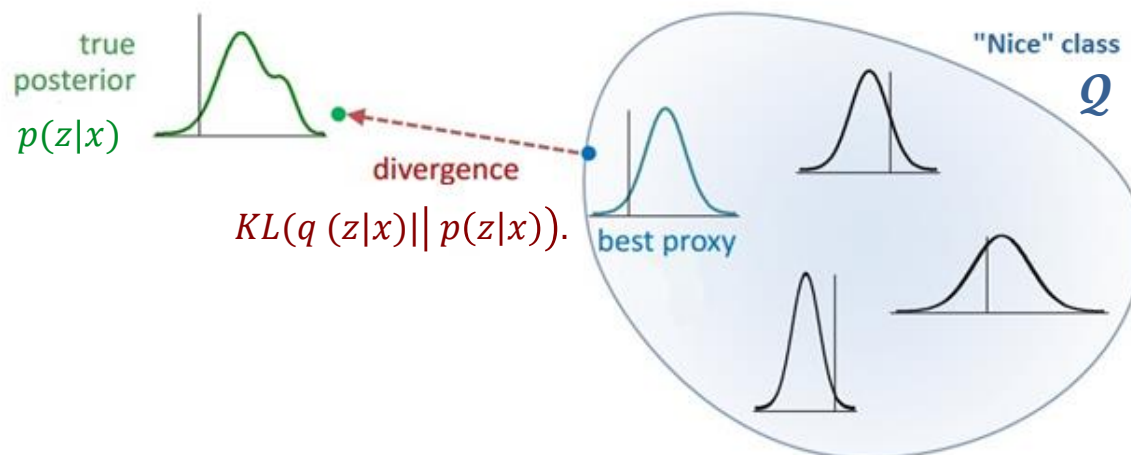
In other words, we are finding the **projection** of $p(z|x)$ onto \mathcal{Q} .

Variational methods for approximating posteriors

Gibbs variational principle: Let $p(z, x)$ be a joint distribution over latent variables and observables. Then,

$$p(z|x) = \operatorname{argmax}_{q(z|x): \text{distribution over } Z} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$

$$\log p(x) = -(-H(q(z|x)) - \mathbb{E}_{z \sim q}[\log p(z, x)]) + KL(q(z|x) || p(z|x))$$



Variational methods for approximating posteriors

Gibbs variational principle: Let $p(z, x)$ be a joint distribution over latent variables and observables. Then,

$$p(z|x) = \operatorname{argmax}_{q(z|x): \text{distribution over } Z} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$
$$\log p(x) = -(-H(q(z|x)) - \mathbb{E}_{z \sim q}[p(z, x)]) + KL(q(z|x) || p(z|x))$$

Why is this useful?

(1) Instead of finding the argmax over **all** distributions over Z , we can maximize over some **simpler** parametric family \mathcal{Q} , i.e. we can solve

$$\max_{q(z|x) \in \mathcal{Q}} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$

There are several common families \mathcal{Q} that are used for which the above optimization is solveable – we will see **mean-field** family today, **neural-net** parametrized families when we study variational autoencoders.

Variational methods for approximating posteriors

Gibbs variational principle: Let $p(z, x)$ be a joint distribution over latent variables and observables. Then,

$$p(z|x) = \operatorname{argmax}_{q(z|x): \text{distribution over } Z} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$
$$\log p(x) = -(-H(q(z|x)) - \mathbb{E}_{z \sim q}[p(z, x)]) + KL(q(z|x) || p(z|x))$$

Why is this useful?

(2) Provides a lower bound on $\log p(x)$ -- sometimes called the **ELBO (evidence lower bound)**, since

$$\log p(x) \geq \max_{q(z|x) \in \mathcal{Q}} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$

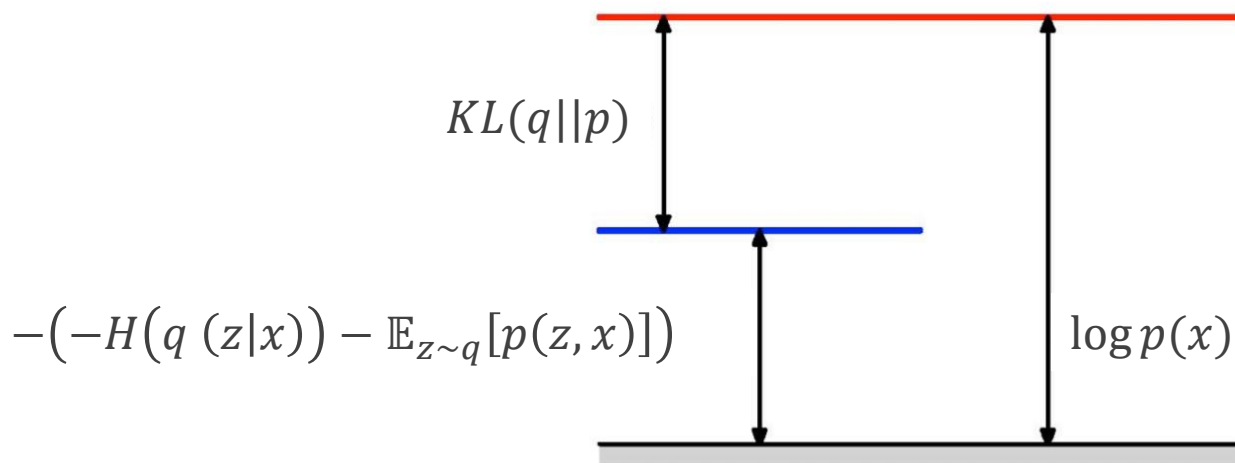
This will be useful when learning latent-variable directed models (stay tuned !).

Variational methods for approximating posteriors

Gibbs variational principle: Let $p(z, x)$ be a joint distribution over latent variables and observables. Then,

$$p(z|x) = \operatorname{argmax}_{q(z|x): \text{distribution over } Z} \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x)$$

$$\log p(x) = -(-H(q(z|x)) - \mathbb{E}_{z \sim q}[p(z, x)]) + KL(q(z|x) || p(z|x))$$



Solving the mean-field relaxation: coordinate ascent

Inspiration from physics: consider the case where \mathcal{Q} contains product distributions, that is, for every $q(\cdot | x) \in \mathcal{Q}$:

$$q(z|x) = \prod_{i=1}^d q_i(z_i|x).$$

Consider updating a **single** coordinate of the mean-field distribution, that is keep $q_{-i}(z_i|x)$ fixed, and optimize for $q_i(z_i|x)$. We have:

$$\begin{aligned} KL(q(z|x) || p(z|x)) &= \mathbb{E}_{q(z|x)} \log q(z|x) - \mathbb{E}_{q(z|x)} \log p(z, x) \\ &= \sum_i \mathbb{E}_{q_i(z_i|x)} \log q_i(z_i|x) - \mathbb{E}_{q_i(z_i|x)} \left[\mathbb{E}_{q_{-i}(z_{-i}|x)} \log p(z_i, z_{-i}, x) \right] \\ &= \mathbb{E}_{q_i(z_i|x)} \log q_i(z_i|x) - \mathbb{E}_{q_i(z_i|x)} [\log \tilde{p}(z_i, x)] + C \end{aligned}$$

Renormalize to make it a distribution

Solving the mean-field relaxation: coordinate ascent

Inspiration from physics: consider the case where \mathcal{Q} contains product distributions, that is, for every $q(\cdot | x) \in \mathcal{Q}$:

$$q(z|x) = \prod_{i=1}^d q_i(z_i|x).$$

Consider updating a **single** coordinate of the mean-field distribution, that is keep $q_{-i}(z_{-i}|x)$ fixed, and optimize for $q_i(z_i|x)$. We have:

$$KL(q(z|x) || p(z|x)) = \mathbb{E}_{q_i(z_i|x)} \log q_i(z_i|x) - \mathbb{E}_{q_i(z_i|x)} [\log \tilde{p}(z_i, x)] + C$$

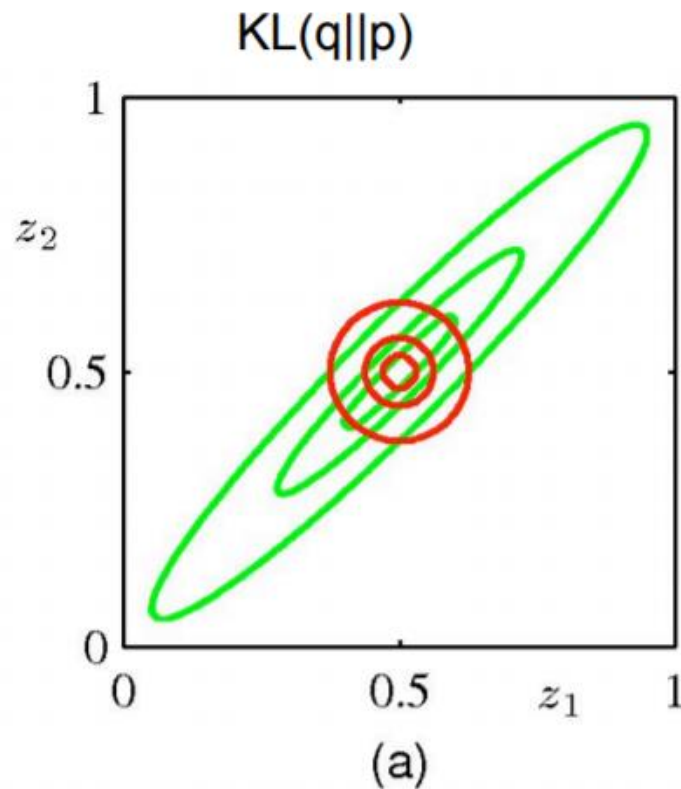
$$= KL(q_i(z_i|x) || \tilde{p}(z_i, x)) + C$$

Optimum is $q_i(z_i|x) = \tilde{p}(z_i, x)$

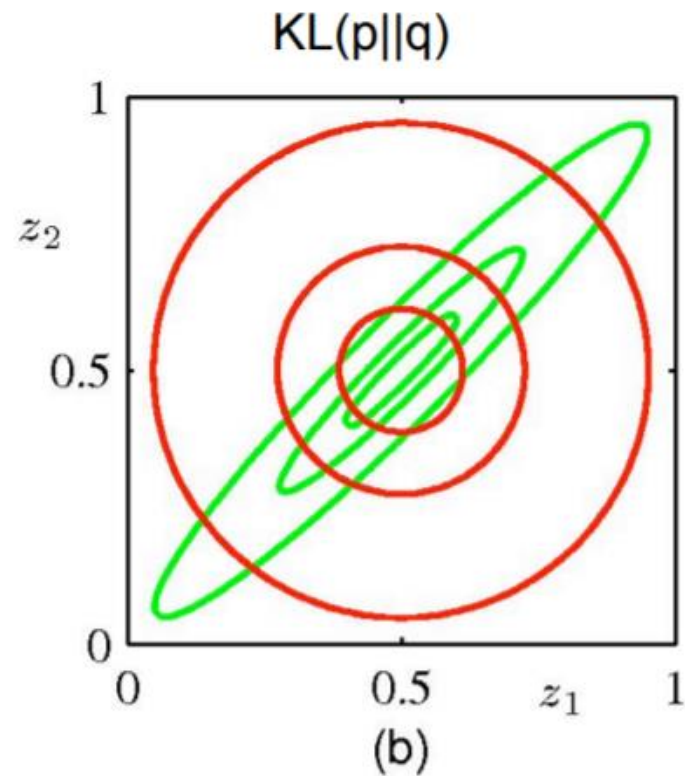
$$= \frac{\mathbb{E}_{q_{-i}(z_{-i}|x)} \log p(z_i, z_{-i}, x)}{\int_{z_i} \mathbb{E}_{q_{-i}(z_{-i}|x)} \log p(z_i, z_{-i}, x)}$$

Coordinate ascent: iterate above updates!

What if we changed the order of p, q in KL divergence?



Approximation is too compact.



Approximation is too spread.

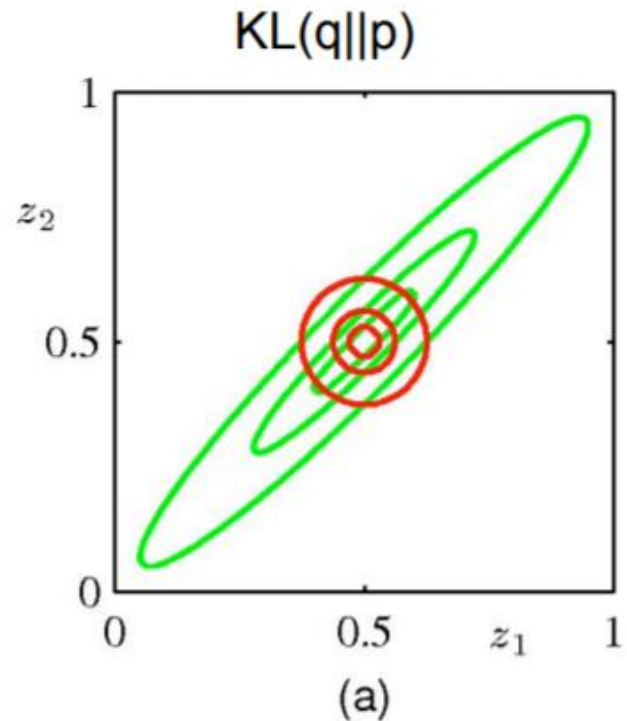
What if we changed the order of p, q in KL divergence?

$$\text{KL}(q||p) = - \int q(\mathbf{Z}) \ln \frac{p(\mathbf{Z})}{q(\mathbf{Z})} d\mathbf{Z}.$$

There is a large positive contribution to the KL divergence from regions of \mathbf{Z} space in which:

- $p(\mathbf{Z})$ is near zero
- unless $q(\mathbf{Z})$ is also close to zero.

Minimizing $\text{KL}(q||p)$ leads to distributions $q(\mathbf{Z})$ that **avoid regions in which $p(\mathbf{Z})$ is small.**



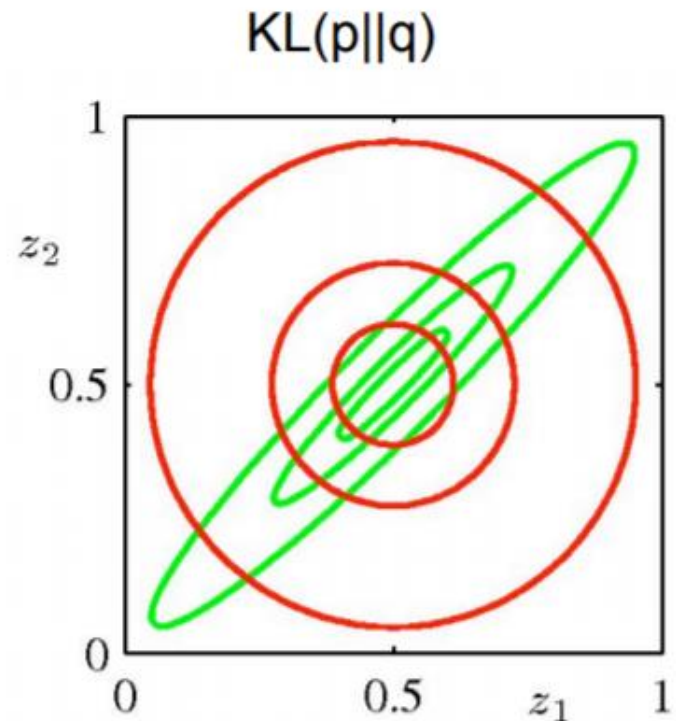
What if we changed the order of p, q in KL divergence?

$$\text{KL}(p||q) = - \int p(\mathbf{Z}) \ln \frac{q(\mathbf{Z})}{p(\mathbf{Z})} d\mathbf{Z}.$$

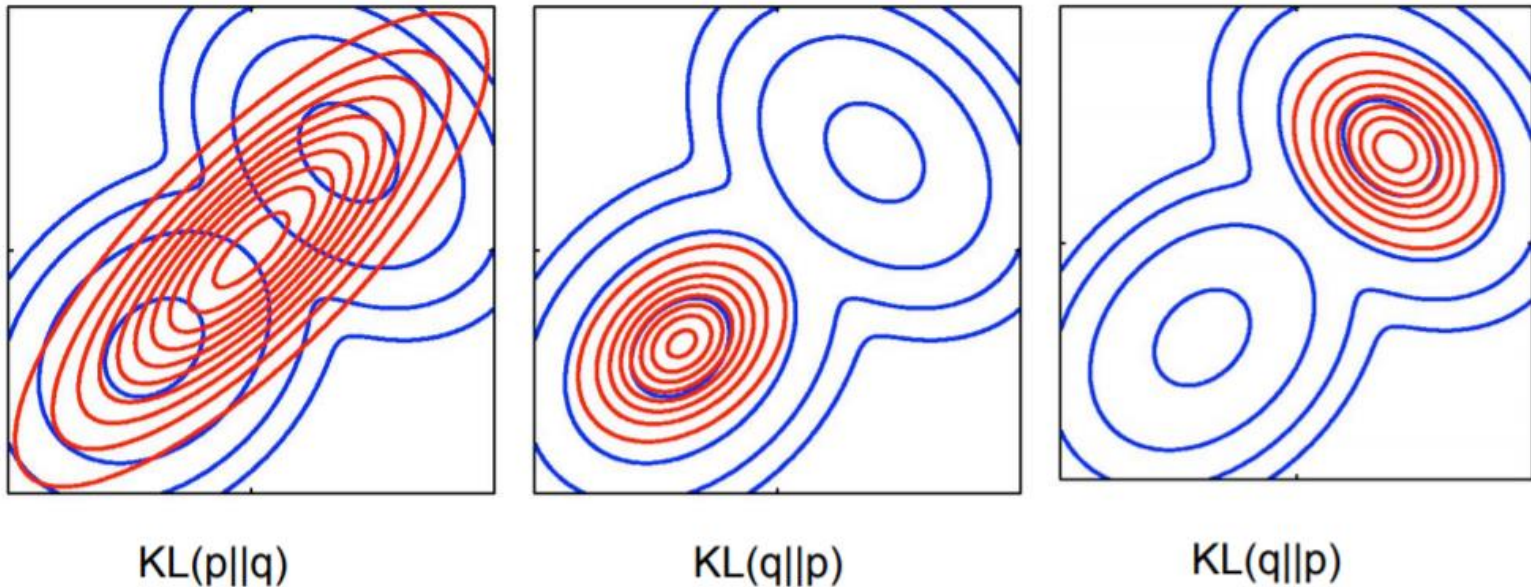
There is a large positive contribution to the KL divergence from regions of \mathbf{Z} space in which:

- $q(\mathbf{Z})$ is near zero,
- unless $p(\mathbf{Z})$ is also close to zero.

Minimizing $\text{KL}(p||q)$ leads to distributions $q(\mathbf{Z})$ that **are nonzero in regions where $p(\mathbf{Z})$ is nonzero.**



What happens when posterior class is not rich enough?



Blue contours show bimodal distribution, red contours single Gaussian distribution that best approximates it.

$KL(q||p)$ will tend to find a single mode, whereas $KL(p||q)$ will average across all of the modes.

Part II: learning latent-variable directed models

Learning latent-variable directed graphical models

How should we try to learn the parameters of a graphical model?

The most obvious strategy: maximum likelihood estimation

Given data x_1, x_2, \dots, x_n , solve the optimization problem

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

Latent variables: we will use the Gibbs variational principle again!

$$\log_{\theta} p(x) = \max_{q(z|x): \text{distribution over } \mathcal{Z}} H(q(z|x)) + \mathbb{E}_{q(z|x)}[\log p_{\theta}(x, z)]$$

Hence, MLE objective can be written as double maximization:

$$\max_{\theta \in \Theta} \max_{\{q_i(z|x_i)\}} \sum_{i=1}^n H(q_i(z|x_i)) + \mathbb{E}_{q_i(z|x_i)}[\log p_{\theta}(x_i, z)]$$

Expectation-maximization/ variational inference

The canonical algorithm for learning a single-layer latent-variable Bayesian network is an iterative algorithm as follows.

Consider the max-likelihood objective, rewritten as in the previous slide:

$$\max_{\theta \in \Theta} \max_{\{q_i(z|x_i) \in \mathcal{Q}\}} \sum_{i=1}^n H(q_i(z|x_i)) + \mathbb{E}_{q_i(z|x_i)}[\log p_{\theta}(x_i, z)]$$

Algorithm maintains iterates $\theta^t, \{q_i^t(z|x_i)\}$, and updates them iteratively

(1) Expectation (E)-step:

Keep θ^t fixed, set $\{q_i^{t+1}(z|x_i) \in \mathcal{Q}\}$, s.t. they maximize the objective above.

(2) Maximization (M)-step:

Keep $\{q_i^t(z|x_i)\}$ fixed, set θ^{t+1} s.t. it maximizes the objective above.

Clearly, every step cannot make the objective worse!

Does *not* mean it converges to global optimum – could, e.g. get stuck in a local minimum.

Expectation-maximization/ variational inference

The canonical algorithm for learning a single-layer latent-variable Bayesian network is an iterative algorithm as follows.

Consider the max-likelihood objective, rewritten as in the previous slide:

$$\max_{\theta \in \Theta} \max_{q_i(z|x_i)} \sum_{i=1}^n H(q_i(z|x_i)) + \mathbb{E}_{q_i(z|x_i)}[\log p_{\theta}(x_i, z)]$$

Algorithm maintains iterates $\theta^t, q_i^t(z|x_i)$, and updates them iteratively

(1) Expectation step:

Keep θ^t and set $q_i^{t+1}(z|x_i)$, s.t. they maximize the objective above.

If the class is infinitely rich, the optimum is $q_i^{t+1}(z|x_i) = p_{\theta^t}(z|x_i)$

This is called **expectation-maximization (EM)**.
If class is not infinitely rich, it's called **variational inference**.

Examples

1: Mixtures of spherical Gaussians

Consider a mixture of K Gaussians with unknown means $p = \sum_{i=1}^K \frac{1}{K} \mathcal{N}(\mu_i, I_d)$

Let's try to calculate the E and M steps.


E-step: the optimal $q_i^{t+1}(z|x_i)$ is $p_{\theta^t}(z|x_i)$. Can we calculate this?

By Bayes rule, $p_{\theta^t}(z = k|x_i) \propto p(x_i|z = k) \propto e^{-\|x_i - \mu_k^t\|^2}$

Writing out the normalizing constant, we have

$$p_{\theta^t}(z = k|x_i) = \frac{e^{-\|x_i - \mu_k^t\|^2}}{\sum_{k'} e^{-\|x_i - \mu_{k'}^t\|^2}}$$

*“Soft” version of assigning
point to nearest cluster*



Examples


1: Mixtures of spherical Gaussians

Consider a mixture of K Gaussians with unknown means $p = \sum_{i=1}^K \frac{1}{K} \mathcal{N}(\mu_i, I_d)$

Let's try to calculate the E and M steps.

M-step: given a guess $q_i^t(z|x_i)$, we can rewrite the maximization for θ as:

$$\max_{\theta \in \Theta} \sum_{i=1}^n H(q_i^t(z|x_i)) + \mathbb{E}_{q_i^t(z|x_i)} [\log p_{\theta}(x_i, z)]$$



$$= \mathbb{E}_{q_i^t(z|x_i)} [\log q_i^t(z|x_i) + \log p_{\theta}(x|z)]$$
$$\mathbb{E}_{q_i^t(z|x_i)} [\log p_{\theta}(x|z)]$$

Doesn't depend on θ

Examples

1: Mixtures of spherical Gaussians

Consider a mixture of K Gaussians with unknown means $p = \sum_{i=1}^K \frac{1}{K} \mathcal{N}(\mu_i, I_d)$

Let's try to calculate the E and M steps.

M-step: given a guess $q_i^t(z|x_i)$, we can rewrite the maximization for θ as:

$$\max_{\theta} \mathbb{E}_{q_i^t(z|x_i)} [\log p_{\theta}(x|z)] = \max_{\theta} - \sum_{i=1}^n \sum_{k=1}^K q_i^t(z = k|x_i) \|x_i - \mu_k\|^2$$

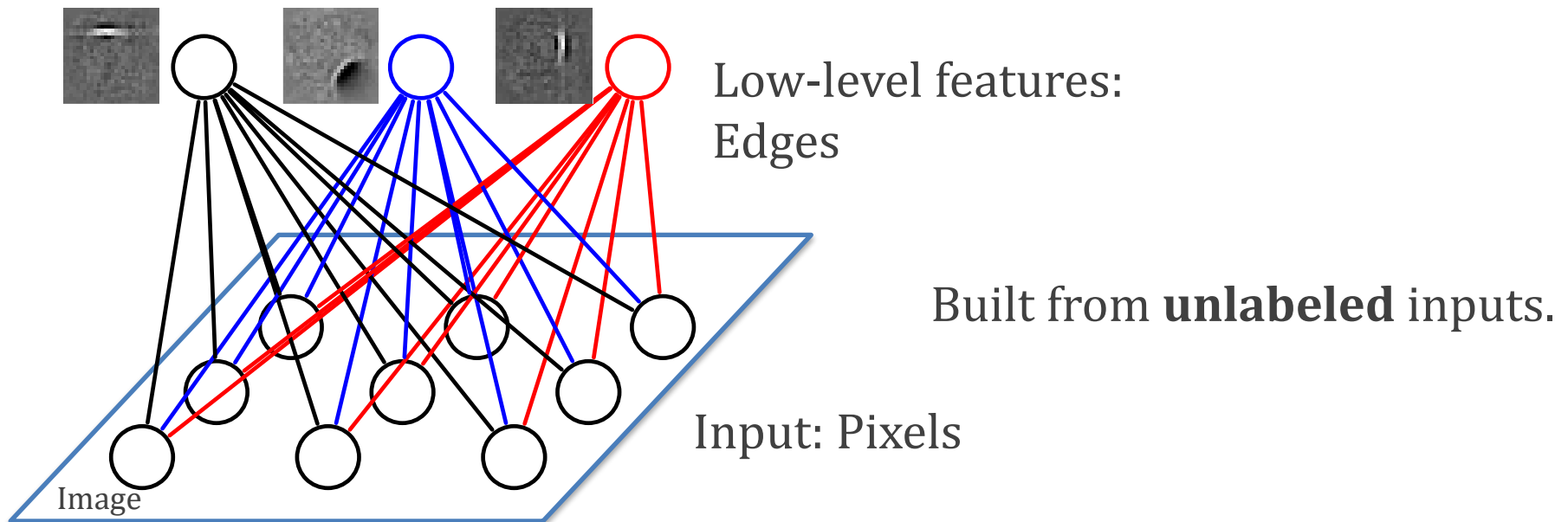
Setting the derivative wrt
to μ_k to 0, we have:

$$\mu_k^{t+1} = \sum_{i=1}^n \frac{e^{-\|x_i - \mu_k^t\|^2}}{\sum_{k'} e^{-\|x_i - \mu_{k'}^t\|^2}} x_i$$

*Average points,
weighing nearby
points more*

Part III: Deep Belief Networks (DBNs)

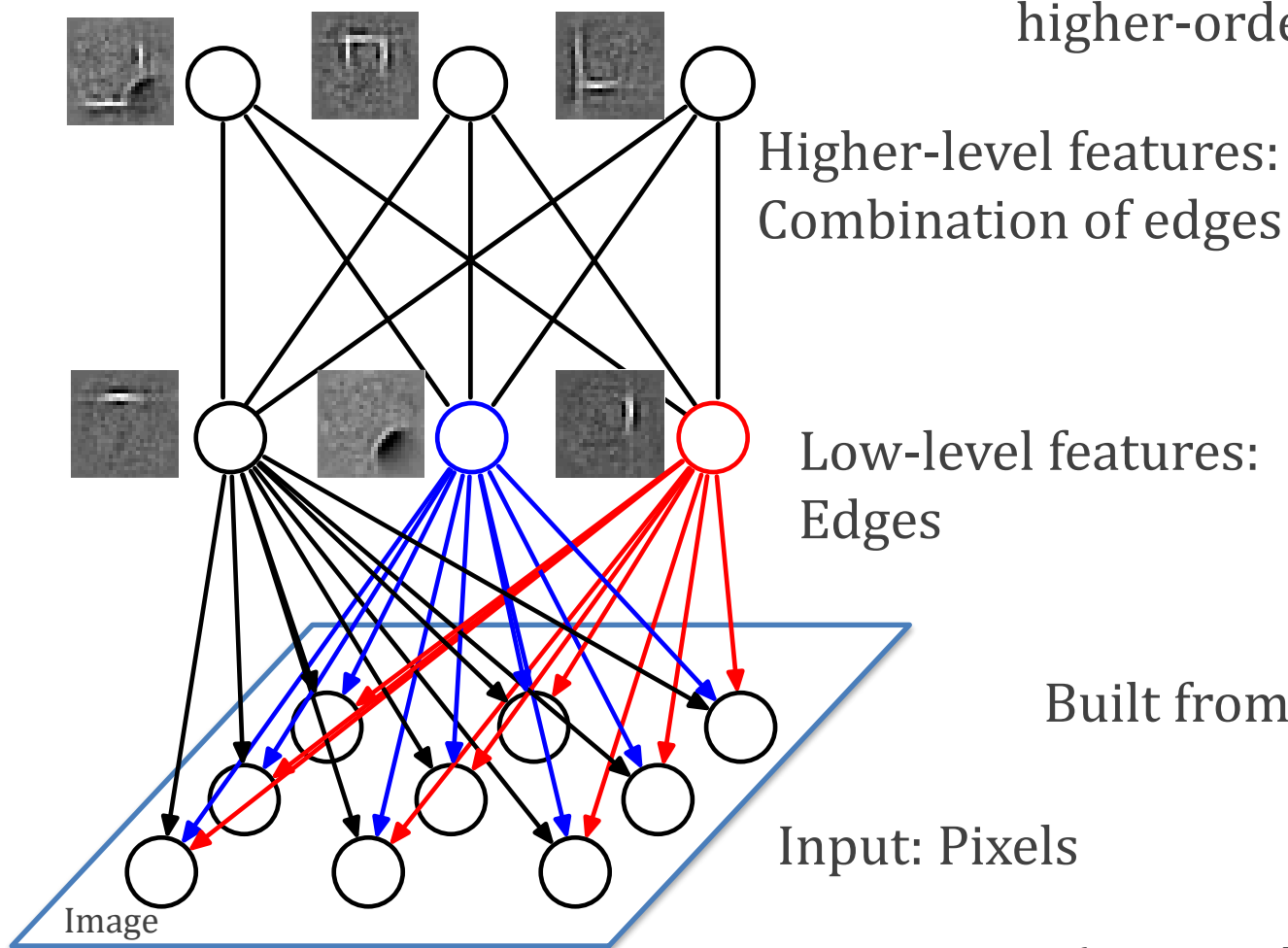
Deep Belief Network



(Hinton et.al. Neural Computation 2006)

Deep Belief Network

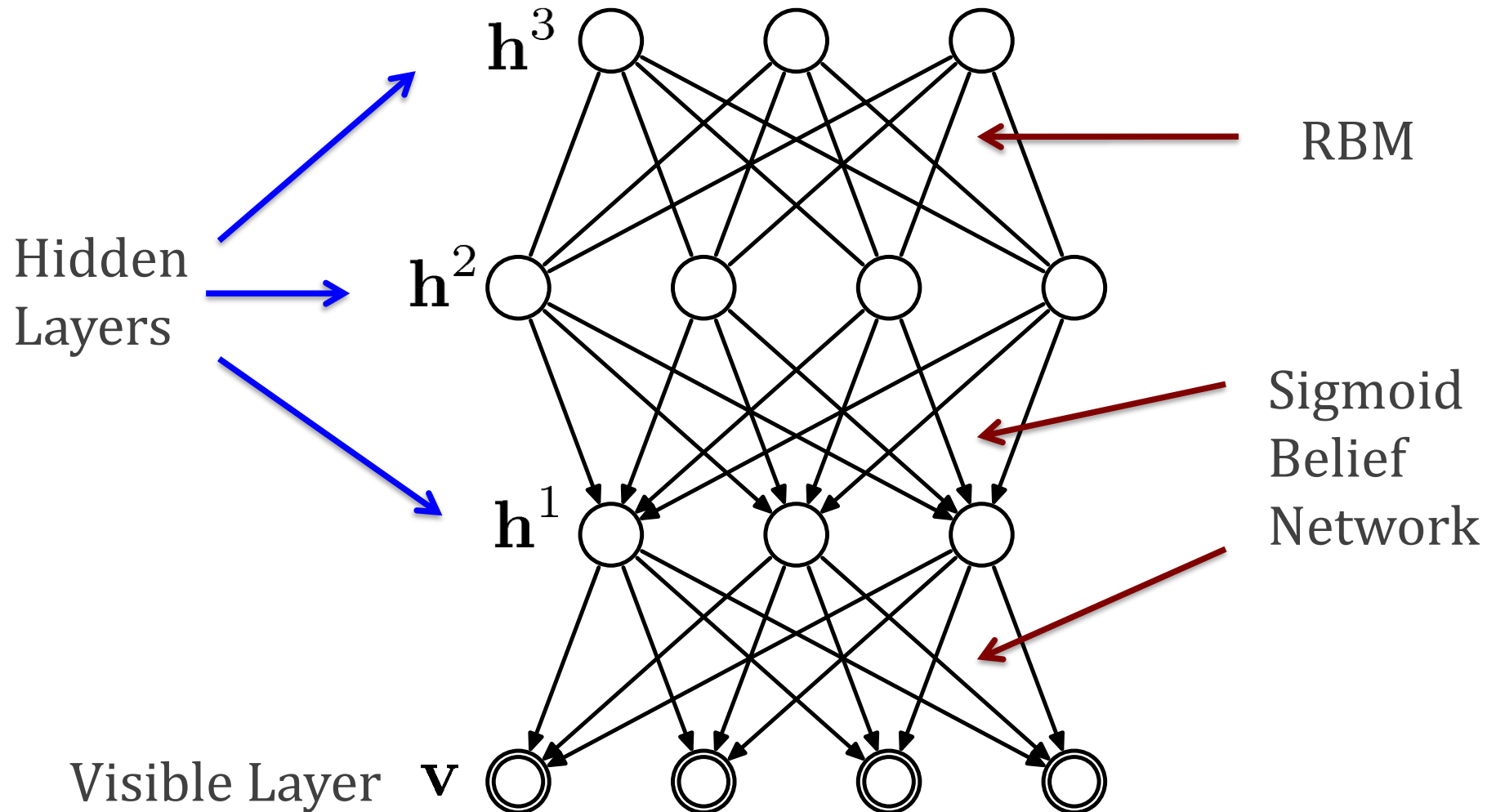
Internal representations capture higher-order statistical structure



Built from **unlabeled** inputs.

(Hinton et.al. Neural Computation 2006)

Deep Belief Network

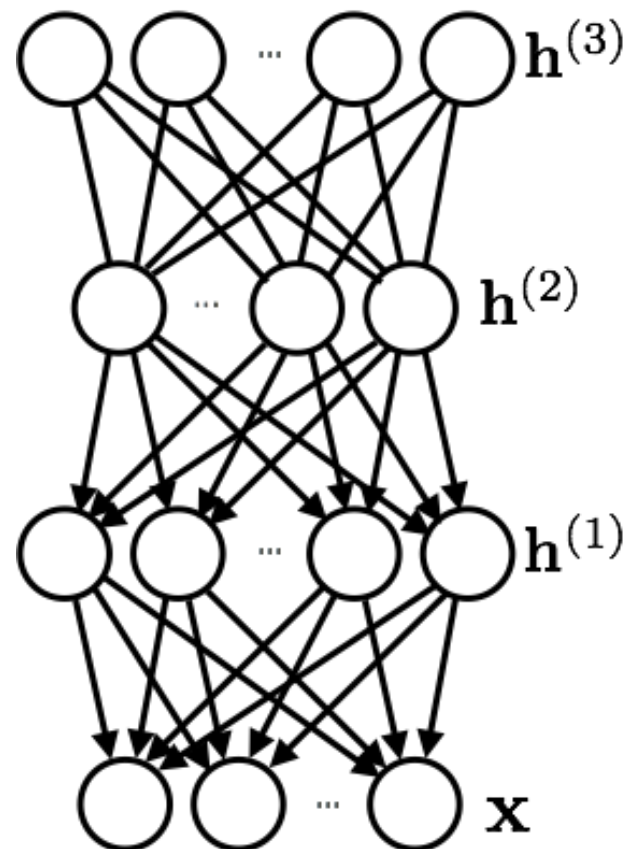


Deep Belief Network

- 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:

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

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



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

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

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

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

(I realize this looks odd.)

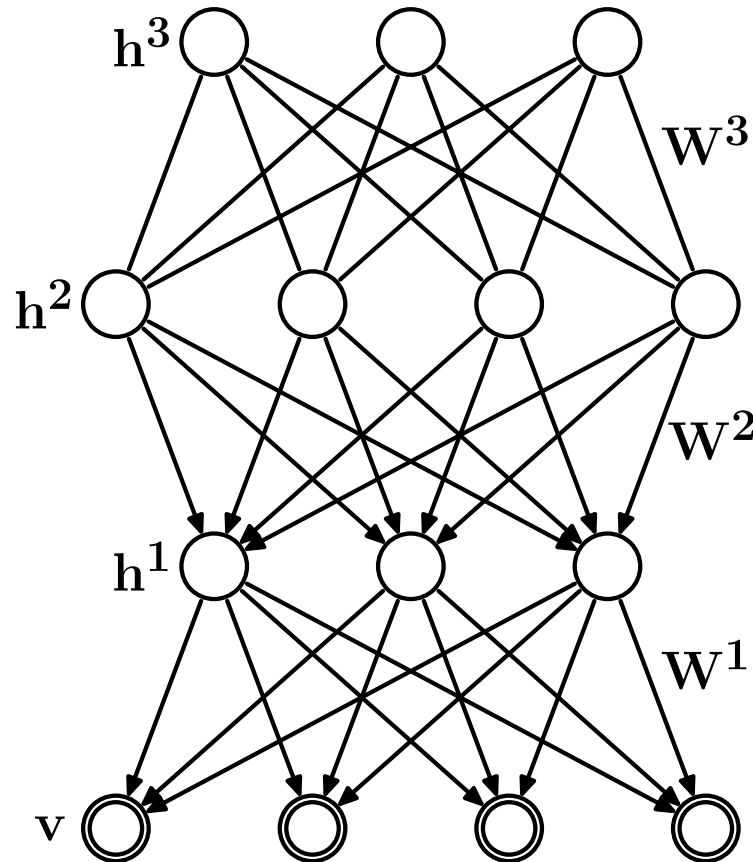
DBN Layer-wise Training

Approximate
Inference

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

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

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



Generative
Process

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

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

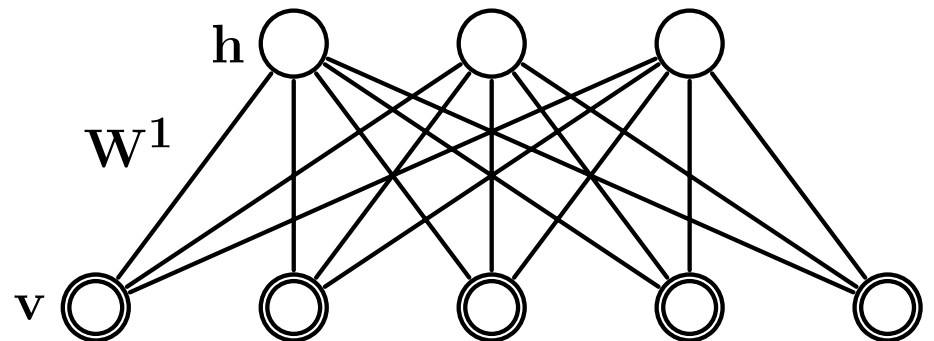
$$P(\mathbf{v} | \mathbf{h}^1)$$

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

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

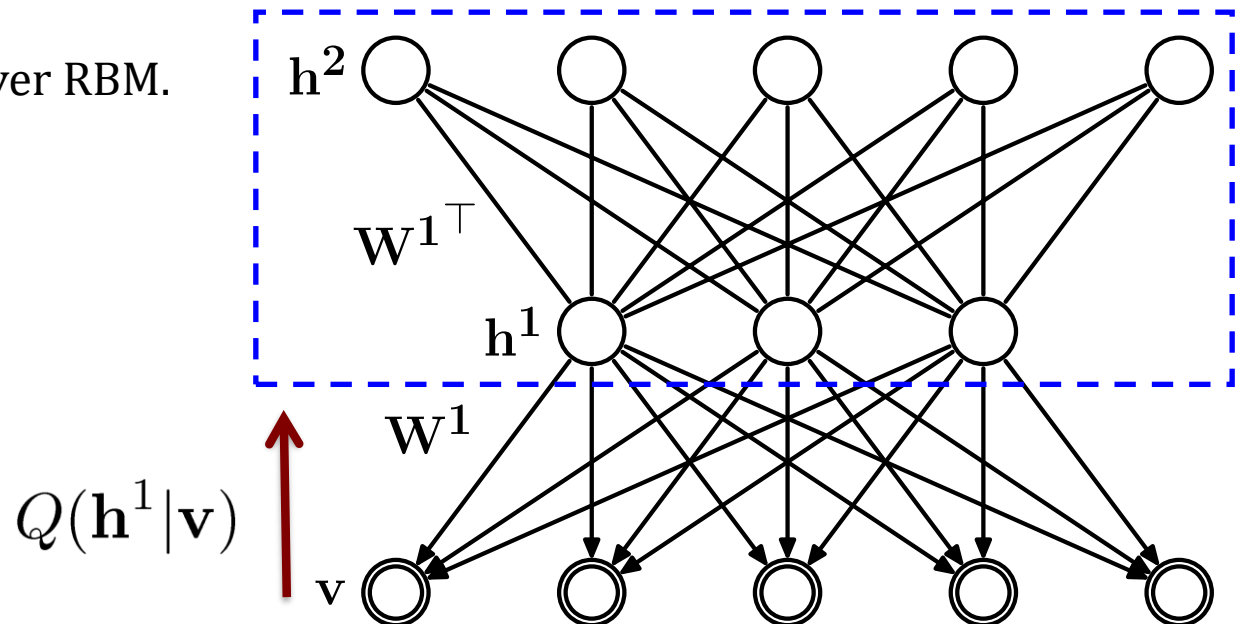
DBN Layer-wise Training

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



DBN Layer-wise Training

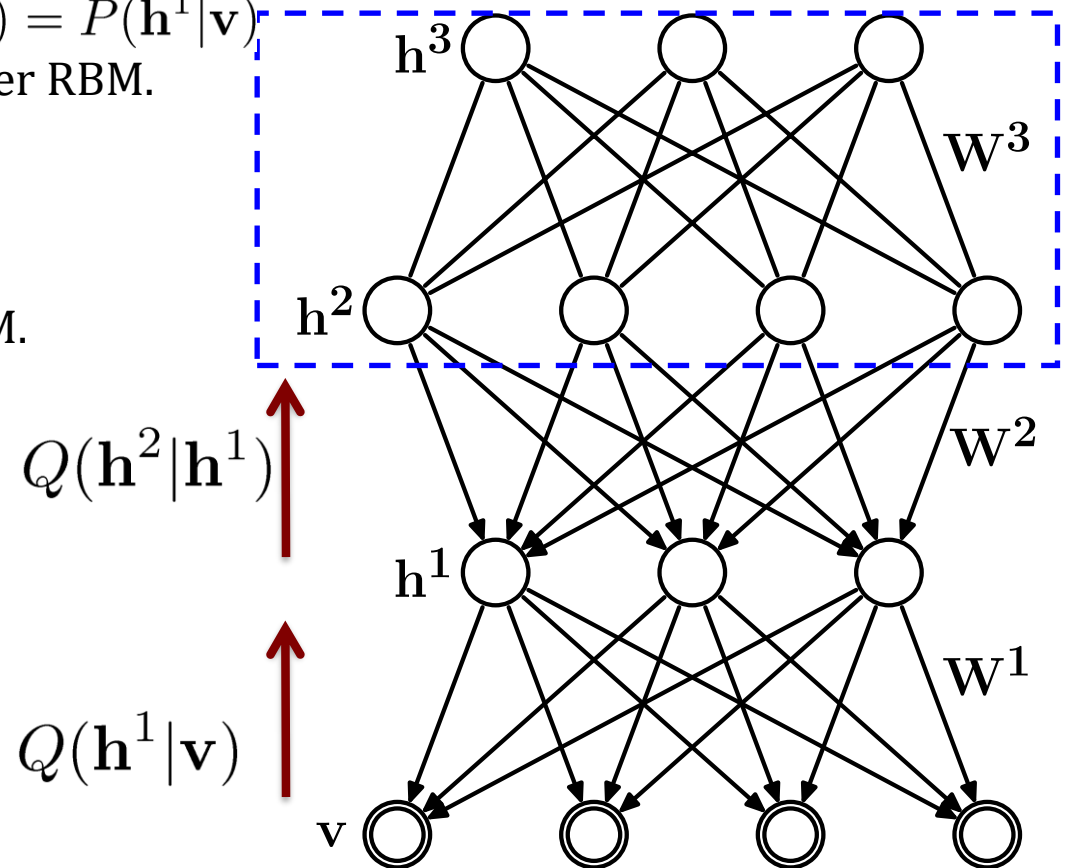
- Learn an RBM with an input layer $\mathbf{v}=\mathbf{x}$ and a hidden layer \mathbf{h} .
- Treat inferred values $Q(\mathbf{h}^1|\mathbf{v}) = P(\mathbf{h}^1|\mathbf{v})$ as the data for training 2nd-layer RBM.
- Learn and freeze 2nd layer RBM.



DBN Layer-wise Training

- Learn an RBM with an input layer $\mathbf{v}=\mathbf{x}$ and a hidden layer \mathbf{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.
- Proceed to the next layer.

Unsupervised Feature Learning.

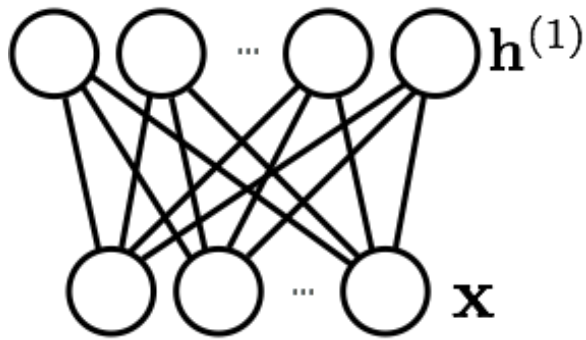


Where does this training come from??

Variational intuitions

Let's write the marginal $p(\mathbf{x})$ in terms of the **Gibbs variational principle**.

As $p(\mathbf{x}) = \sum_{\mathbf{h}^{(1)}} p(\mathbf{x}, \mathbf{h}^{(1)})$ (i.e. the normalizing constant for $p(\mathbf{h}^{(1)}) \propto p(\mathbf{x}, \mathbf{h}^{(1)})$), we have:



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

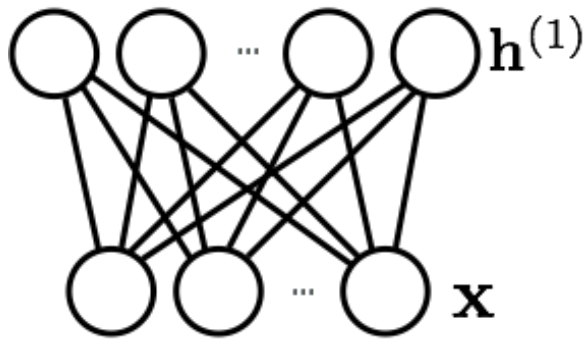
$$\begin{aligned} \log p(\mathbf{x}) &\geq \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{h}^{(1)}) \\ &\quad - \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log q(\mathbf{h}^{(1)}|\mathbf{x}) \end{aligned}$$

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

Variational intuitions

Let's write the marginal $p(\mathbf{x})$ in terms of the **Gibbs variational principle**.

As $p(\mathbf{x}) = \sum_{\mathbf{h}^{(1)}} p(\mathbf{x}, \mathbf{h}^{(1)})$ (i.e. the normalizing constant for $p(\mathbf{h}^{(1)}) \propto p(\mathbf{x}, \mathbf{h}^{(1)})$), we have:




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

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

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

Variational intuitions

adding 2nd layer means
untying the parameters


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


- 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



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

- we can train the parameters of the **bound**. This is equivalent to maximizing the lower bound when the other terms are constant:

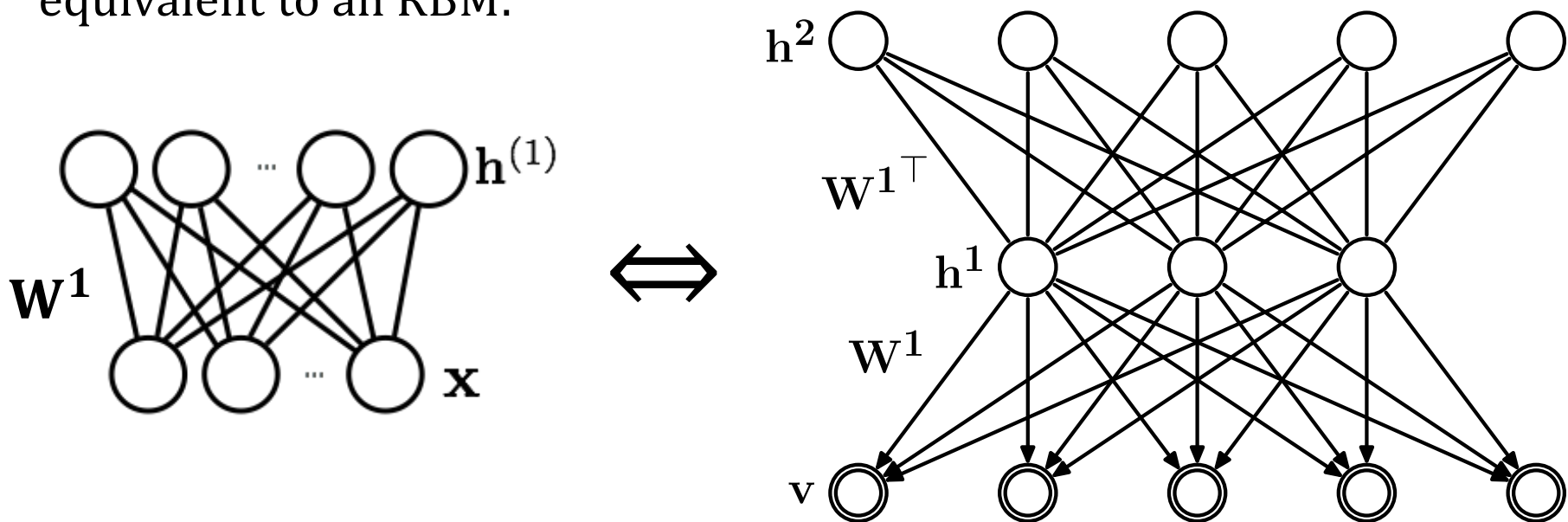
$$- \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log p(\mathbf{h}^{(1)})$$

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

Layerwise training
improves variational
lower bound

Does the lower bound improve?

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



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 \mathbf{x} given $\mathbf{h}^{(1)}$ converges to model distribution in second.
- The steps in these two random walks are **exactly** the same.

Does the lower bound improve?

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

Does the lower bound improve?

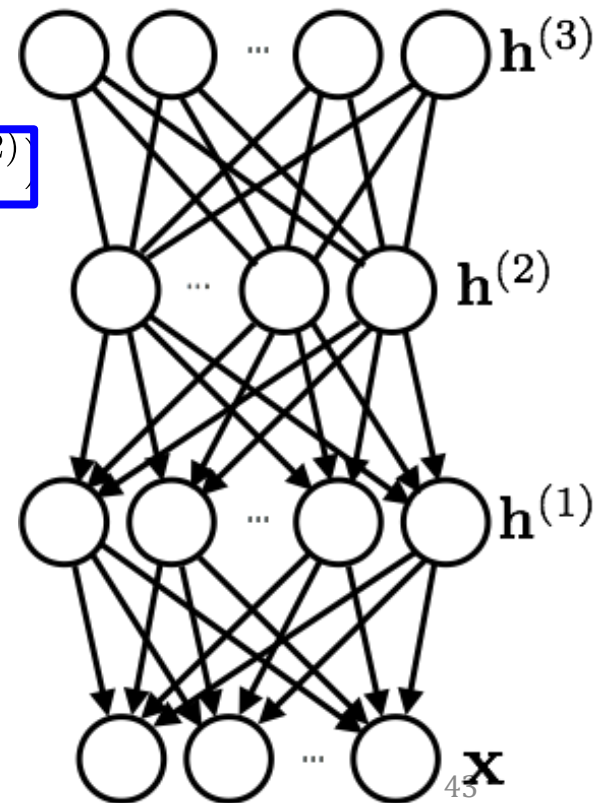
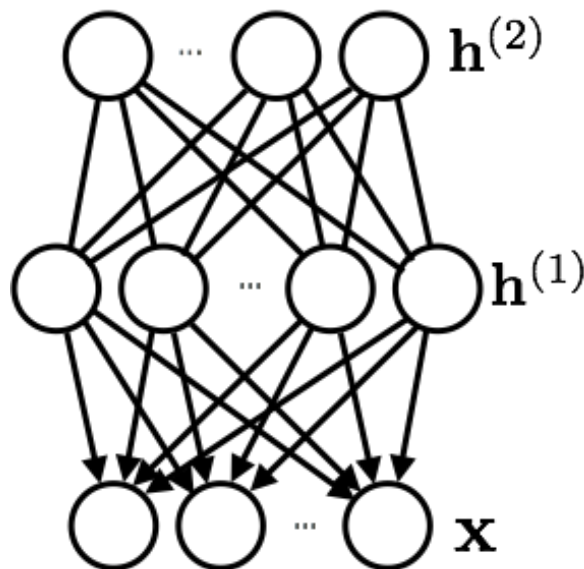
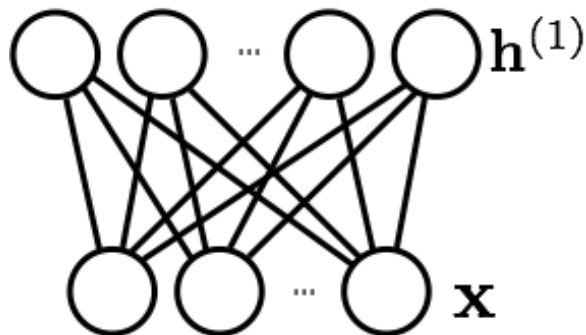
This is where the RBM stacking procedure comes from:

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

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

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

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



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

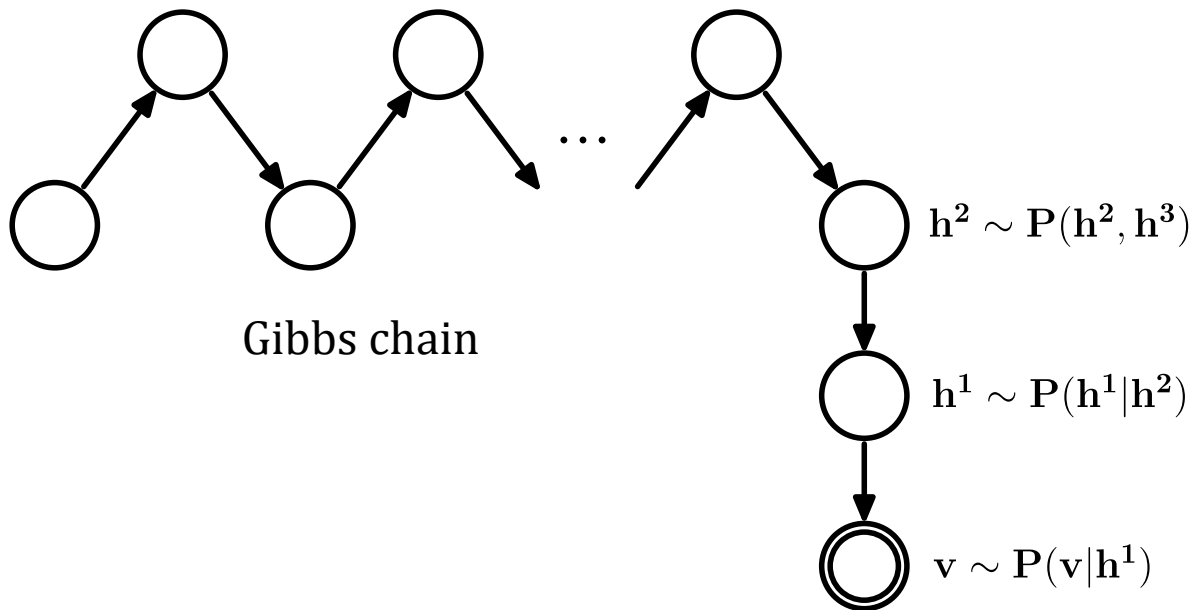
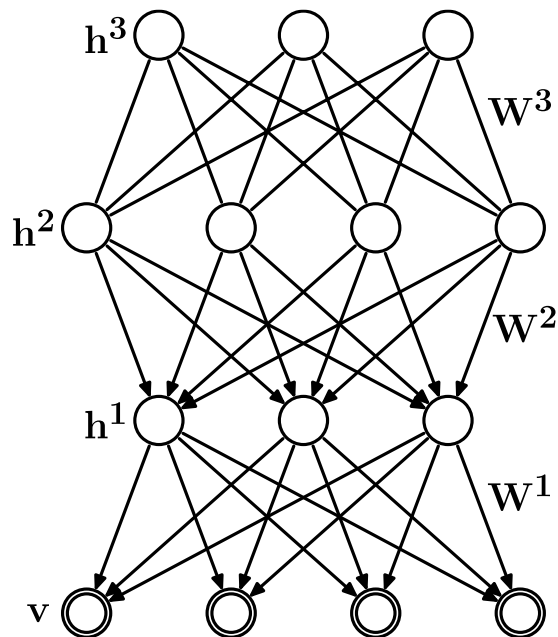
- A fast learning algorithm for deep belief nets. Hinton, Teh, Osindero, 2006.

Sampling from DBNs

- To sample from the DBN model:

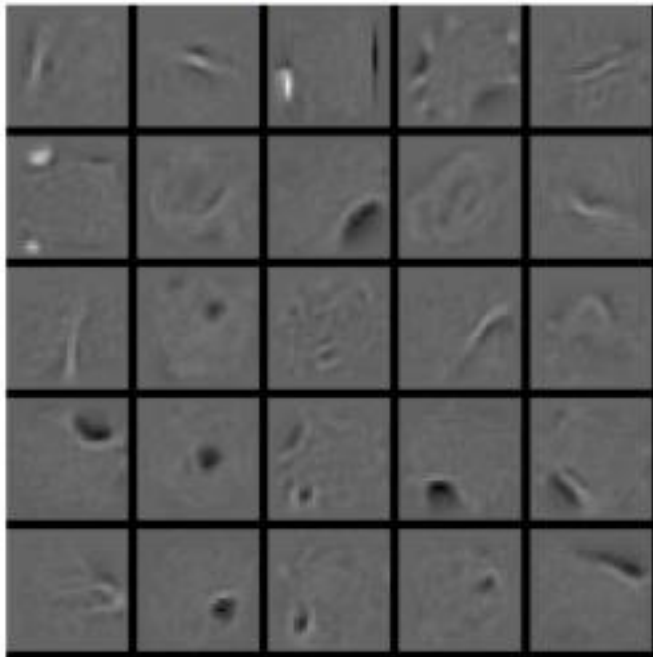
$$P(\mathbf{v}, \mathbf{h}^1, \mathbf{h}^2, \mathbf{h}^3) = P(\mathbf{v}|\mathbf{h}^1)P(\mathbf{h}^1|\mathbf{h}^2)P(\mathbf{h}^2, \mathbf{h}^3)$$

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

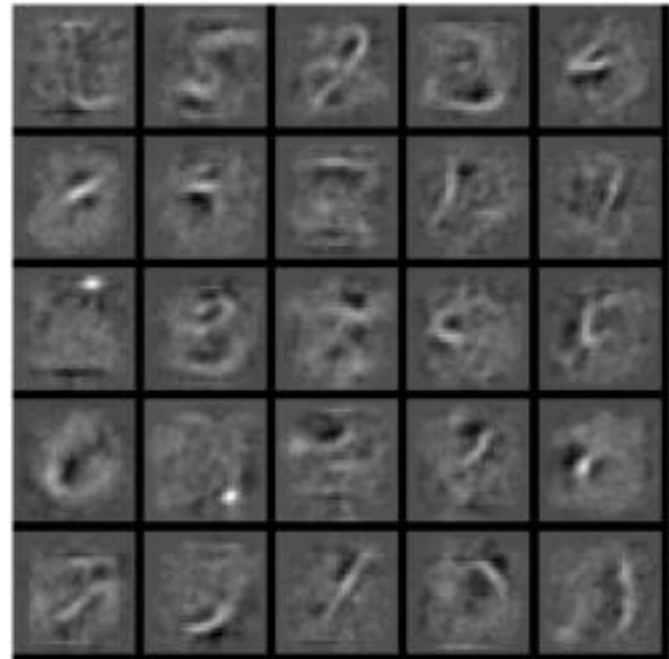


Learned Features

1st-layer features

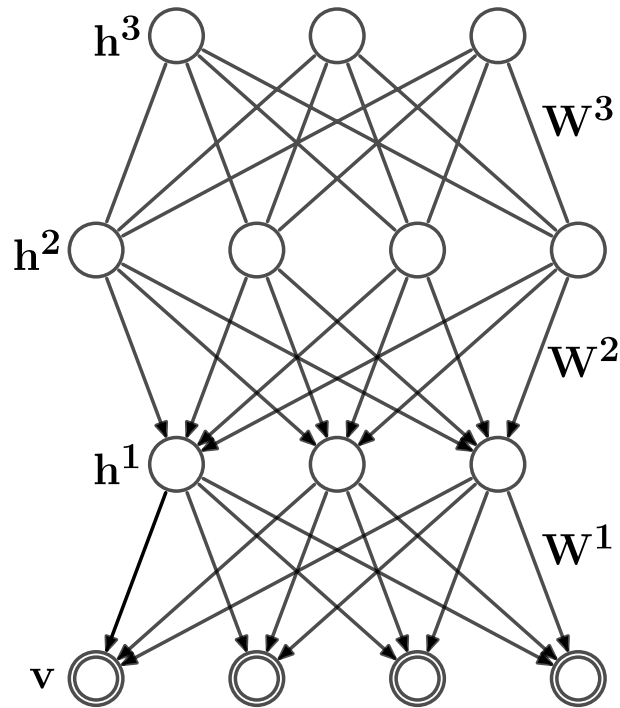


2nd-layer features

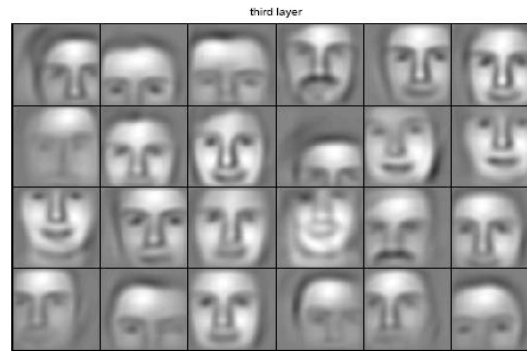


Learning Part-based Representation

Convolutional DBN



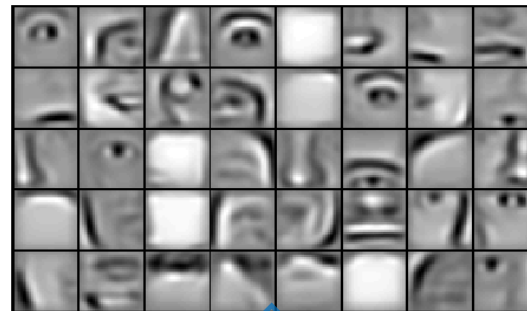
Faces



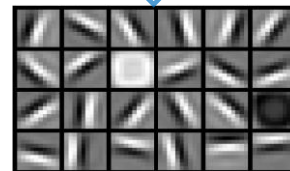
Groups of parts.



second layer



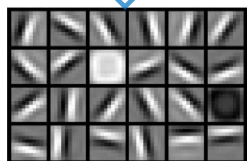
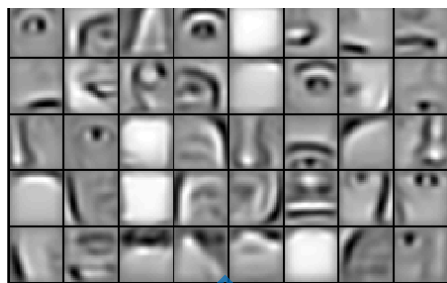
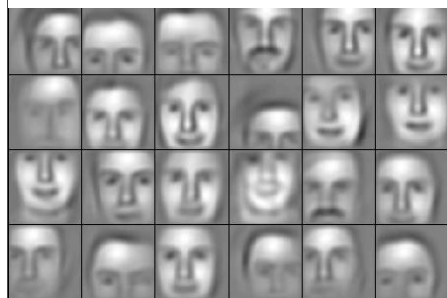
Object Parts



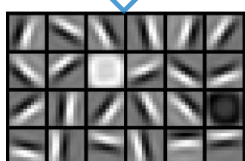
Trained on face images.

Learning Part-based Representation

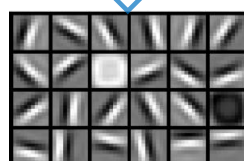
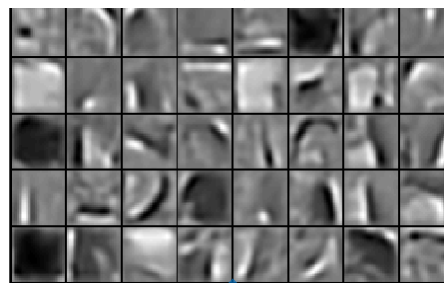
Faces



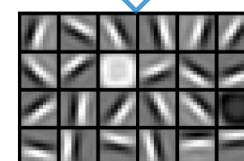
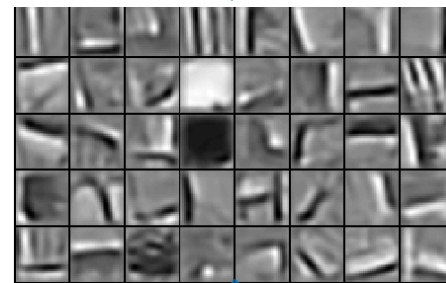
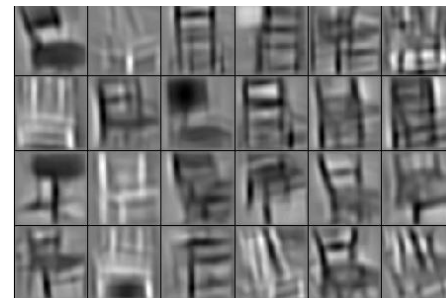
Cars



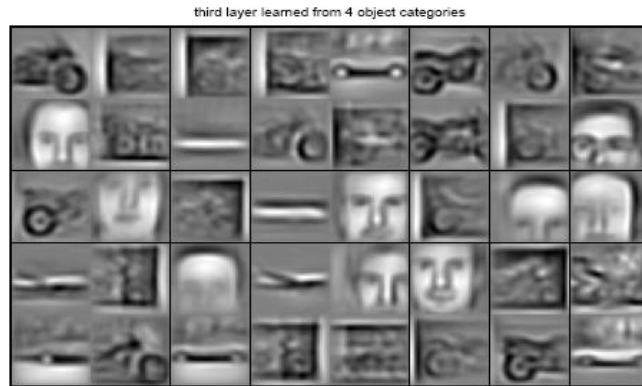
Elephants



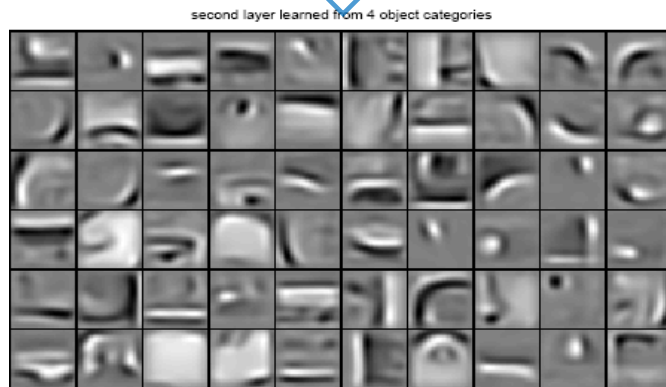
Chairs



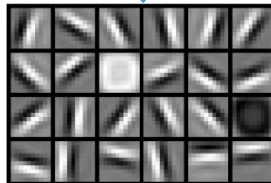
Learning Part-based Representation



Groups of parts.



Class-specific object parts



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