10417-617
Deep Learning: Fall 2020

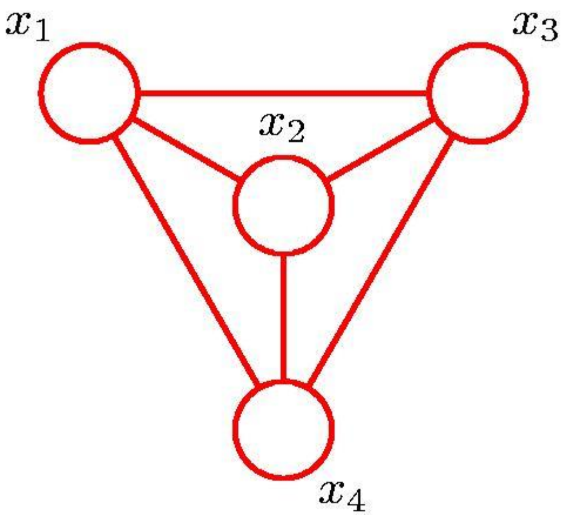
Andrej Risteski

Machine Learning Department

Lecture 13:
Variational methods

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 ✗
- Easy to sample posterior distribution over latents ✓

Directed models

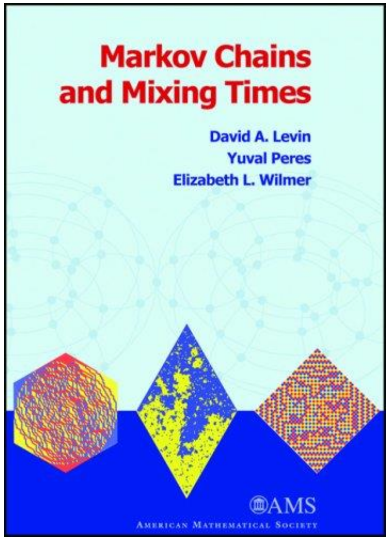
- Easy to draw samples ✓
- Hard to sample posterior distribution over latents ✗

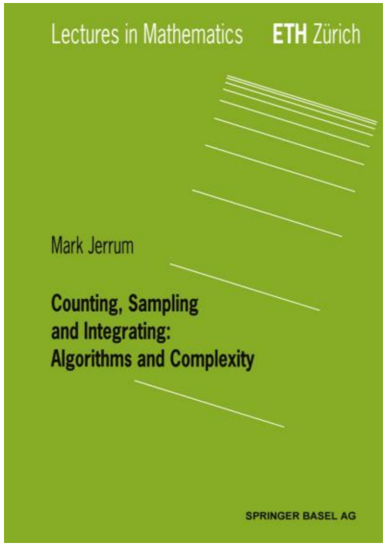
Algorithmic approaches

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

MARKOV CHAIN MONTE CARLO

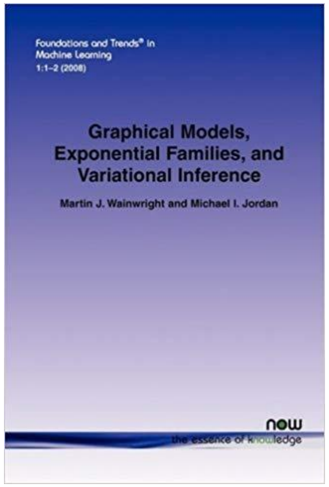
- Random walk w/ equilibrium distribution the one we are trying to sample from.





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**:

$$P(\text{Diseases}, \text{Symptoms}) = P(\text{Diseases}) \;\; P(\text{Symptoms}|\text{Diseases})$$

Latent

Data

Simple, explicit

By Bayes rule, $P(\text{Diseases}|\text{Symptoms}) \propto P(\text{Diseases}, \text{Symptoms})$

Up to normalizing const, simple…

Complicated partition function:

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

Variational methods for approximating posteriors

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

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

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

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

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

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

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

Why: $$0 \leq KL(q\,(z|x)||\, p(z|x)) = \mathbb{E}_{q\,(z|x)} \log q\,(z|x) - \mathbb{E}_{q\,(z|x)} p(z|x)$$

$$= -H\big(q\,(z|x)\big) - \mathbb{E}_{q\,(z|x)} \log \frac{p(z,x)}{p(x)}$$

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

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,

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

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

Why is this useful?

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

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

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

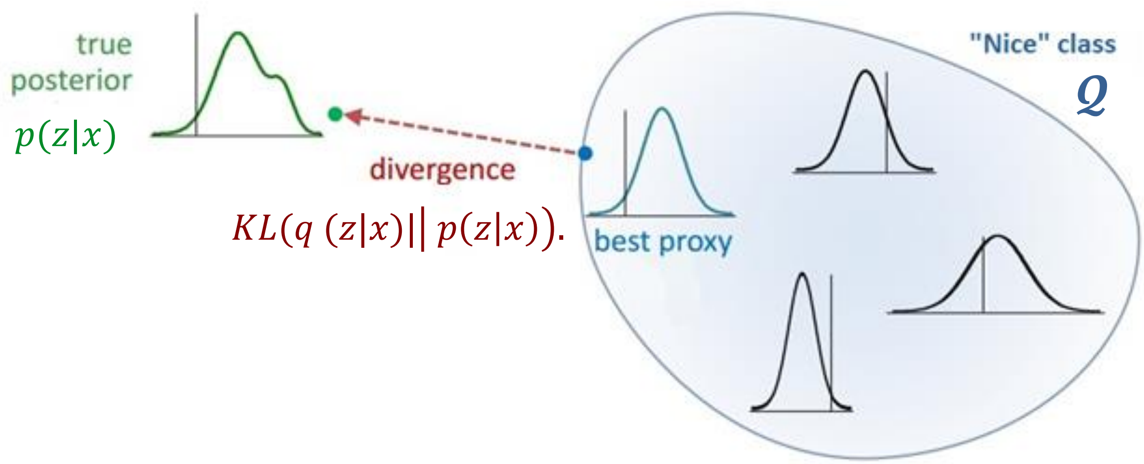
In other words, we are finding the **projection** of $p(z|x)$ onto Q.

Variational methods for approximating posteriors

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

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

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



Variational methods for approximating posteriors

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

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

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

Why is this useful?

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

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

There are several common families 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,

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

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

Why is this useful?

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

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

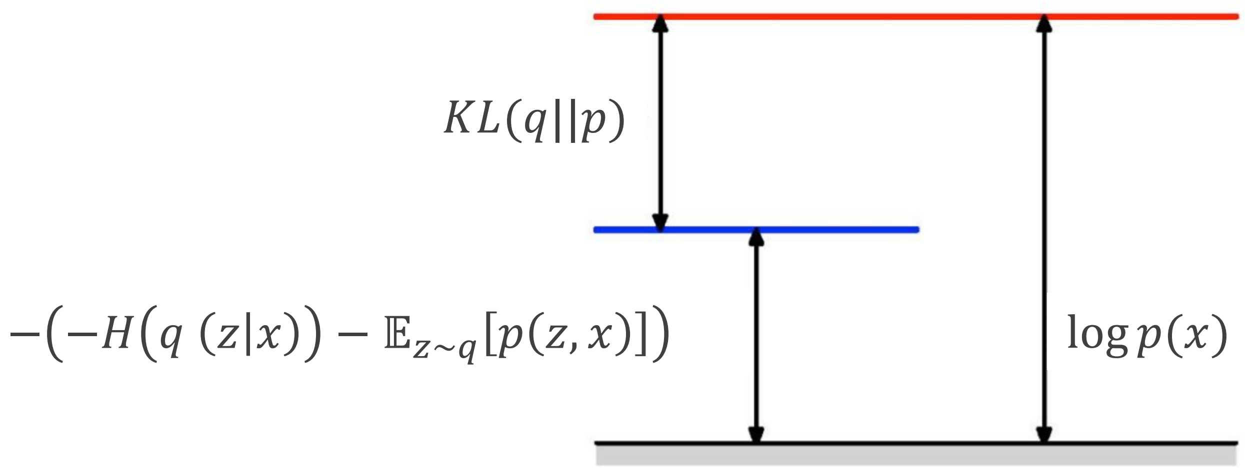
This will be useful when learning latent-variable directed models (stay tuned !).

Variational methods for approximating posteriors

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

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

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



Solving the mean-field relaxation: coordinate ascent

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

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

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:

$$\min_{q(Z|X)\in\mathcal{Q}} KL(q\,(z|x)||\,p(z|x)) = \min_{q(Z|X)\in\mathcal{Q}} \mathbb{E}_{q\,(z|x)} \log q\,(z|x) - \mathbb{E}_{q\,(z|x)} \log p\,(z,x)$$

$$= \min_{q(Z|X)\in\mathcal{Q}} \sum_i \mathbb{E}_{q_i\,(z_i|x)} \log q_i\,(z_i|x) - \mathbb{E}_{q_i\,(z_i|x)} \left[\mathbb{E}_{q_{-i}(z_{-i}|x)} \log p\,(z_i, z_{-i}, x)\right]$$

$$= \min_{q(Z|X)\in\mathcal{Q}} \mathbb{E}_{q_i\,(z_i|x)} \log q_i\,(z_i|x) - \mathbb{E}_{q_i\,(z_i|x)}[\log \tilde{p}\,(z_i,x)] + C$$

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 $q(\cdot\,|x) \in \mathcal{Q}$:

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

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:

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

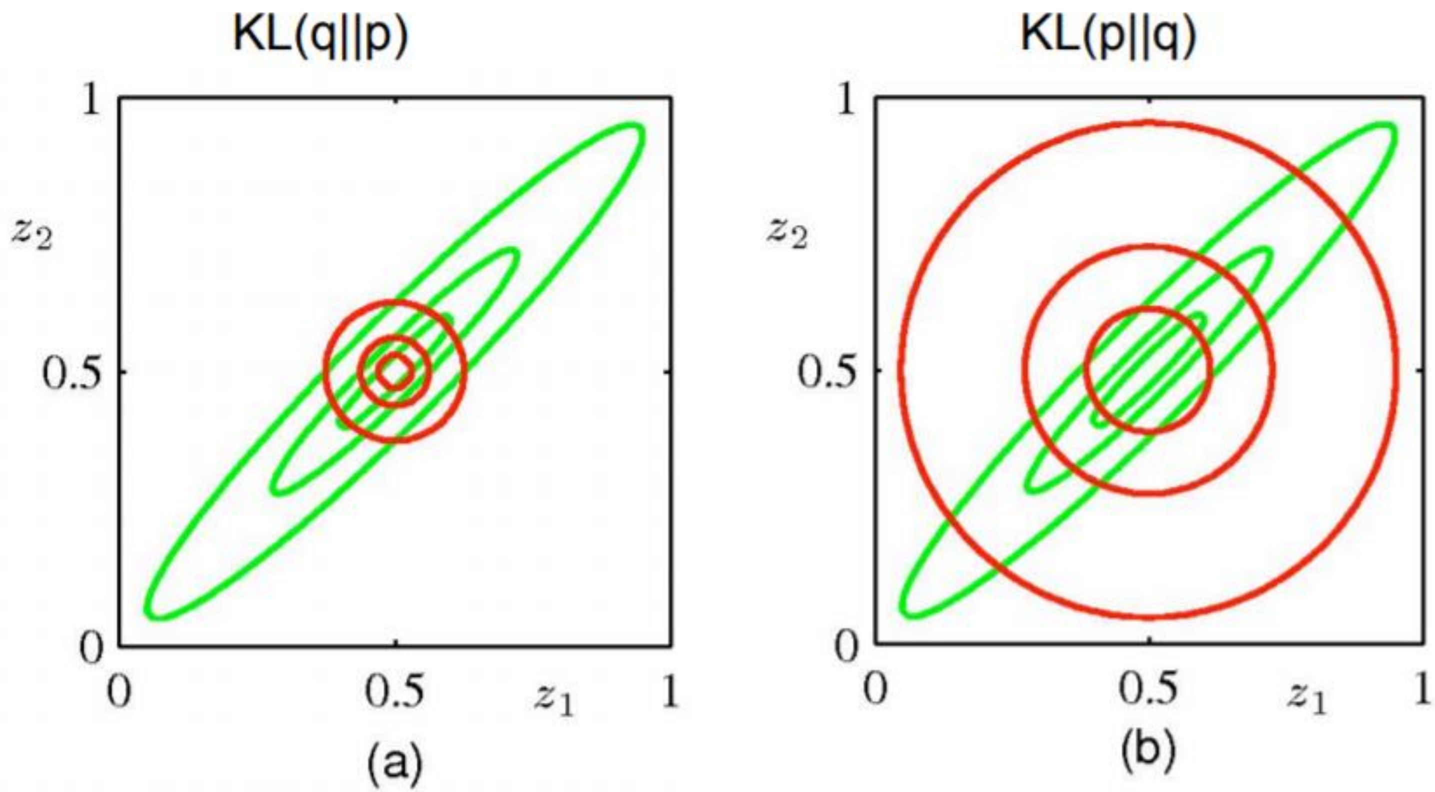
$$= \min_{q(z|x)\in\mathcal{Q}} KL(q_i\,(z_i|x)||\,\tilde{p}(z_i,x)) + C$$

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!

A tale of two KL divergences



Approximation is too compact.

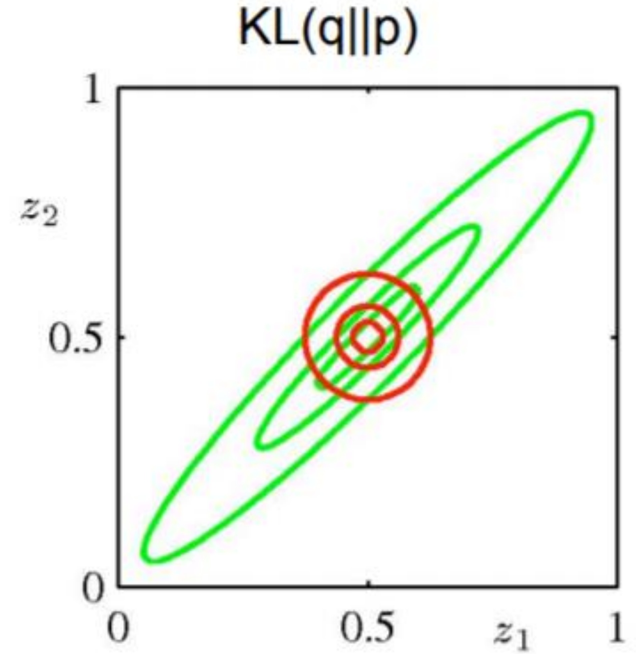
Approximation is too spread.

The “variational” KL divergence

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

There is a large positive contribution to the KL divergence from regions of Z space in which:
- p(Z) is near zero
- unless q(Z) is also close to zero.

Minimizing KL(q||p) leads to distributions q(Z) that avoid regions in which p(Z) is small.



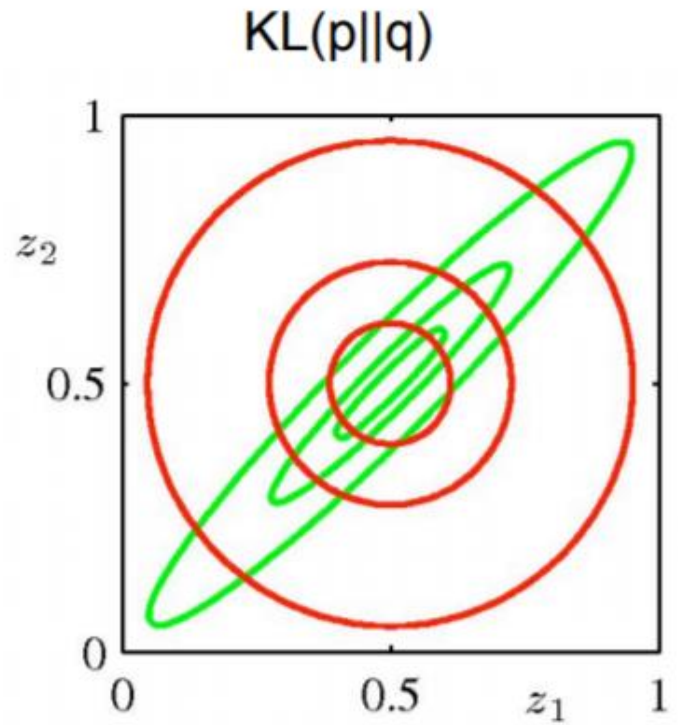
(a)

The “maximum likelihood” KL divergence

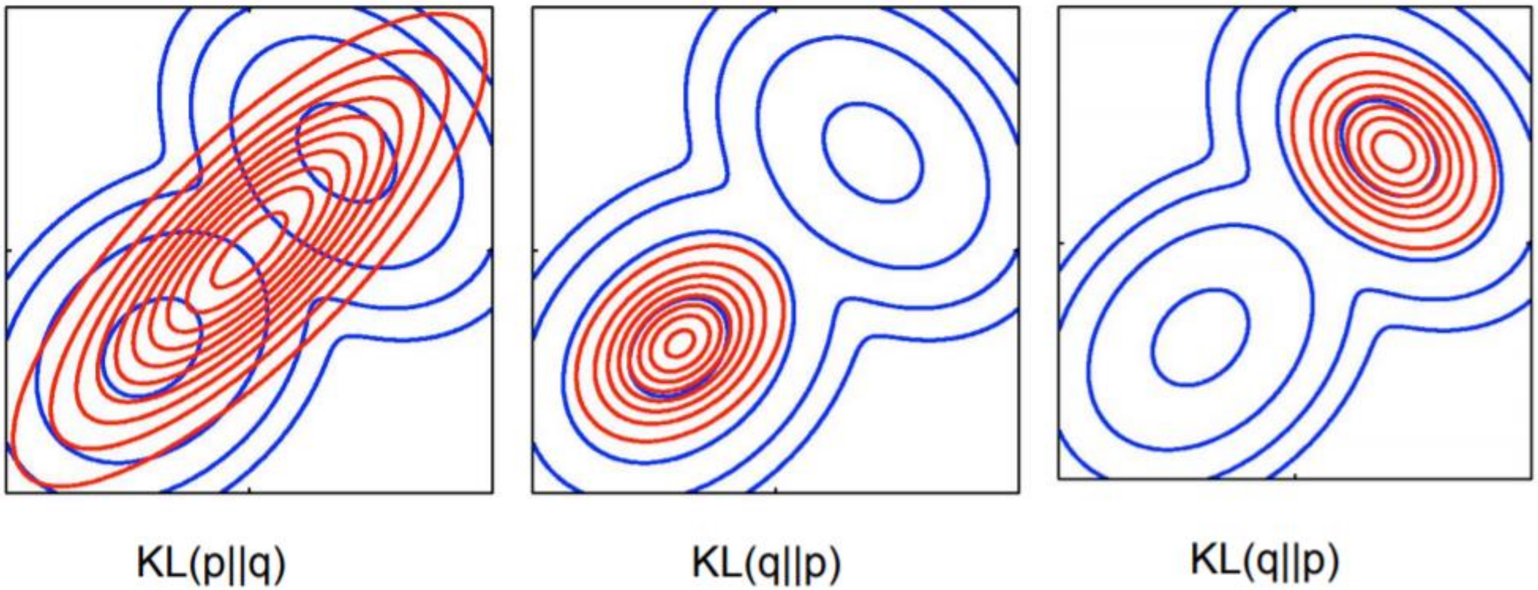
$$\mathrm{KL}(p||q) = -\int p(\mathbf{Z}) \ln \frac{q(\mathbf{Z})}{p(\mathbf{Z})} \mathrm{d}\mathbf{Z}.$$

There is a large positive contribution to the KL divergence from regions of Z space in which:
- q(Z) is near zero,
- unless p(Z) is also close to zero.

Minimizing KL(p||q) leads to distributions q(Z) that are nonzero in regions where p(Z) is nonzero.



What happens when distribution class for Q 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 $x_1, x_2, \ldots, x_n$, 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!

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

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**.

Example

<u>Mixture of spherical Gaussians</u>

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

Writing out the normalizing constant, we have

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

"Soft" version of assigning point to nearest cluster

Example

<u>Mixture of spherical Gaussians</u>

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 quess $q_i^t(z|x_i)$, we can rewrite the maximization for θ as:

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

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

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

Doesn't depend on θ

Example

<u>Mixture of spherical Gaussians</u>

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 quess $q_i^t(z|x_i)$, we can rewrite the maximization for θ as:

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

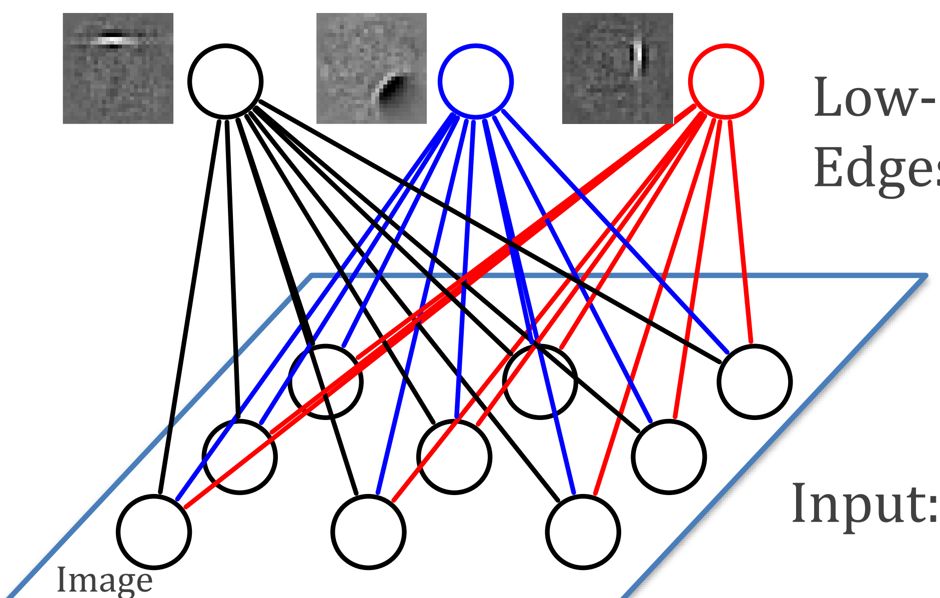
Setting the derivative wrt to μ_k to 0, we have:

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

Average points, weighing nearby points more

Part III: Deep Belief Networks (DBNs)

Deep Belief Network



Low-level features:
Edges

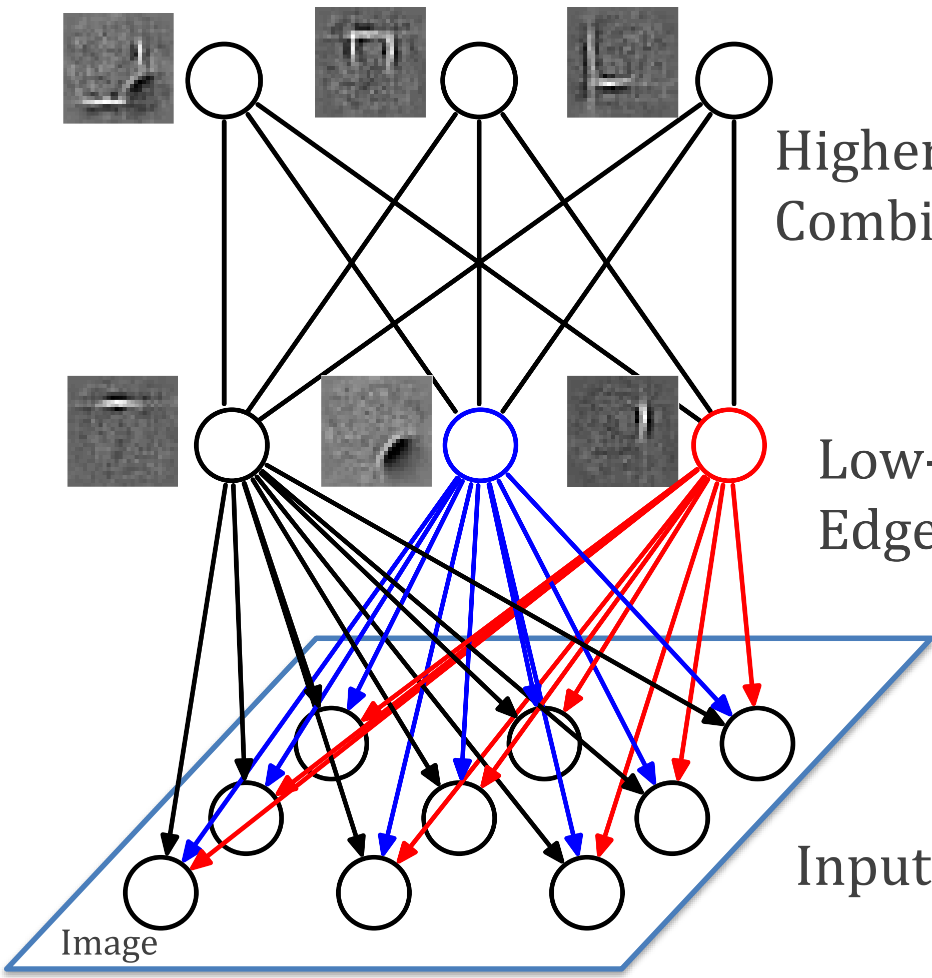
Built from **unlabeled** inputs.

Input: Pixels

(Hinton et.al. Neural Computation 2006)

Deep Belief Network

Internal representations capture higher-order statistical structure



Higher-level features: Combination of edges

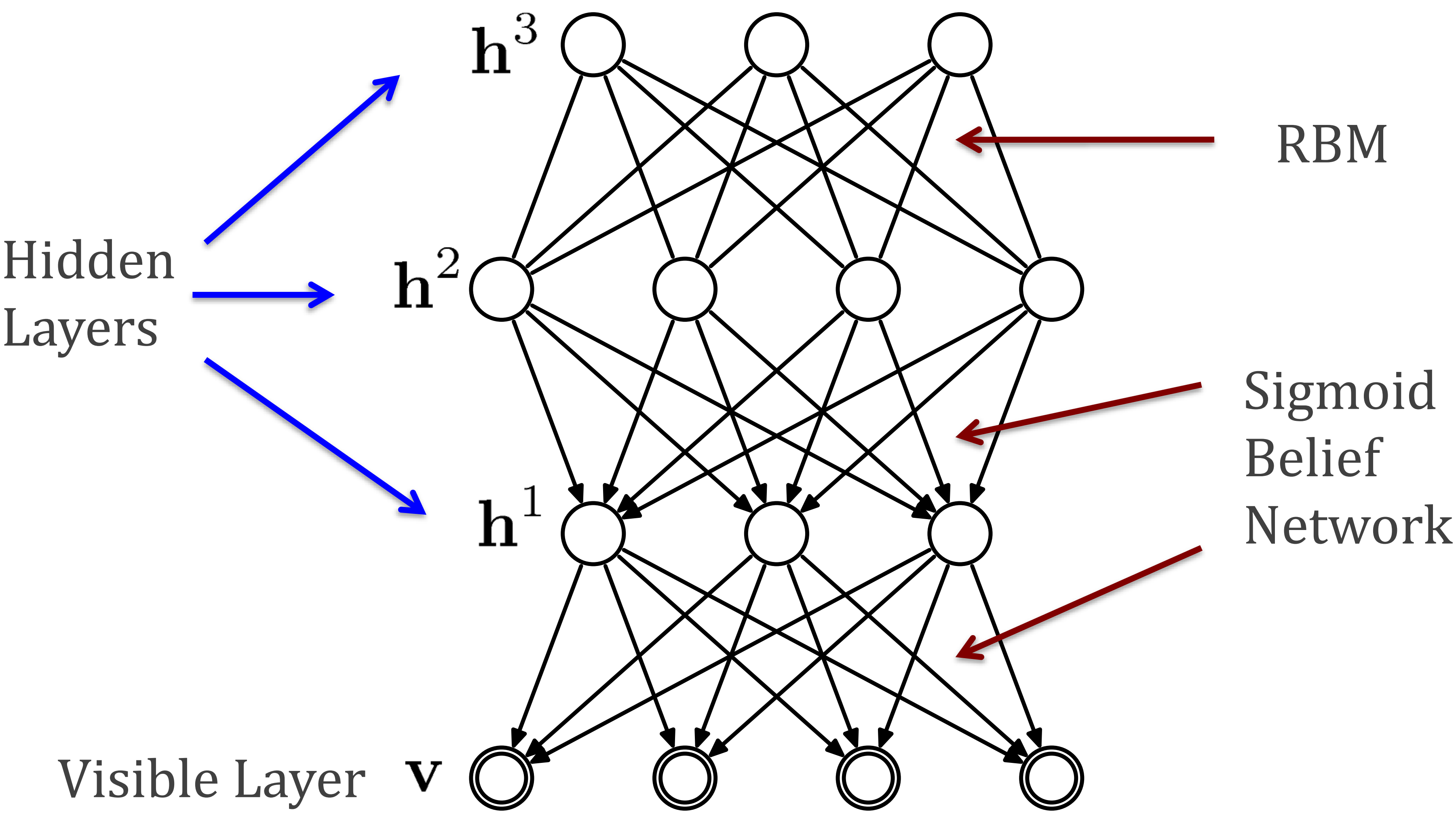
Low-level features: Edges

Built from **unlabeled** inputs.

Input: Pixels

(Hinton et.al. Neural Computation 2006)

Deep Belief Network

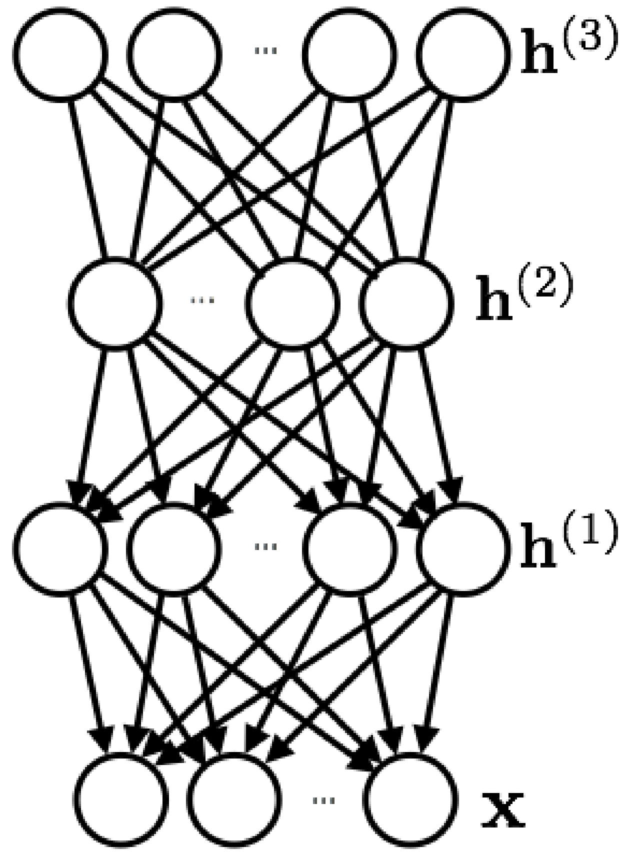


Deep Belief Network

- 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:

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

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



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

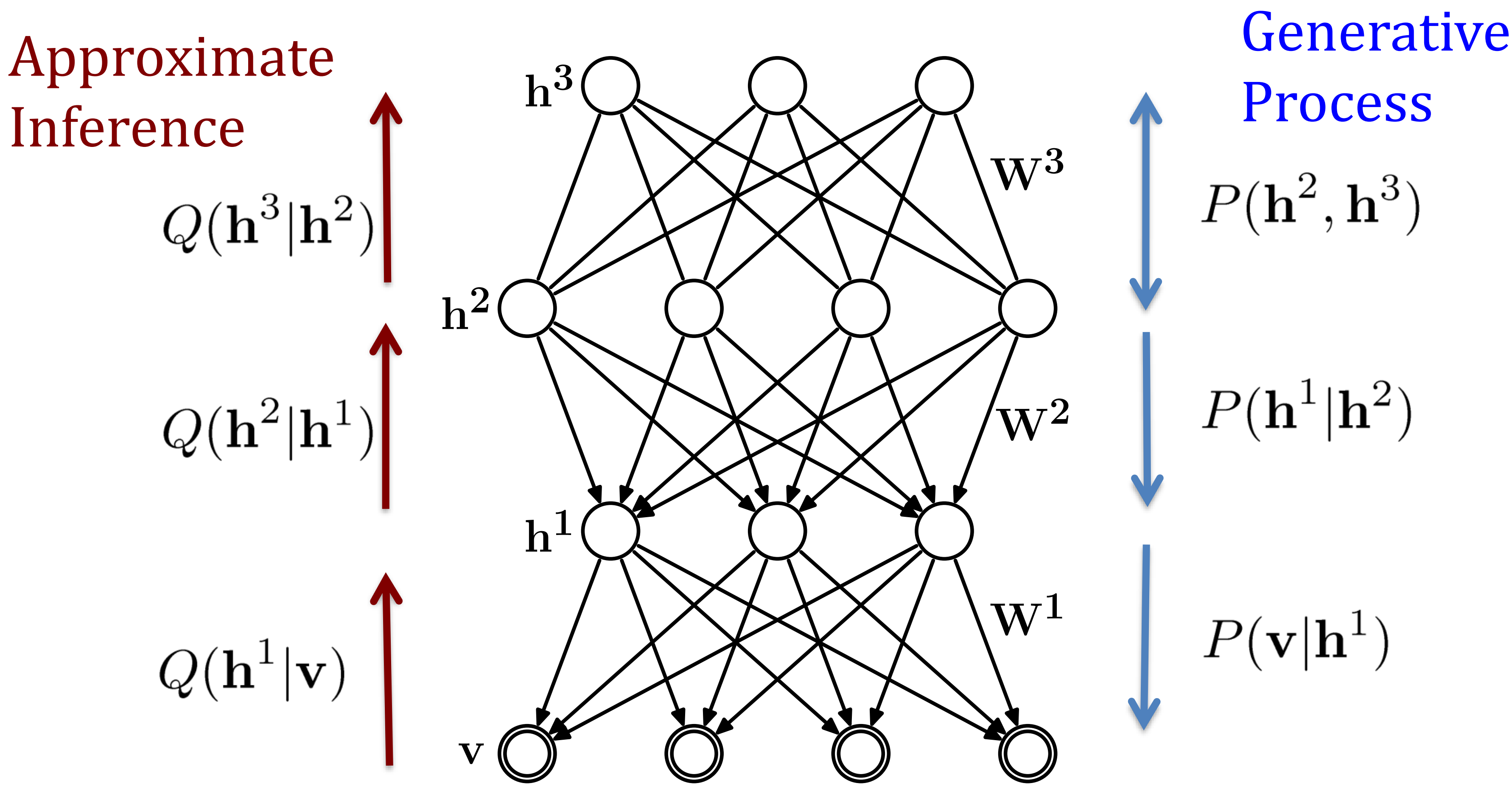
$$p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \exp\left(\mathbf{h}^{(2)}{}^{\top}\mathbf{W}^{(3)}\mathbf{h}^{(3)} + \mathbf{b}^{(2)}{}^{\top}\mathbf{h}^{(2)} + \mathbf{b}^{(3)}{}^{\top}\mathbf{h}^{(3)}\right)/Z$$

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

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

(I realize this looks odd.)

DBN Layer-wise Training

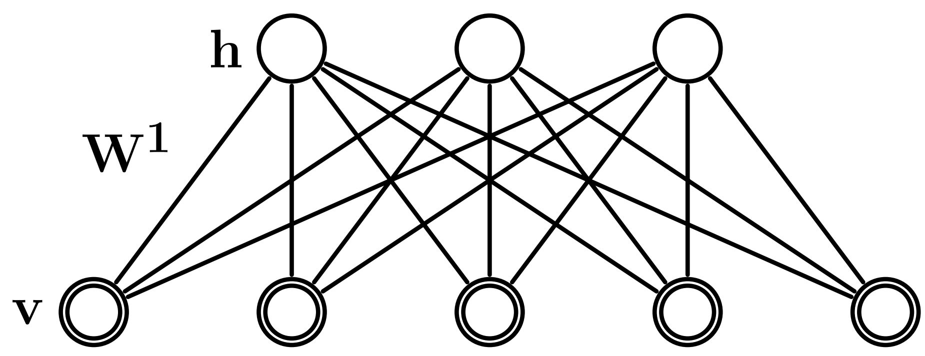


$Q(h^t|h^{t-1}), P(h^{t-1}|h^t)$ are product distributions, s.t.:

$$Q\left((h^t)_j = 1\middle|\, h^{t-1}\right) = \frac{1}{1 + \exp(W_{t,\cdot} h^{t-1})} \quad P\left((h^{t-1})_j = 1\middle|\, h^t\right) = \frac{1}{1 + \exp((h^t)^T W_{\cdot,t})}$$

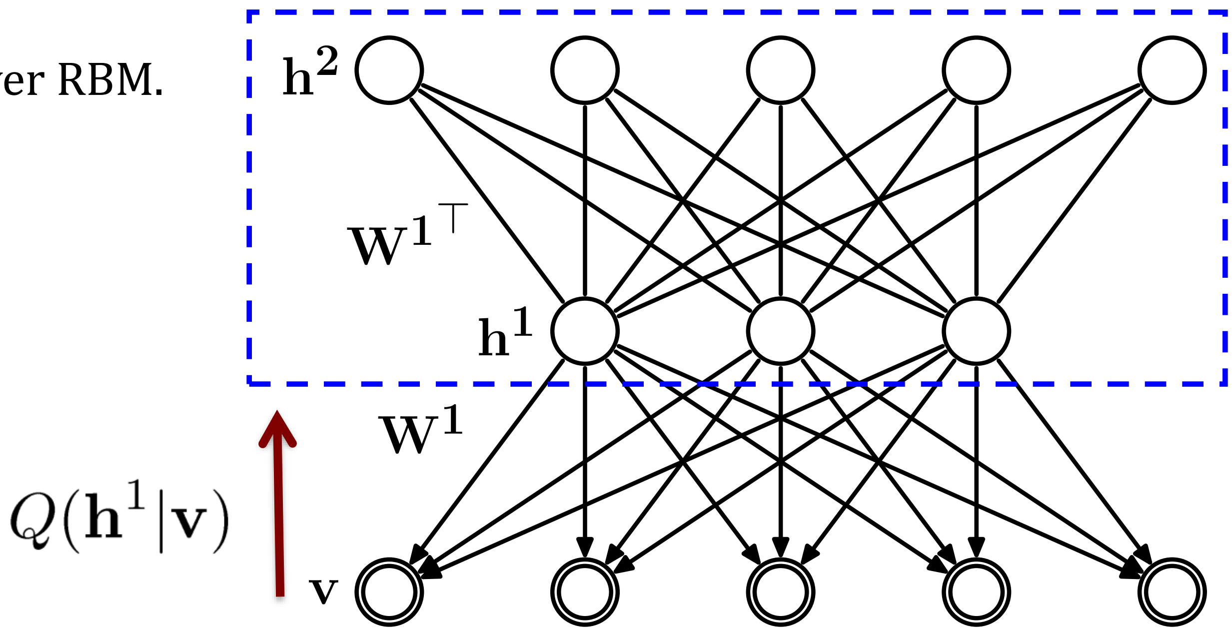
DBN Layer-wise Training

- 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

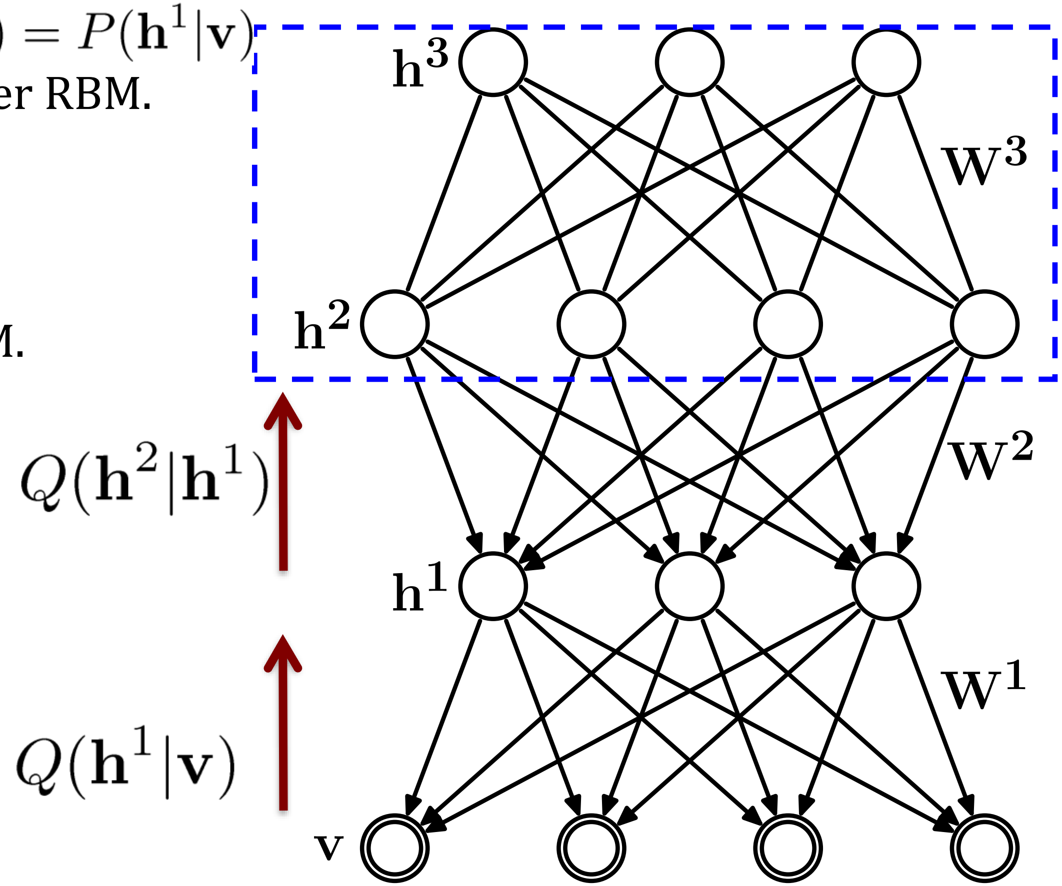
- Learn an RBM with an input layer v=x and a hidden layer h.

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.

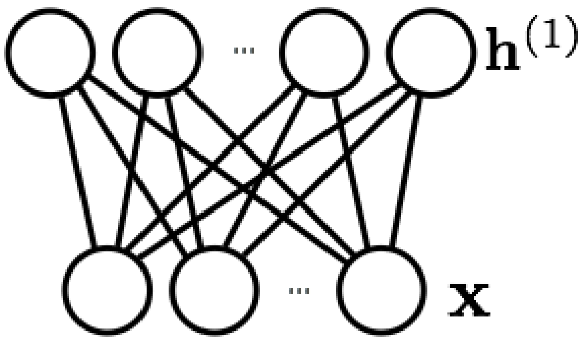


Where does this training come from??

Variational intuitions

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

Recall, we have:



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

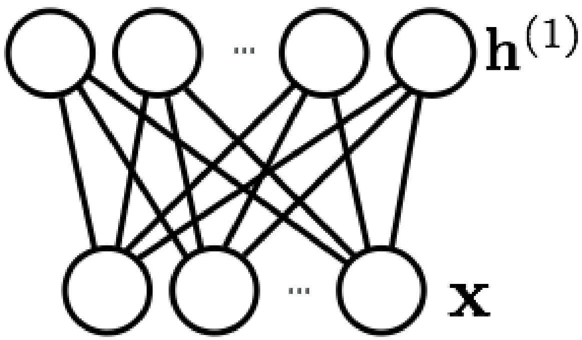
$$
\begin{aligned}
\log p(\mathbf{x}) \quad &\geq \quad \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{h}^{(1)}) \\
&\quad - \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log q(\mathbf{h}^{(1)}|\mathbf{x})
\end{aligned}
$$

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

Variational intuitions

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

Recall, we have:



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

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

*The idea will be to add layers, s.t. we improve the **variational bound (i.e. the right-hand side)***

Variational intuitions

adding 2nd layer means
untying the parameters

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

- 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 o the 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 $q(\mathbf{h}^{(1)}|\mathbf{x})$!

Layerwise training improves variational lower bound

Stacking the layers

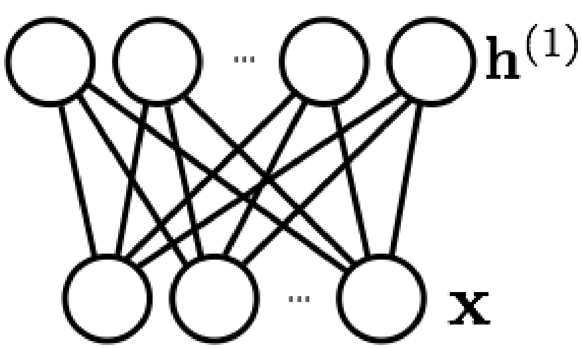
This is where the RBM stacking procedure comes from:

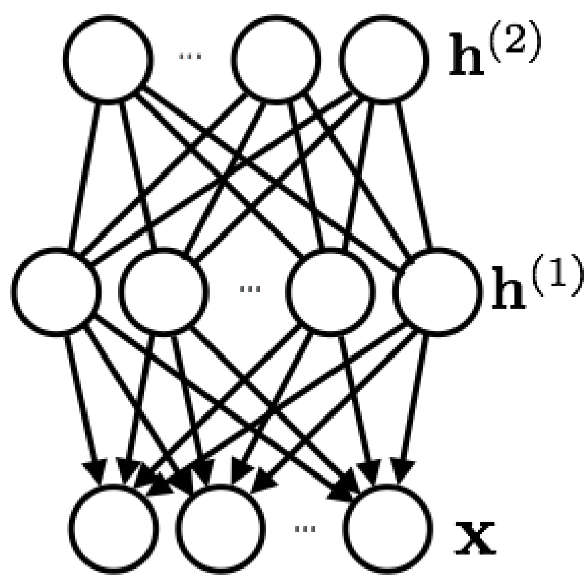
- **idea**: improve prior on last layer by adding another hidden layer

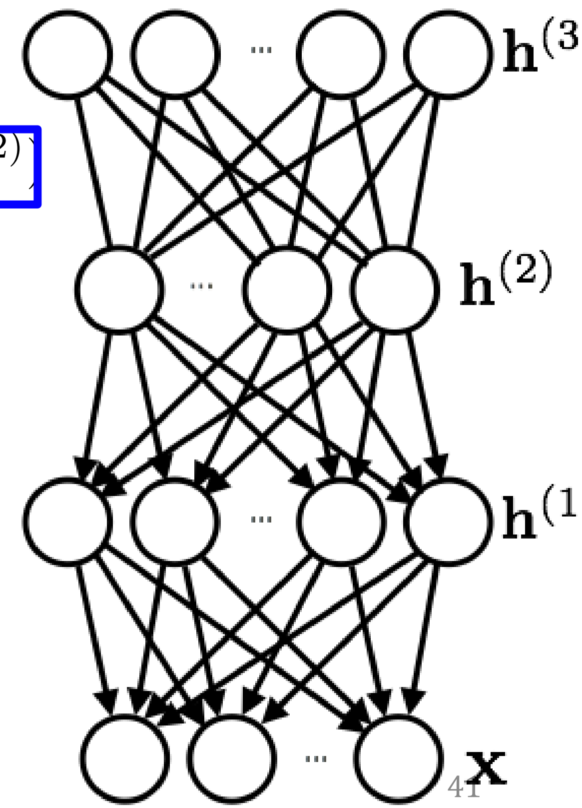
$$p(\mathbf{h}^{(1)}, \mathbf{h}^{(2)}) = p(\mathbf{h}^{(1)}|\mathbf{h}^{(2)}) \sum_{\mathbf{h}^{(3)}} p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)})$$

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

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

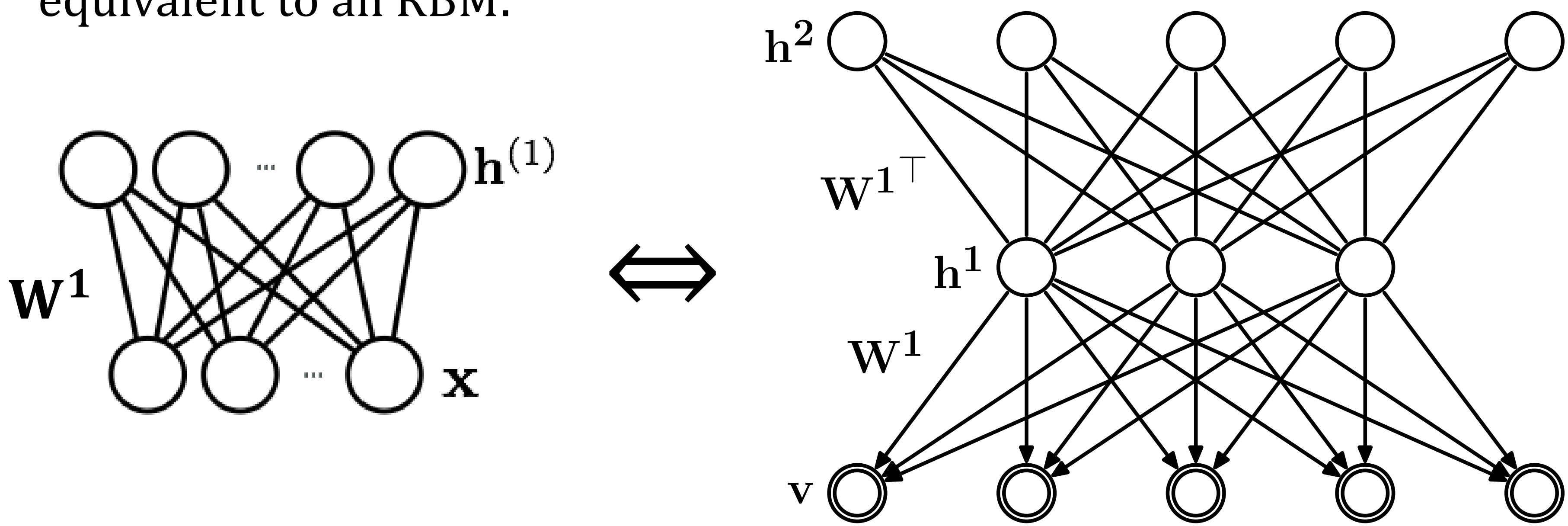






Improvement at initialization: weight-tied DBN is equivalent to a RBM

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

Improvement at initialization: weight-tied DBN is equivalent to a RBM

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**.
- 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 $\mathrm{q}(\mathbf{h}^{(1)}|\mathbf{x})$

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

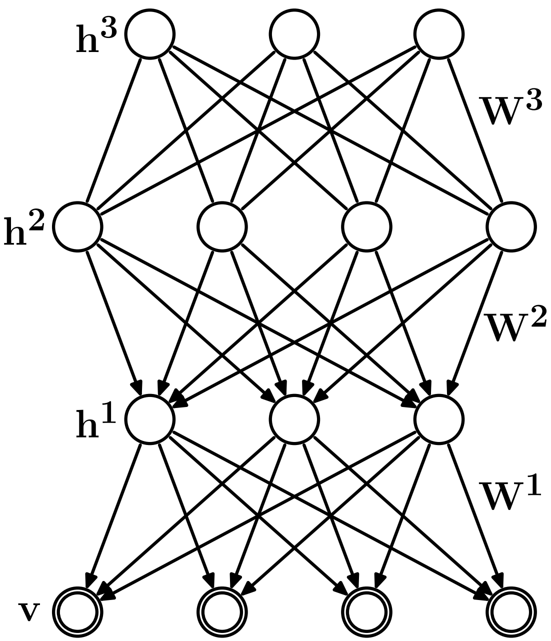
- A fast learning algorithm for deep belief nets. Hinton, Teh, Osindero, 2006.

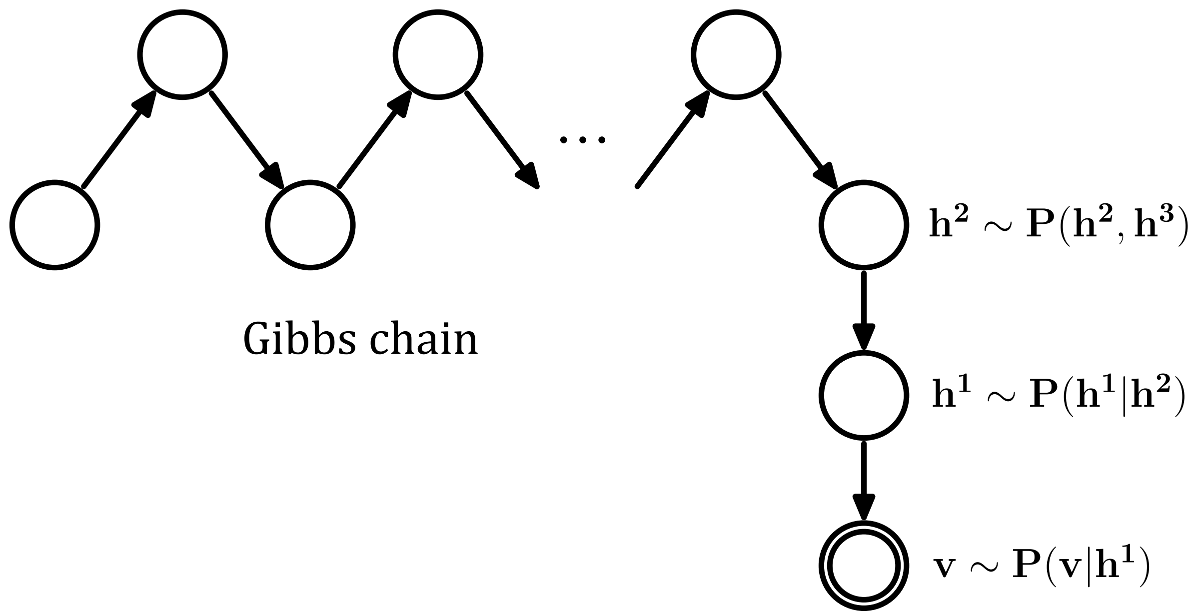
Sampling from DBNs

- To sample from the DBN model:

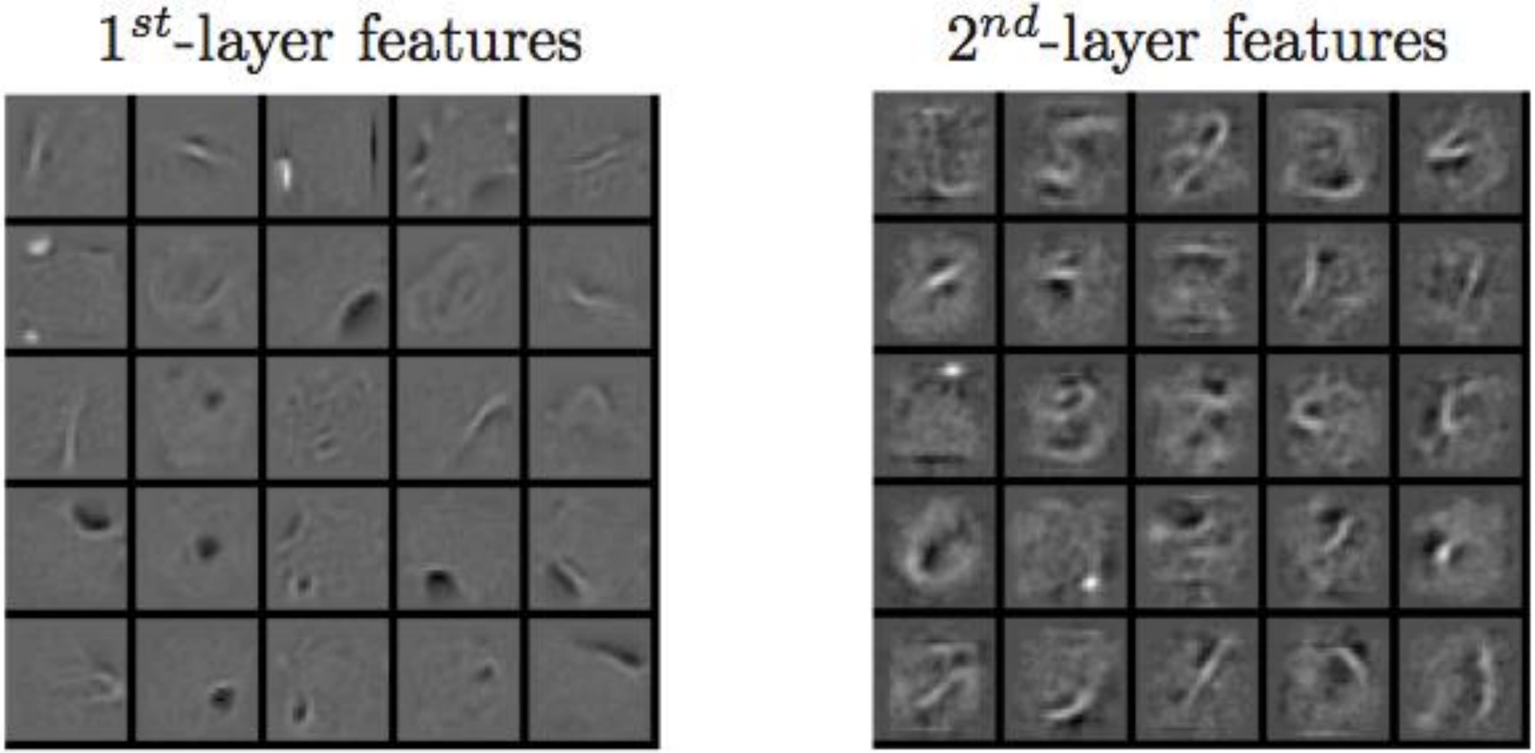
$$P(\mathbf{v}, \mathbf{h}^1, \mathbf{h}^2, \mathbf{h}^3) = P(\mathbf{v}|\mathbf{h}^1)P(\mathbf{h}^1|\mathbf{h}^2)P(\mathbf{h}^2, \mathbf{h}^3)$$

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



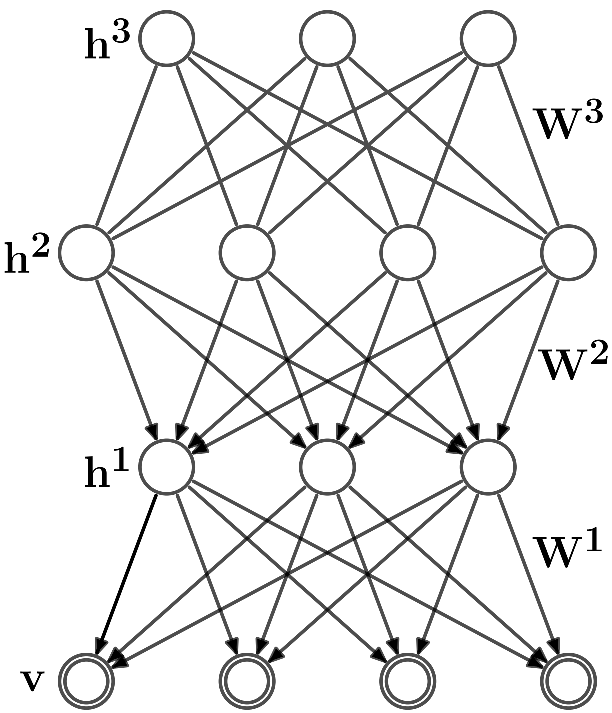


Learned Features

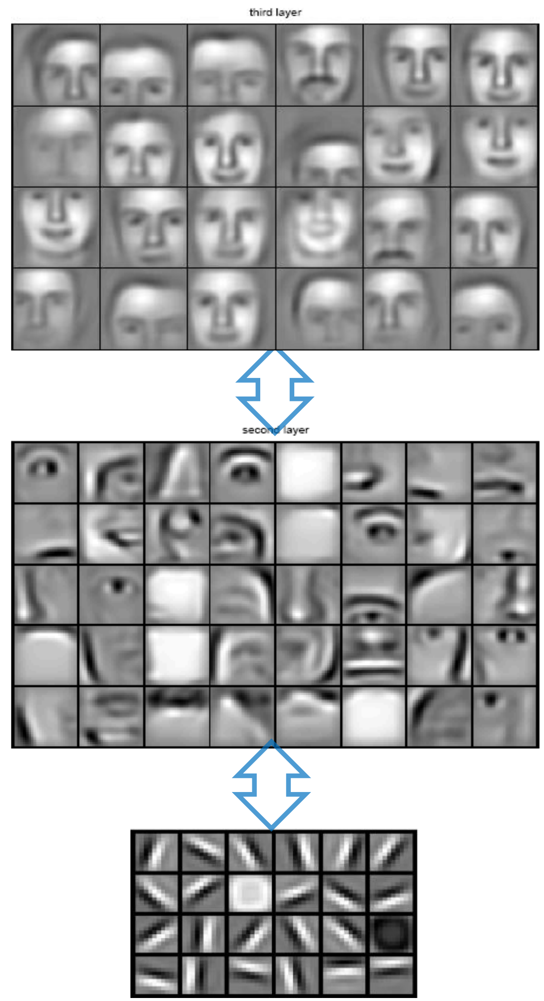


Learning Part-based Representation

Convolutional DBN



Faces



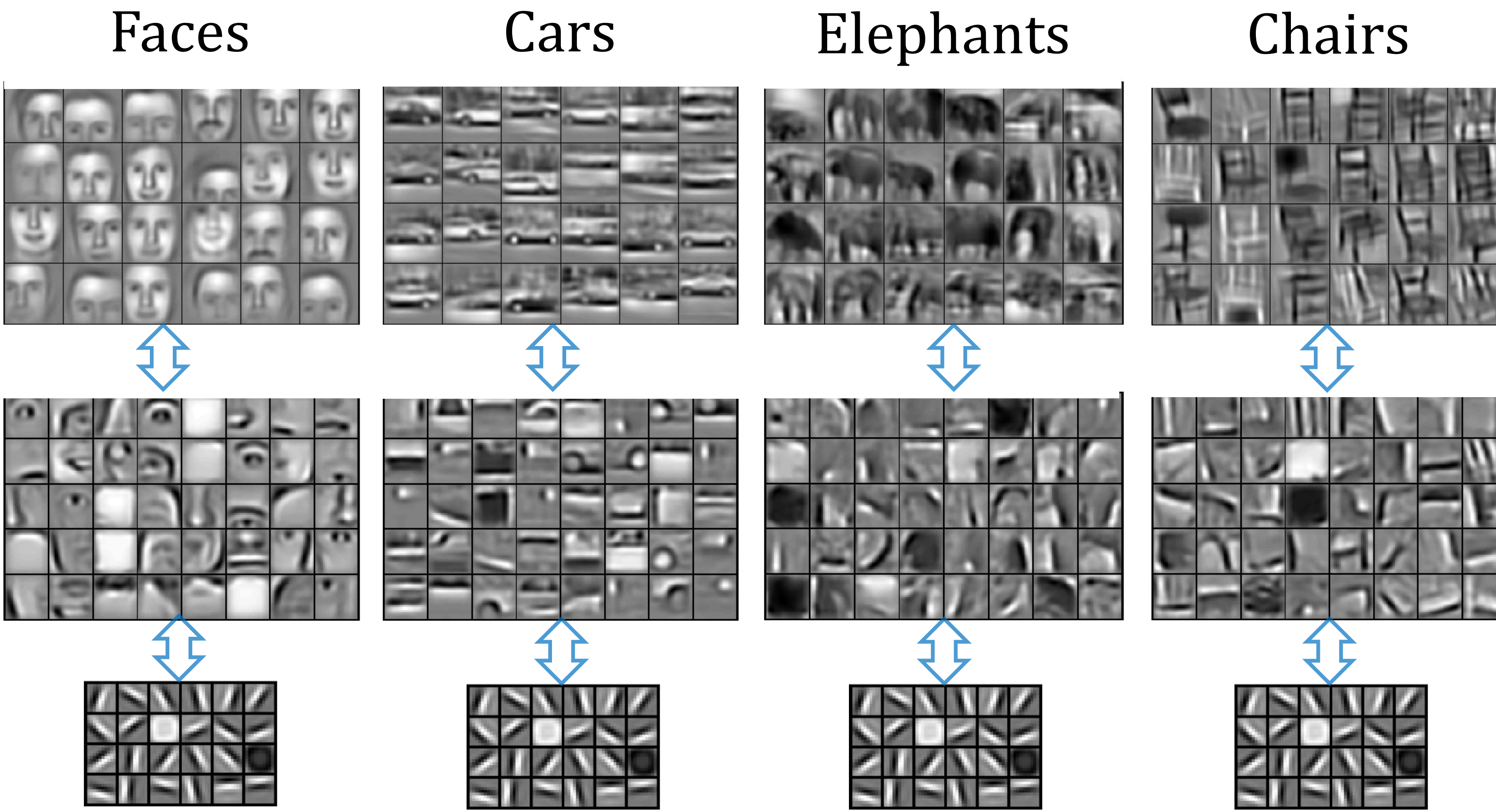
Groups of parts.

Object Parts

Trained on face images.

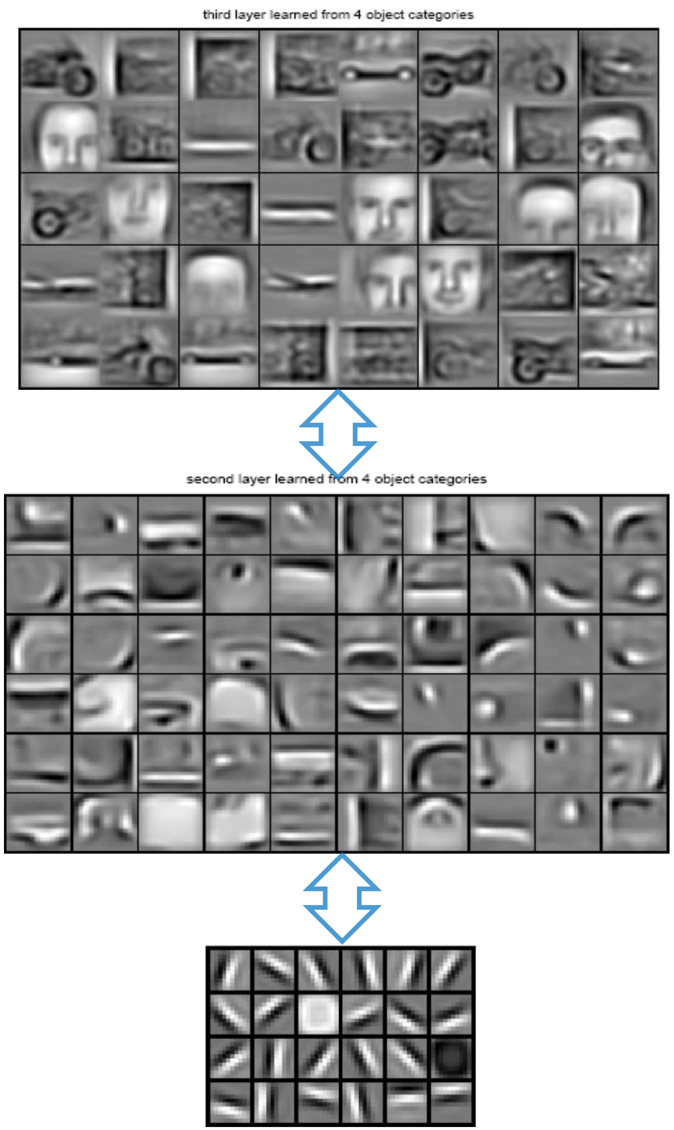
Lee et.al., ICML 2009

Learning Part-based Representation



Lee et.al., ICML 2009

Learning Part-based Representation



Groups of parts.

Class-specific object parts

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

Lee et.al., ICML 2009