## 10707 Deep Learning

Russ Salakhutdinov

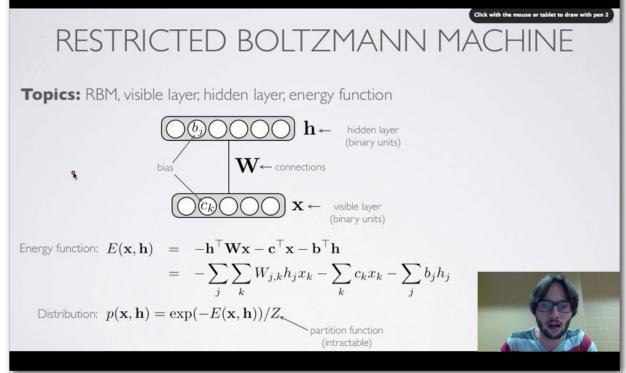
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Deep Belief Networks

#### Neural Networks Online Course

- **Disclaimer**: Much of the material and slides for this lecture were borrowed from Hugo Larochelle's class on Neural Networks: https://sites.google.com/site/deeplearningsummerschool2016/
- Hugo's class covers many other topics: convolutional networks, neural language model, Boltzmann machines, autoencoders, sparse coding, etc.
- We will use his material for some of the other lectures.

http://info.usherbrooke.ca/hlarochelle/neural\_networks



### Multilayer Neural Net

- Consider a network with L hidden layers.
- layer pre-activation for k>0

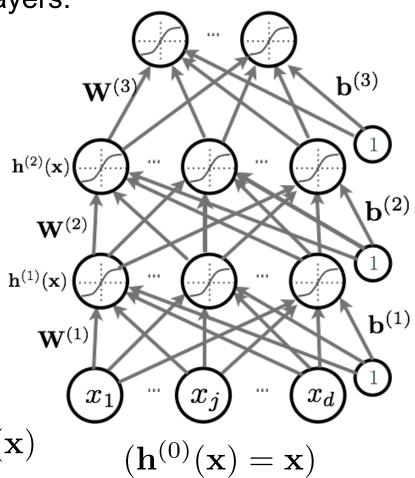
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

hidden layer activation from 1 to L:

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

output layer activation (k=L+1):

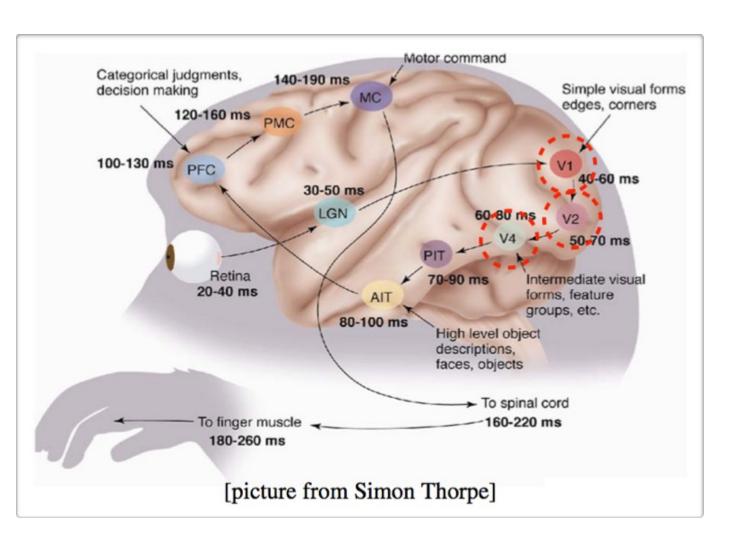
$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$

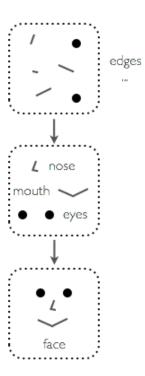


### Learning Distributed Representations

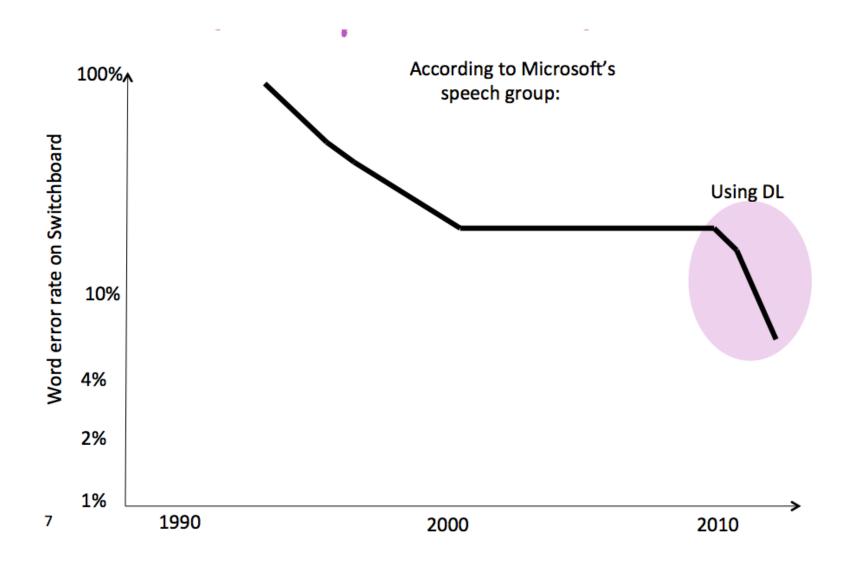
- Deep learning is research on learning models with multilayer representations
  - multilayer (feed-forward) neural networks
  - multilayer graphical model (deep belief network, deep Boltzmann machine)
- Each layer learns "distributed representation"
  - Units in a layer are not mutually exclusive
    - each unit is a separate feature of the input
    - two units can be "active" at the same time
  - Units do not correspond to a partitioning (clustering) of the inputs
    - in clustering, an input can only belong to a single cluster

#### Inspiration from Visual Cortex



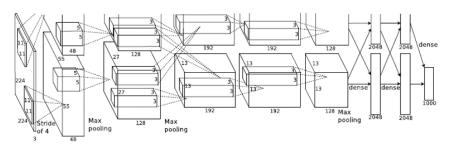


#### Success Story: Speech Recognition



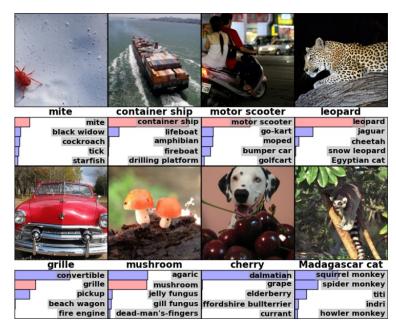
### Success Story: Image Recognition

Deep Convolutional Nets for Vision (Supervised)



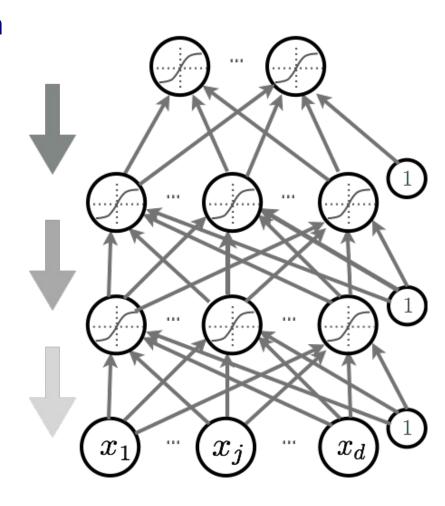


1.2 million training images 1000 classes



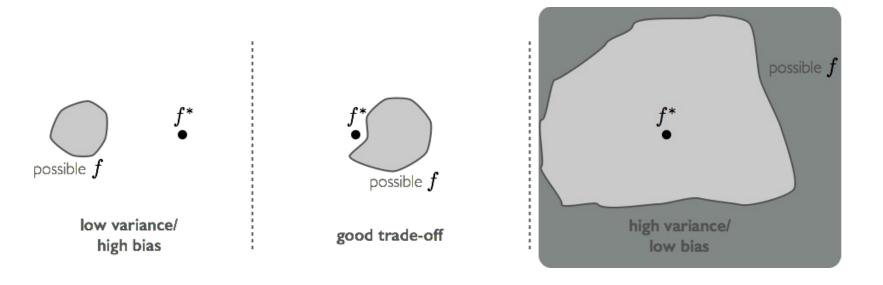
### Why Training is Hard

- First hypothesis: Hard optimization problem (underfitting)
  - vanishing gradient problem
  - saturated units block gradient propagation
- •This is a well known problem in recurrent neural networks



### Why Training is Hard

- Second hypothesis: Overfitting
  - we are exploring a space of complex functions
  - deep nets usually have lots of parameters
- Might be in a high variance / low bias situation

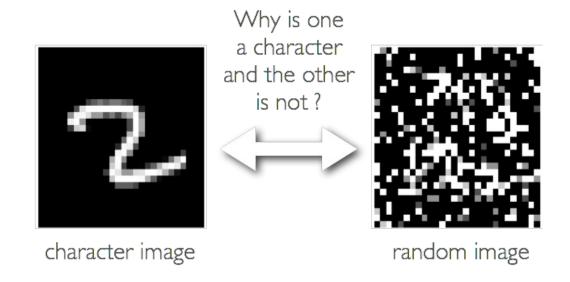


#### Why Training is Hard

- First hypothesis (underfitting): better optimize
  - Use better optimization tools (e.g. batch-normalization, second order methods, such as KFAC)
  - Use GPUs, distributed computing.
- Second hypothesis (overfitting): use better regularization
  - Unsupervised pre-training
  - Stochastic drop-out training
- For many large-scale practical problems, you will need to use both: better optimization and better regularization!

#### **Unsupervised Pre-training**

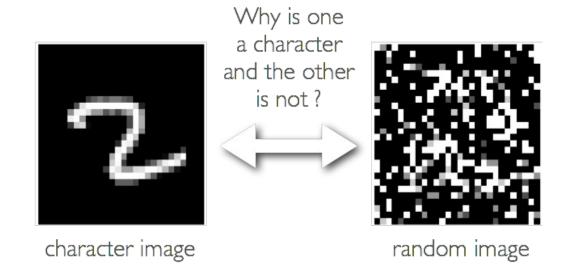
- Initialize hidden layers using unsupervised learning
  - Force network to represent latent structure of input distribution



Encourage hidden layers to encode that structure

#### **Unsupervised Pre-training**

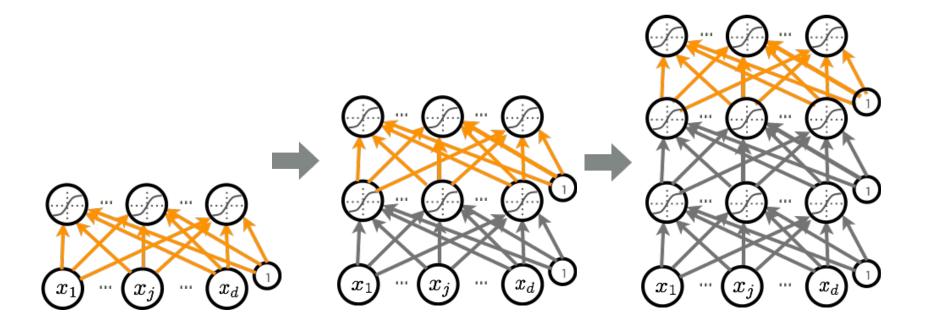
- Initialize hidden layers using unsupervised learning
  - This is a harder task than supervised learning (classification)



Hence we expect less overfitting

#### Pre-training

- We will use a greedy, layer-wise procedure
  - > Train one layer at a time with unsupervised criterion
  - > Fix the parameters of previous hidden layers
  - Previous layers viewed as feature extraction



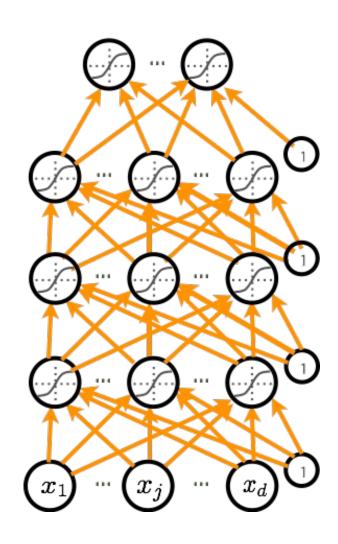
#### Pre-training

- Unsupervsed Pre-training
  - first layer: find hidden unit features that are more common in training inputs than in random inputs
  - second layer: find combinations of hidden unit features that are more common than random hidden unit features
  - third layer: find combinations of combinations of ...

 Pre-training initializes the parameters in a region such that the near local optima overfit less the data

### Fine-tuning

- Once all layers are pre-trained
  - add output layer
  - train the whole network using supervised learning
- Supervised learning is performed as in a regular network
  - forward propagation, backpropagation and update
- We call this last phase fine-tuning
  - all parameters are "tuned" for the supervised task at hand
  - representation is adjusted to be more discriminative

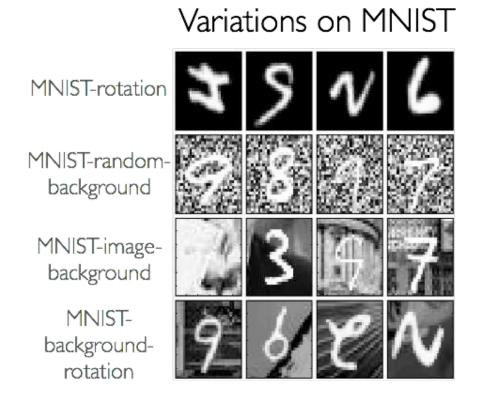


#### Stacking RBMs, Autoencoders

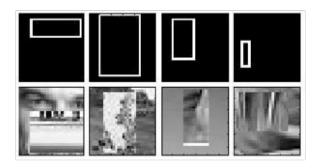
- Stacked Restricted Boltzmann Machines:
  - Hinton, Teh and Osindero suggested this procedure with RBMs,:
     A fast learning algorithm for deep belief nets.
  - To recognize shapes, first learn to generate images. Hinton, 2006.
- Stacked autoencoders, sparse-coding models, etc.
  - Bengio, Lamblin, Popovici and Larochelle (stacked autoencoders)
  - Ranzato, Poultney, Chopra and LeCun (stacked sparse coding models)
- Lots of others started stacking models together.

### Example

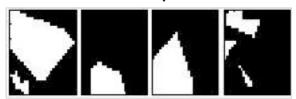
Datasets generated with varying number of factors of variations



Tall or wide?



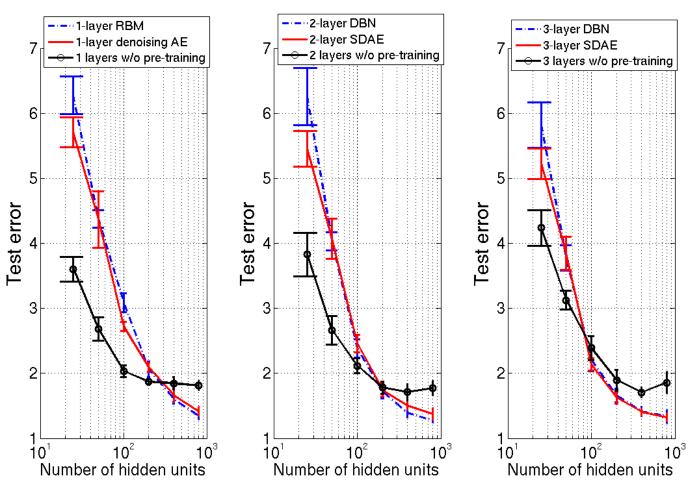
Convex shape or not?



# Impact of Initialization

Network		MNIST-small	MNIST-rotation
Type	Depth	classif. test error	classif. test error
Neural network	1	<b>4.14</b> % ± 0.17	$15.22 \% \pm 0.31$
	2	<b>4.03</b> % ± 0.17	<b>10.63</b> % ± 0.27
Deep net	3	<b>4.24</b> % ± 0.18	$11.98 \% \pm 0.28$
	4	$4.47 \% \pm 0.18$	$11.73 \% \pm 0.29$
Deep net +	1	$3.87 \% \pm 0.17$	$11.43\% \pm 0.28$
' .	2	<b>3.38</b> % ± 0.16	$9.88~\% \pm 0.26$
autoencoder	3	<b>3.37</b> % ± 0.16	<b>9.22</b> % ± 0.25
	4	<b>3.39</b> % ± 0.16	<b>9.20</b> % ± 0.25
Doop not +	1	$3.17 \% \pm 0.15$	$10.47 \% \pm 0.27$
Deep net +	2	<b>2.74</b> % ± 0.14	$9.54~\% \pm 0.26$
RBM	3	<b>2.71</b> % ± 0.14	<b>8.80</b> % ± 0.25
	4	<b>2.72</b> % ± 0.14	<b>8.83</b> % ± 0.24

### Impact of Pretraining



Acts as a regularizer: overfits less with large capacity, underfits with small capacity

#### Performance on Different Datasets

Stacked	Stacked	Stacked
Autoencoders	RBMS	Denoising Autoencoders
SAA-3	DBN-3	$\mathbf{SdA-3}\;(\nu)$
$3.46 \pm 0.16$	$3.11 \pm 0.15$	<b>2.80</b> ± <b>0.14</b> (10%)
$10.30{\pm}0.27$	$10.30{\pm}0.27$	10.29 $\pm$ 0.27 (10%)
$11.28 \pm 0.28$	$6.73 {\pm} 0.22$	$10.38 \pm 0.27 \ (40\%)$
$23.00 \pm 0.37$	$16.31{\pm}0.32$	<b>16.68</b> ± <b>0.33</b> (25%)
$51.93 \pm 0.44$	$47.39 \pm 0.44$	$44.49\pm0.44$ (25%)
$2.41 \pm 0.13$	$2.60 {\pm} 0.14$	$1.99 \pm 0.12 \ (10\%)$
$24.05 \pm 0.37$	$22.50 {\pm} 0.37$	21.59±0.36 (25%)
$18.41 {\pm} 0.34$	$18.63{\pm}0.34$	<b>19.06</b> ± <b>0.34</b> (10%)

#### Deep Autoencoder

Pre-training can be used to initialize a deep autoencoder

Pre-training initializes the optimization problem in a region with better local optima of the training objective

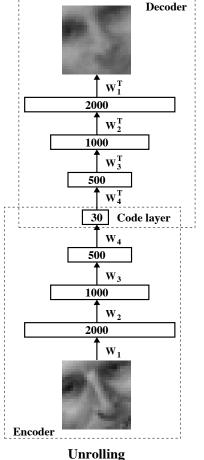
Each RBM used to initialize parameters both in encoder and decoder ("unrolling")

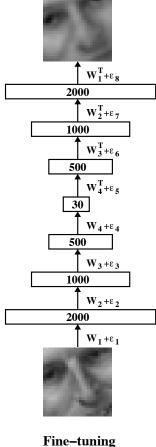
Better optimization algorithms can also help: Deep learning via Hessian-free optimization.

Martens, 2010

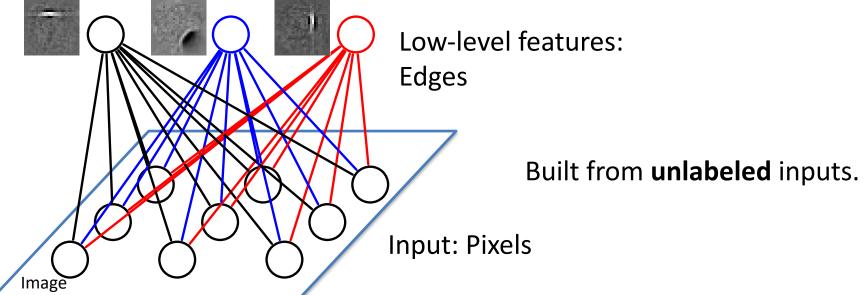
Top **RBM**  $\mathbf{W}_{3}$ **RBM** 1000 2000 RBM 2000 RBM

**Pretraining** 

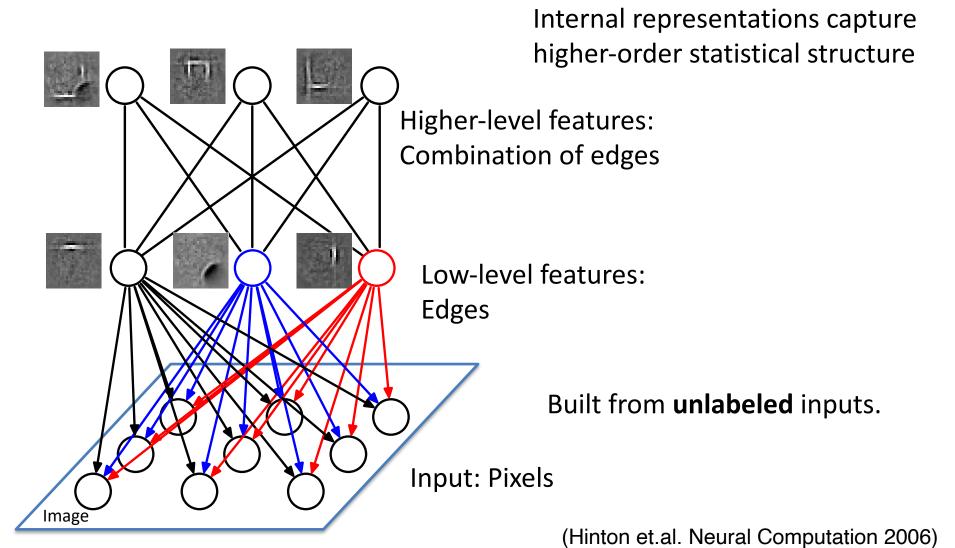


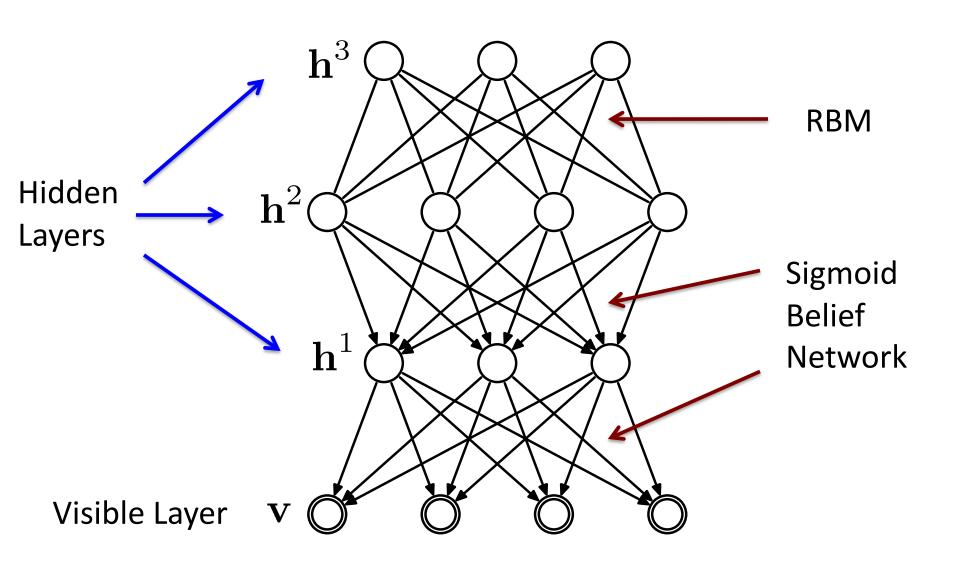


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(Hinton et.al. Neural Computation 2006)





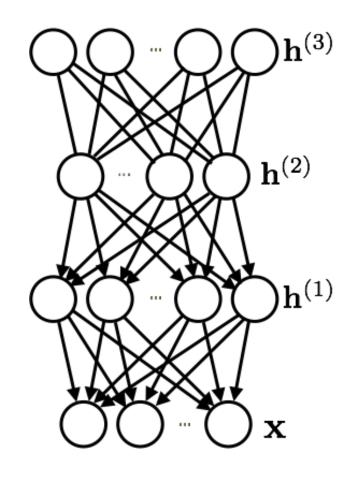
#### Deep Belief Networks:

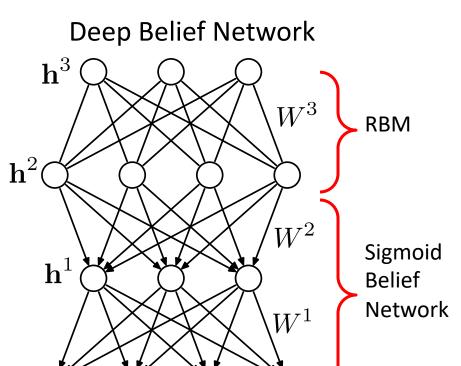
- it is a generative model that mixes undirected and directed connections between variables
- > top 2 layers' distribution  $p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)})$  is an RBM!
- other layers form a Bayesian network with conditional distributions:

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

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

This is not a feed-forward neural network





- > top 2 layers' distribution  $p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)})$  is an RBM
- other layers form a Bayesian network with conditional distributions:

$$p(h_j^{(1)} = 1 | \mathbf{h}^{(2)}) = \text{sigm}(\mathbf{b}^{(1)} + \mathbf{W}^{(2)}^{\top} \mathbf{h}^{(2)})$$
  
 $p(x_i = 1 | \mathbf{h}^{(1)}) = \text{sigm}(\mathbf{b}^{(0)} + \mathbf{W}^{(1)}^{\top} \mathbf{h}^{(1)})$ 

The joint distribution of a DBN is as follows

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

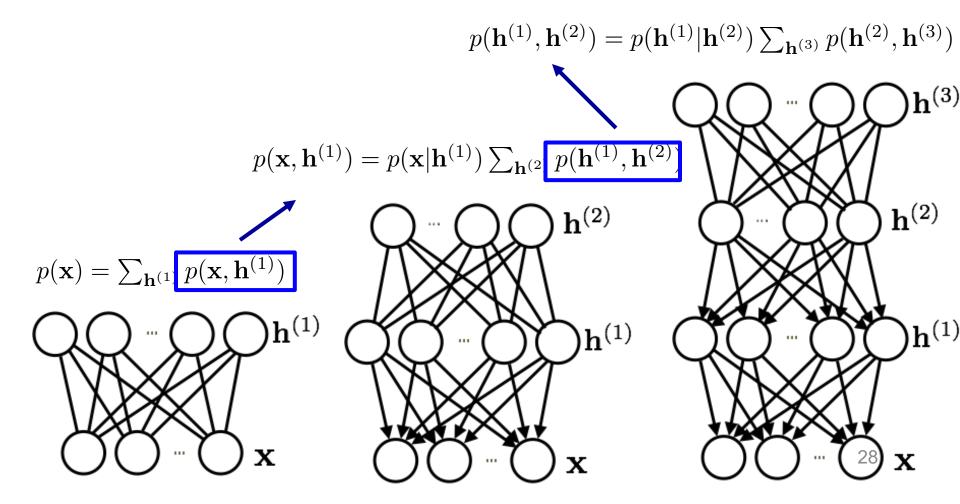
where

$$p(\mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \exp\left(\mathbf{h}^{(2)^{\top}} \mathbf{W}^{(3)} \mathbf{h}^{(3)} + \mathbf{b}^{(2)^{\top}} \mathbf{h}^{(2)} + \mathbf{b}^{(3)^{\top}} \mathbf{h}^{(3)}\right) / Z$$
$$p(\mathbf{h}^{(1)} | \mathbf{h}^{(2)}) = \prod_{j} p(h_j^{(1)} | \mathbf{h}^{(2)})$$
$$p(\mathbf{x} | \mathbf{h}^{(1)}) = \prod_{i} p(x_i | \mathbf{h}^{(1)})$$

As in a deep feed-forward network, training a DBN is hard

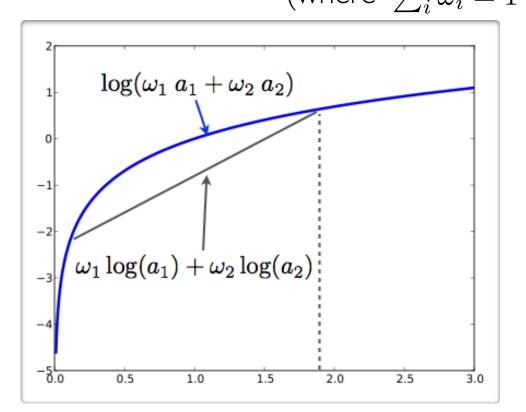
#### Layer-wise Pretraining

- This is where the RBM stacking procedure comes from:
  - idea: improve prior on last layer by adding another hidden layer



#### Concavity

$$\log(\sum_i \omega_i \ a_i) \geq \sum_i \omega_i \log(a_i)$$
 (where  $\sum_i \omega_i = 1$  and  $\omega_i \geq 0$ )



• For any model  $p(\mathbf{x}, \mathbf{h}^{(1)})$  with latent variables  $\mathbf{h}^{(1)}$  we can write:

$$\log p(\mathbf{x}) = \log \left( \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \frac{p(\mathbf{x}, \mathbf{h}^{(1)})}{q(\mathbf{h}^{(1)}|\mathbf{x})} \right)$$

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

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

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

where  $q(\mathbf{h}^{(1)}|\mathbf{x})$  is any approximation to  $p(\mathbf{h}^{(1)}|\mathbf{x})$ 

This is called a variational bound

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

- ightharpoonup if  $q(\mathbf{h}^{(1)}|\mathbf{x})$  is equal to the true conditional  $p(\mathbf{h}^{(1)}|\mathbf{x})$ , then we have an equality the bound is tight!
- the more  $q(\mathbf{h}^{(1)}|\mathbf{x})$  is different from  $p(\mathbf{h}^{(1)}|\mathbf{x})$  the less tight the bound is.

This is called a variational bound

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

In fact, difference between the left and right terms is the KL divergence between  $q(\mathbf{h}^{(1)}|\mathbf{x})$  and  $p(\mathbf{h}^{(1)}|\mathbf{x})$ :

$$KL(q||p) = \sum_{\mathbf{h}^{(1)}} q(\mathbf{h}^{(1)}|\mathbf{x}) \log \left( \frac{q(\mathbf{h}^{(1)}|\mathbf{x})}{p(\mathbf{h}^{(1)}|\mathbf{x})} \right)$$

This is called a variational bound

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

- for a single hidden layer DBN (i.e. an RBM), both the likelihood  $p(\mathbf{x}|\mathbf{h}^{(1)})$  and the prior  $p(\mathbf{h}^{(1)})$  depend on the parameters of the first layer.
- > we can now improve the model by building a better prior  $p(\mathbf{h}^{(1)})$

This is called a variational bound

adding 2nd layer means untying the parameters

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

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

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

This is called a variational bound

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 other terms are constant:

Layerwise pretraining improves variational lower bound

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

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

This is called a variational bound

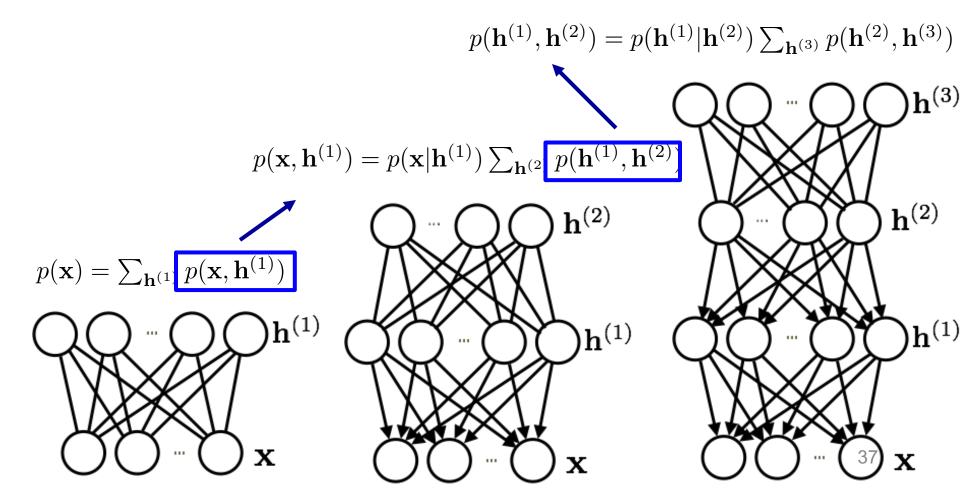
adding 2nd layer means untying the parameters

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

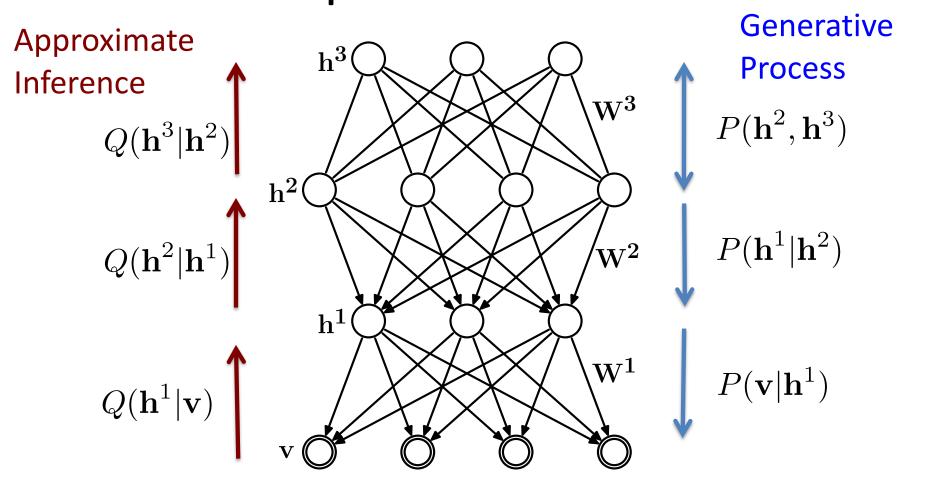
- for  $q(\mathbf{h}^{(1)}|\mathbf{x})$  we use the posterior of the first layer RBM. This is equivalent to a feed-forward (sigmoidal) layer, followed by sampling
- by initializing the weights of the second layer RBM as the transpose of the first layer weights, the bound is initially tight!
- a 2-layer DBN with tied weights is equivalent to a 1-layer RBM

### Layer-wise Pretraining

- This is where the RBM stacking procedure comes from:
  - idea: improve prior on last layer by adding another hidden layer

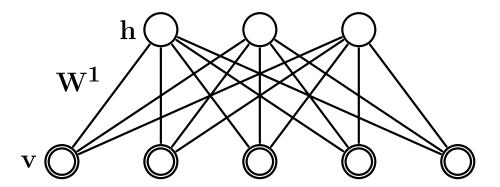


# Deep Belief Network

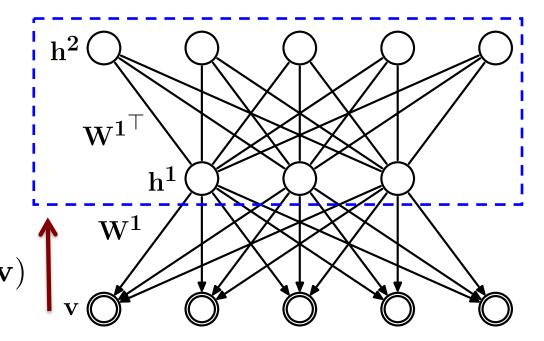


$$Q(\mathbf{h}^t | \mathbf{h}^{t-1}) = \prod_j \sigma \left( \sum_i W^t h_i^{t-1} \right) \qquad P(\mathbf{h}^{t-1} | \mathbf{h}^t) = \prod_j \sigma \left( \sum_i W^t h_i^t \right)$$

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



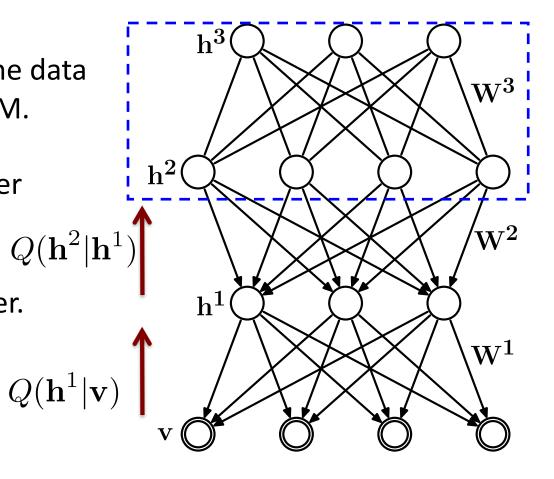
- Learn an RBM with an input layer v=x and a hidden layer h.
- Treat inferred values  $Q(\mathbf{h}^1|\mathbf{v}) = P(\mathbf{h}^1|\mathbf{v}) \text{ as the data}$  for training 2<sup>nd</sup>-layer RBM.
- Learn and freeze 2<sup>nd</sup> layer RBM.



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

Unsupervised Feature Learning.

- Treat inferred values  $Q(\mathbf{h}^1|\mathbf{v}) = P(\mathbf{h}^1|\mathbf{v}) \text{ as the data}$  for training 2<sup>nd</sup>-layer RBM.
- Learn and freeze 2<sup>nd</sup> layer RBM.
- Proceed to the next layer.



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

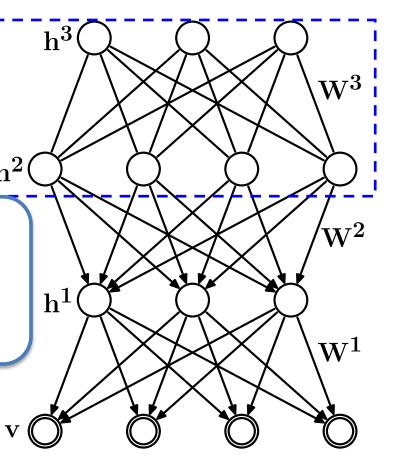
**RBM** 

Layerwise pretraining

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.

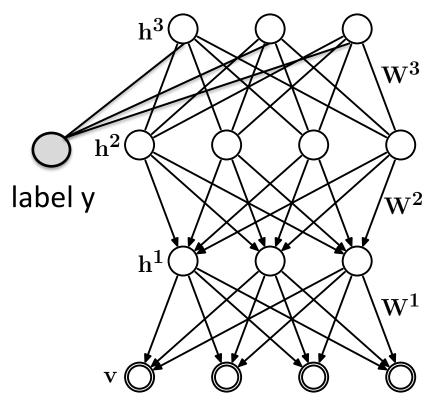
## Supervised Learning with DBNs

 If we have access to label information, we can train the joint generative model by maximizing the joint log-likelihood of data and labels

$$\log P(\mathbf{y}, \mathbf{v})$$

- Discriminative fine-tuning:
  - Use DBN to initialize a multilayer neural network.
  - Maximize the conditional distribution:

$$\log P(\mathbf{y}|\mathbf{v})$$

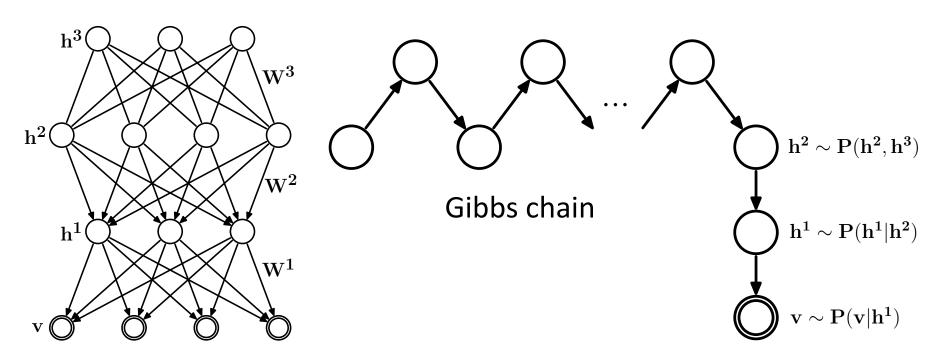


## Sampling from DBNs

• To sample from the DBN model:

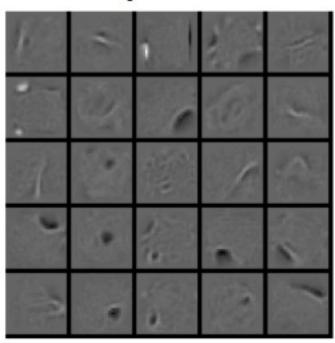
$$P(\mathbf{v}, \mathbf{h}^1, \mathbf{h}^2, \mathbf{h}^3) = P(\mathbf{v}|\mathbf{h}^1)P(\mathbf{h}^1|\mathbf{h}^2)P(\mathbf{h}^2, \mathbf{h}^3)$$

- Sample h<sup>2</sup> using alternating Gibbs sampling from RBM.
- Sample lower layers using sigmoid belief network.

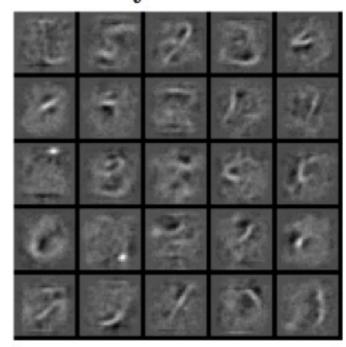


### Learned Features

 $1^{st}$ -layer features

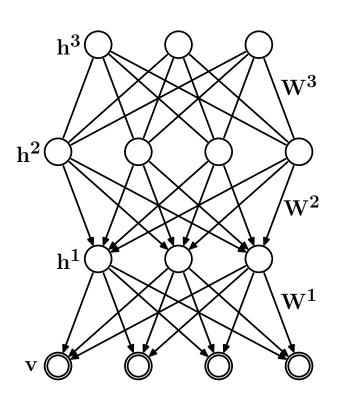


 $2^{nd}$ -layer features

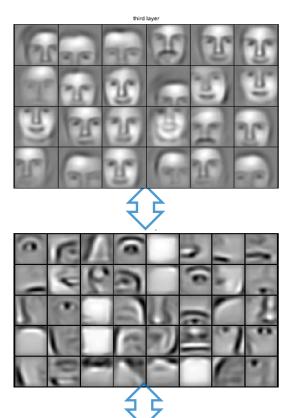


### Learning Part-based Representation

#### Convolutional DBN



#### **Faces**

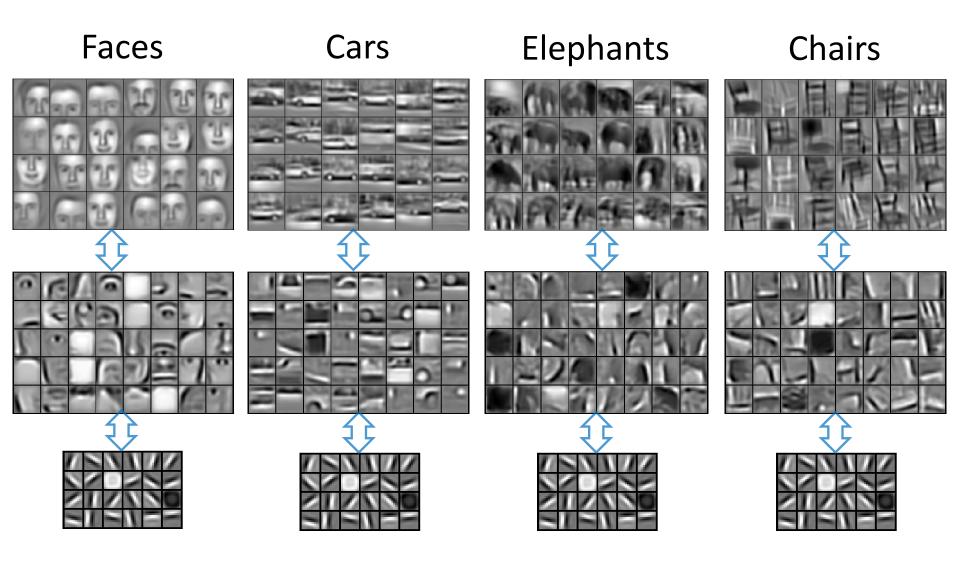


Groups of parts.

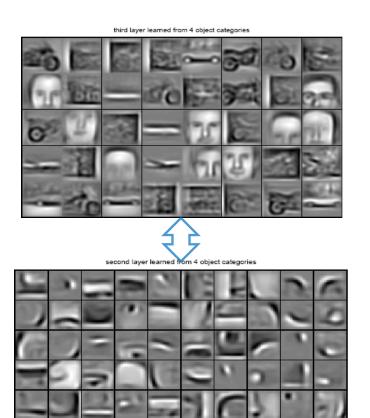
**Object Parts** 

Trained on face images.

## Learning Part-based Representation

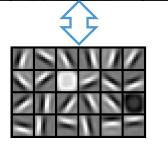


### Learning Part-based Representation



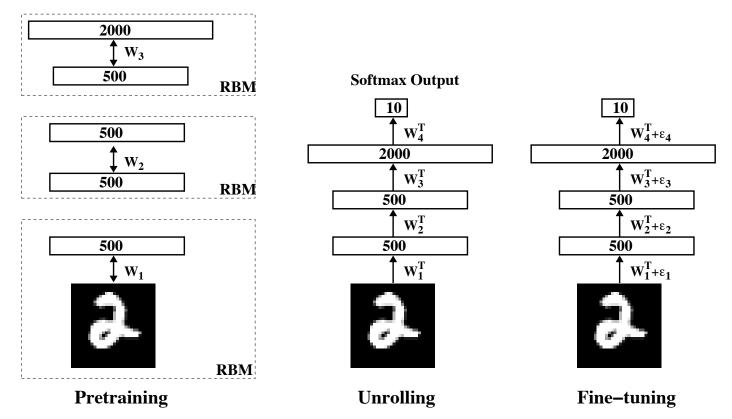
Groups of parts.

Class-specific object parts



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

### **DBNs** for Classification



- After layer-by-layer unsupervised pretraining, discriminative fine-tuning by backpropagation achieves an error rate of 1.2% on MNIST. SVM's get 1.4% and randomly initialized backprop gets 1.6%.
- Clearly unsupervised learning helps generalization. It ensures that most of the information in the weights comes from modeling the input data.

## **DBNs** for Regression

Predicting the orientation of a face patch



**Test Data** 



**Training Data:** 1000 face patches of 30 training people.

**Test Data:** 1000 face patches of **10 new people**.

**Regression Task:** predict orientation of a new face.

Gaussian Processes with spherical Gaussian kernel achieves a RMSE (root mean squared error) of 16.33 degree.

## **DBNs** for Regression

#### **Training Data**



Additional Unlabeled Training Data: 12000 face patches from 30 training people.

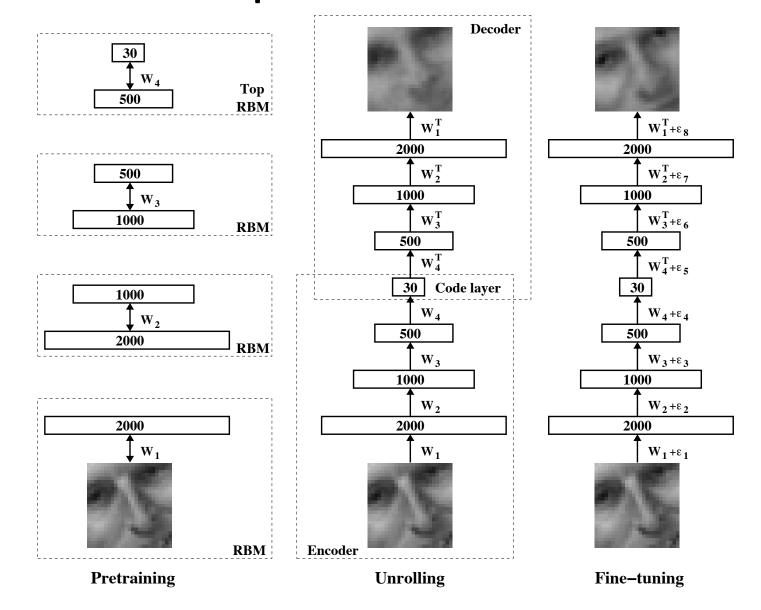
- Pretrain a stack of RBMs: 784-1000-1000-1000.
- Features were extracted with no idea of the final task.

The same GP on the top-level features: RMSE: 11.22

GP with fine-tuned covariance Gaussian kernel: RMSE: 6.42

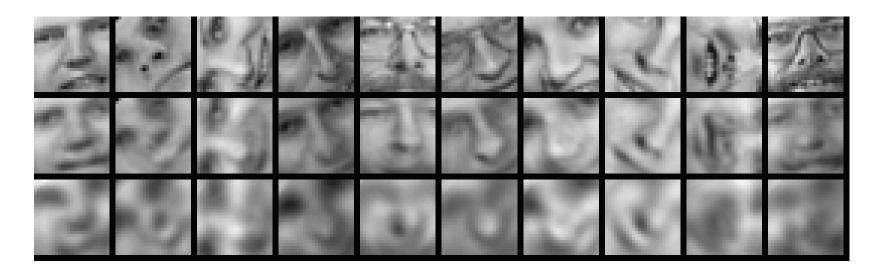
Standard GP without using DBNs: RMSE: 16.33

# Deep Autoencoders



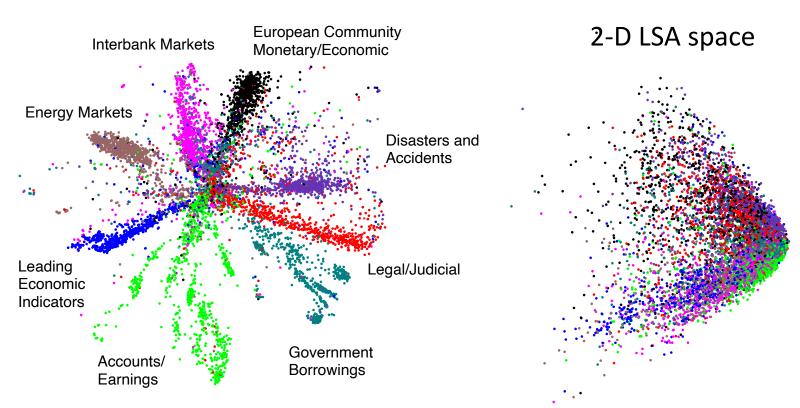
## Deep Autoencoders

• We used 25x25 - 2000 - 1000 - 500 - 30 autoencoder to extract 30-D real-valued codes for Olivetti face patches.



- **Top**: Random samples from the test dataset.
- Middle: Reconstructions by the 30-dimensional deep autoencoder.
- **Bottom**: Reconstructions by the 30-dimentinoal PCA.

### Information Retrieval



- The Reuters Corpus Volume II contains 804,414 newswire stories (randomly split into 402,207 training and 402,207 test).
- "Bag-of-words" representation: each article is represented as a vector containing the counts of the most frequently used 2000 words in the training set.

  (Hinton and Salakhutdinov, Science 2006)