Artificial Neural Networks II

STAT 27725/CMSC 25400: Machine Learning

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- Things we will look at today

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  - Regularization in Neural Networks

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  - Generative Neural Methods

A Short Primer on Regularization: Empirical Risk

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- Ideally, our goal is to minimize the *expected loss*, called the *risk*

$$R(\mathbf{w}) = \mathbb{E}_{(x_0,y_0)\sim p(x,y)}[L(f(x_0;\mathbf{w}), y_0)]$$

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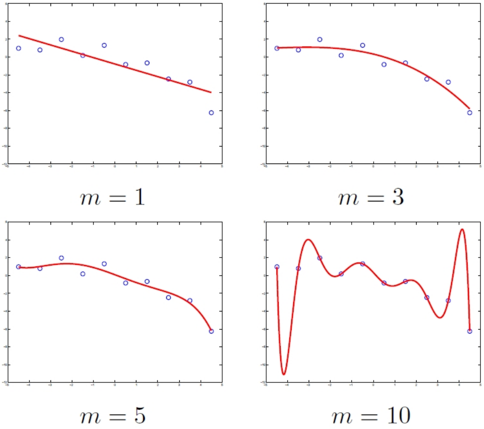
- The true distribution is unknown. So, we instead work with a proxy that is measurable: Empirical loss on the training set

$$L(\mathbf{w}, X, y) = \frac{1}{N}\sum_{i=1}^{N} L(f(x_i; \mathbf{w}), y_i)$$

Model Complexity and Overfitting

Consider data drawn from a 3rd order model:



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How to avoid overfitting?

- If a model overfits (is too sensitive to the data), it would be unstable and will not generalize well.
- Intuitively, the complexity of the model can be measured by the number of "degrees of freedom" (independent parameters) (previous example?)
- Idea: Directly penalize by the number of parameters (called the Akaike Information criterion): minimize

$$\sum_{i=1}^{N} L(f(x_i; \mathbf{w}), y_i) + \#\text{params}$$

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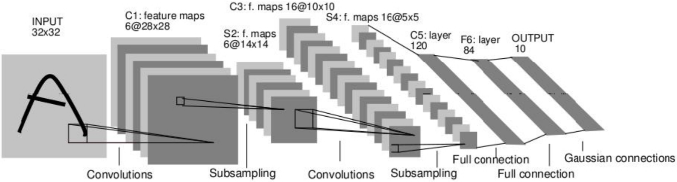
- Regularization is basically a way to implement Occam's Razor

Regularization in Neural Networks

- We have infact already looked at one method (for vision tasks)



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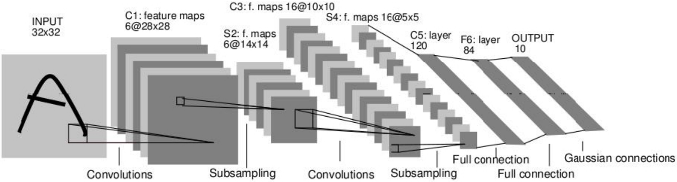

- How is this a form of regularization?

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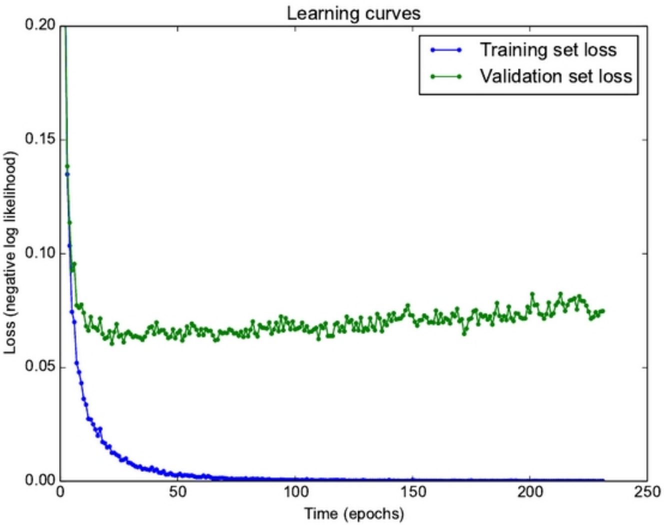
- Why is it called Weight decay?
- **Parameter sharing** (CNNs, RNNs)
- **Dataset Augmentation** ImageNet 2012, discussed last time was won by significant dataset augmentation

Regularization in Neural Networks

- **Early Stoppping:**



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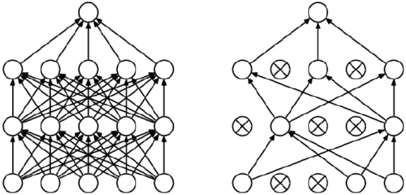
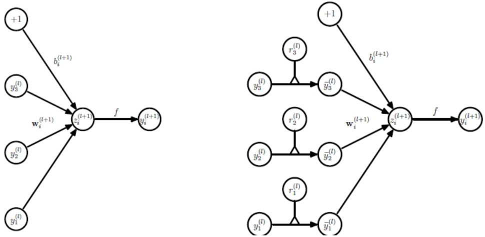


(a) Standard Neural Net (b) After applying dropout.

Dropout: A simple way to prevent neural networks from overfitting, N Srivastava, G Hinton, A Krizhevsky, I Sutskever, R Salakhutdinov, JMLR 2014

Dropout: Feedforward Operation



Without dropout: $z_i^{(l+1)} = w_i^{(l+1)} y^l + b_i^{(l+1)}$, and $y_i^{l+1} = f(z_i^{(l+1)})$

With dropout:

$r_j^{(l)} =$ Bernoulli(p)

$\tilde{y}^{(l)} = r^{(l)} * y^{(l)}$

$z_i^{(l+1)} = w_i^{(l+1)} \tilde{y}^l + b_i^{(l+1)}$

$y_i^{l+1} = f(z_i^{(l+1)})$

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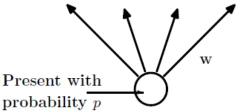
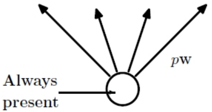


(a) At training time



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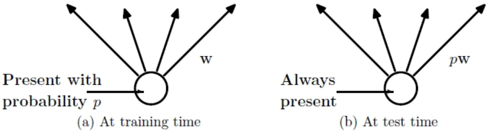
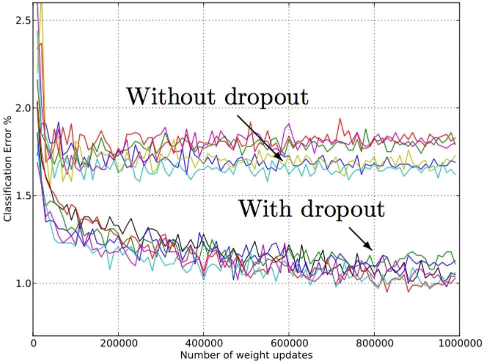


- Extreme form of bagging

Dropout: Performance

These architectures have 2 to 4 hidden layers with 1024 to 2048 hidden units

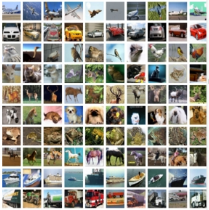


Dropout: Performance

(a) Street View House Numbers (SVHN)

Method	Error %
Binary Features (WDCH) (Netzer et al., 2011)	36.7
HOG (Netzer et al., 2011)	15.0
Stacked Sparse Autoencoders (Netzer et al., 2011)	10.3
KMeans (Netzer et al., 2011)	9.4
Multi-stage Conv Net with average pooling (Sermanet et al., 2012)	9.06
Multi-stage Conv Net + L2 pooling (Sermanet et al., 2012)	5.36
Multi-stage Conv Net + L4 pooling + padding (Sermanet et al., 2012)	4.90
Conv Net + max-pooling	3.95
Conv Net + max pooling + dropout in fully connected layers	3.02
Conv Net + stochastic pooling (Zeiler and Fergus, 2013)	2.80
Conv Net + max pooling + dropout in all layers	2.55
Conv Net + maxout (Goodfellow et al., 2013)	**2.47**
Human Performance	2.0

Table 3: Results on the Street View House Numbers data set.



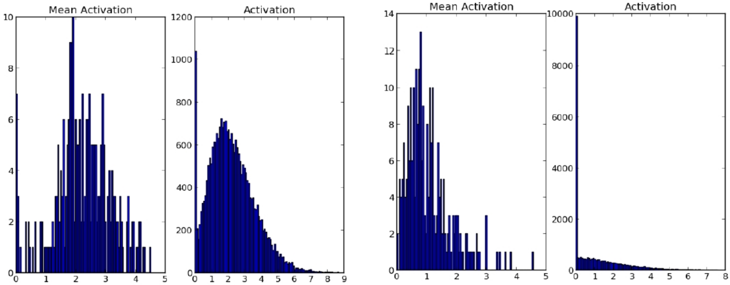
(b) CIFAR-10

Method	CIFAR-10	CIFAR-100
Conv Net + max pooling (hand tuned)	15.60	43.48
Conv Net + stochastic pooling (Zeiler and Fergus, 2013)	15.13	42.51
Conv Net + max pooling (Snoek et al., 2012)	14.98	-
Conv Net + max pooling + dropout fully connected layers	14.32	41.26
Conv Net + max pooling + dropout in all layers	12.61	**37.20**
Conv Net + maxout (Goodfellow et al., 2013)	**11.68**	38.57

Table 4: Error rates on CIFAR-10 and CIFAR-100.

Dropout: A simple way to prevent neural networks from overfitting, N Srivastava, G Hinton, A Krizhevsky, I Sutskever, R Salakhutdinov, JMLR 2014

Dropout: Effect on Sparsity



(a) Without dropout (b) Dropout with $p = 0.5$.

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- Thus, dropout with linear regression is equivalent, in expectation to ridge regression with a particular form of Γ

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- Seems plausible that asexual reproduction should be a better way to optimize for individual fitness (in sexual reproduction if a good combination is found, it's split again)
- Criterion for natural selection may not be individual fitness but mixability. Thus role of sexual reproduction is not just to allow useful new genes to propagate but also to ensure that complex coadaptations between genes are broken

Sequence Learning with Neural Networks

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- Recurrent Neural Networks address this issue by having loops.

Some Sequence Tasks

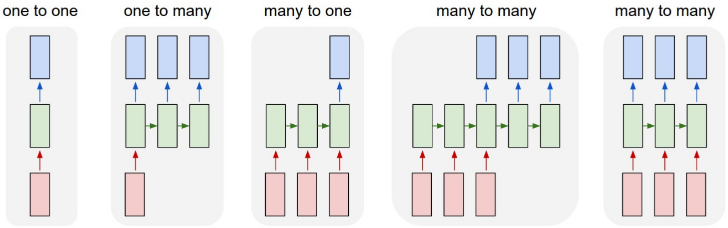
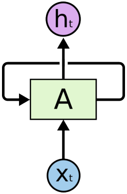


Figure credit: Andrej Karpathy

Recurrent Neural Networks

- The loops in them allow the information to persist



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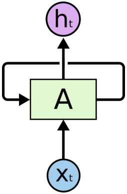

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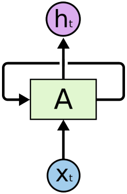

- For some input x_i, we pass it through a hidden state A and then output a value h_i. The loop allows information to be passed from one time step to another
- A RNN can be thought of as multiple copies of the same network, each of which passes a message to its successor

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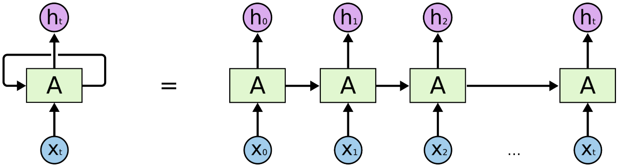

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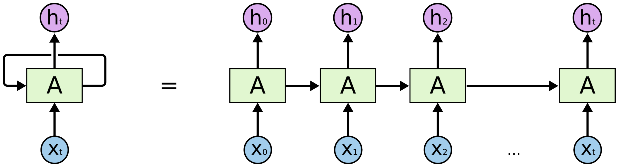

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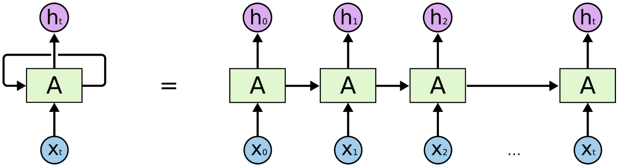

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- RNN is a recurrence of the form:

$$h_t^l = tanh W^l \begin{pmatrix} h_t^{l-1} \\ h_{t-1}^l \end{pmatrix}$$

Illustration credit: Chris Olah

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- "If training vanilla neural nets is optimization over functions, training recurrent nets is optimization over programs"

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- Train the network as if there were no constraints, obtain weights at different time stamps, average them

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- Sometimes the context can be clear immediately: "The clouds are in the *sky*"
- Sometimes the dependency is more long term: "We are basically from Transylvania, although I grew up in Spain, but I can still speak fluent *Romanian*."
- In principle, RNNs should be able to learn long term dependencies with the right parameter choices, but learning those parameters is hard.

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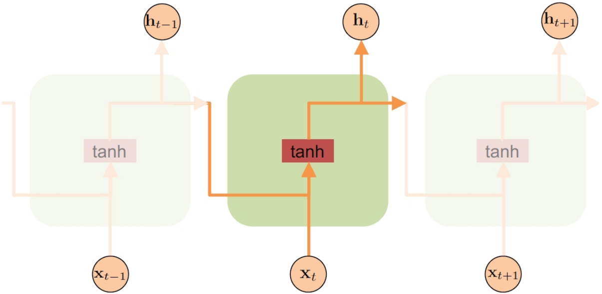
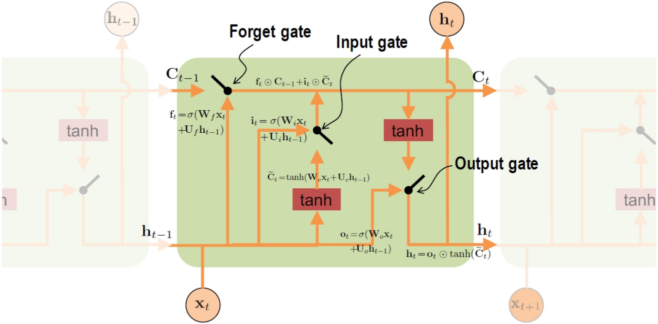
- Consider a language model in which the task is to predict the next word based on the previous
- Sometimes the context can be clear immediately: "The clouds are in the *sky*"
- Sometimes the dependency is more long term: "We are basically from Transylvania, although I grew up in Spain, but I can still speak fluent *Romanian*."
- In principle, RNNs should be able to learn long term dependencies with the right parameter choices, but learning those parameters is hard.
- The Long Short Term Memory was proposed to solve this problem (Hochreiter and Schmidhuber, 1997)

Long Short Term Memory Networks



Vanilla RNN: Error propagation is blocked by a non-linearity *Illustration credit: Chris Olah*

Long Short Term Memory Networks



Long Short Term Memory

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- There are three types of gates in LSTM (e.g. forget gate helps the LSTM to learn to forget)

Long Short Term Memory

- Precise form of the LSTM update is:

$$\begin{pmatrix} i \\ f \\ o \\ \hat{C}_t \end{pmatrix} = \begin{pmatrix} sigm \\ sigm \\ sigm \\ tanh \end{pmatrix} W^l \begin{pmatrix} h_t^{l-1} \\ h_{t-1}^l \end{pmatrix}$$

$$c_t^l = f \odot c_{t-1}^l + i \odot \hat{C}_t, \text{ and } h_t^l = o \odot tanh(c_t^l)$$

Some Applications: Caption Generation

Caption Generation (Karpathy and Li, 2014)

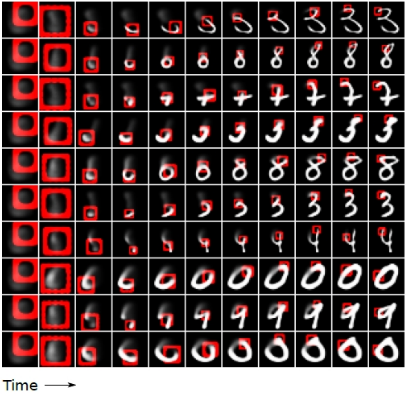
RNN Shakespeare

Using a character level language model trained on all of Shakespeare.

VIOLA: Why, Salisbury must find his flesh and thought That which I am not aps, not a man and in fire, To show the reining of the raven and the wars To grace my hand reproach within, and not a fair are hand, That Caesar and my goodly father's world; When I was heaven of presence and our fleets, We spare with hours, but cut thy council I am great, Murdered and by thy master's ready there My power to give thee but so much as hell: Some service in the noble bondman here, Would show him to her wine.

KING LEAR: O, if you were a feeble sight, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

Image Generation



(Also uses attention mechanism - not discussed) DRAW: A Recurrent Neural Network For Image Generation (Gregor *et al.*, 2015)

Applications

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Generative Neural Models

Recap: Multilayered Neural Networks

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- This is called the softmax and can be used as an estimator of $p(Y = i|x)$

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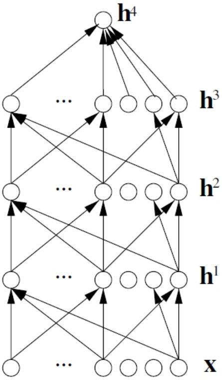

One loss to be considered: $L(h^l, y) = -\log P(Y = y|x)$

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- Purely discriminative. No generative model for the raw input features x (connections go upwards)

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- Use the parameters learned to initialize a feedforward neural network, and fine tune for classification

Sigmoid Belief Networks, 1992

- The generative model is decomposed as:

$$P(x, h^1, \ldots, h^l) = P(h^l)\Big(\prod_{k=1}^{l-1} P(h^k|h^{k+1})\Big)P(x|h^1)$$

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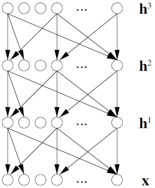

R. Neal, Connectionist learning of belief networks, 1992

Dayan, P., Hinton, G. E., Neal, R., and Zemel, R. S. The Helmholtz Machine, 1995

L. Saul, T. Jaakkola, and M. Jordan, Mean field theory for sigmoid belief networks, 1996

Deep Belief Networks, 2006

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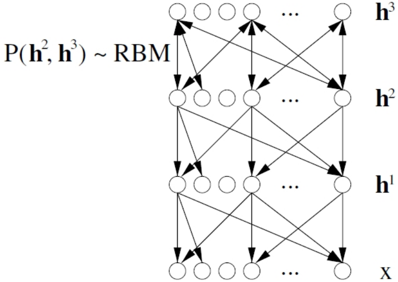

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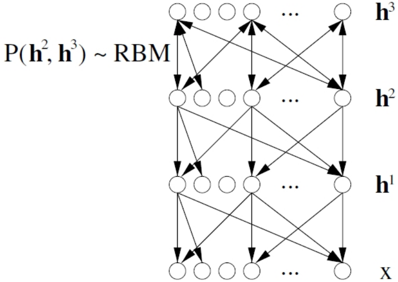

- The joint distribution of the top two layers is a Restricted Boltzmann Machine

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- Such models assign a scalar energy to each configuration of the variables of interest. Learning then corresponds to modifying the energy function so that its shape has desirable properties

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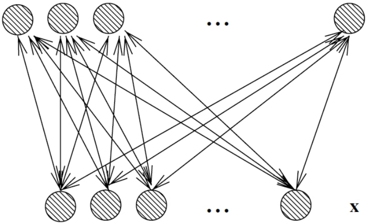
- The data log-likelihood gradient has an interesting form (details skipped)

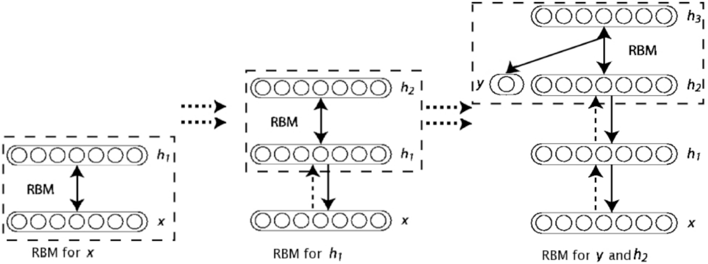
Restricted Boltzmann Machines



$$
\begin{aligned}
P(\mathbf{h}|\mathbf{x}) &= \frac{\exp(\mathbf{b}'\mathbf{x} + \mathbf{c}'\mathbf{h} + \mathbf{h}'W\mathbf{x})}{\sum_{\tilde{\mathbf{h}}} \exp(\mathbf{b}'\mathbf{x} + \mathbf{c}'\tilde{\mathbf{h}} + \tilde{\mathbf{h}}'W\mathbf{x})} \\
&= \frac{\prod_i \exp(\mathbf{c}_i\mathbf{h}_i + \mathbf{h}_i W_i \mathbf{x})}{\prod_i \sum_{\tilde{\mathbf{h}}_i} \exp(\mathbf{c}_i\tilde{\mathbf{h}}_i + \tilde{\mathbf{h}}_i W_i \mathbf{x})} \\
&= \prod_i \frac{\exp(\mathbf{h}_i(\mathbf{c}_i + W_i\mathbf{x}))}{\sum_{\tilde{\mathbf{h}}_i} \exp(\tilde{\mathbf{h}}_i(\mathbf{c}_i + W_i\mathbf{x}))} \\
&= \prod_i P(\mathbf{h}_i|\mathbf{x}).
\end{aligned}
$$

$$x_1 \to h_1 \sim P(h|x_1) \to x_2 \sim P(x|h_1) \to h_2 \sim P(h|x_2) \to \dots$$

Back to Deep Belief Networks



Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)
→ Supervised deep neural network

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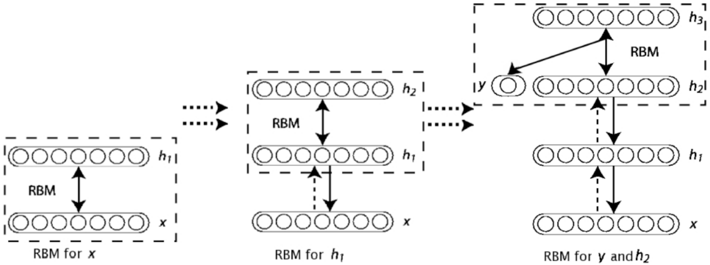

Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)
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- Everything is completely unsupervised till now. We can treat these weights learned as an initialization, treat the network as a feedword network and fine tune using backpropagation

Deep Belief Networks

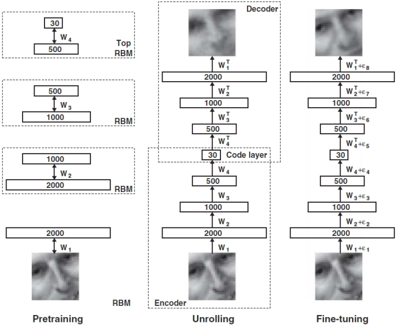
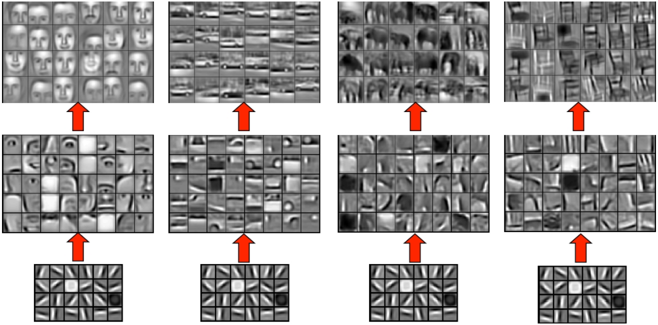


Fig. 1. Pretraining consists of learning a stack of restricted Boltzmann machines (RBMs), each having only one layer of feature detectors. The learned feature activations of one RBM are used as the "data" for training the next RBM in the stack. After the pretraining, the RBMs are "unrolled" to create a deep autoencoder, which is then fine-tuned using backpropagation of error derivatives.

G. E. Hinton, R. R. Salakhutdinov, Reducing the dimensionality of data with neural networks, Science, 2006

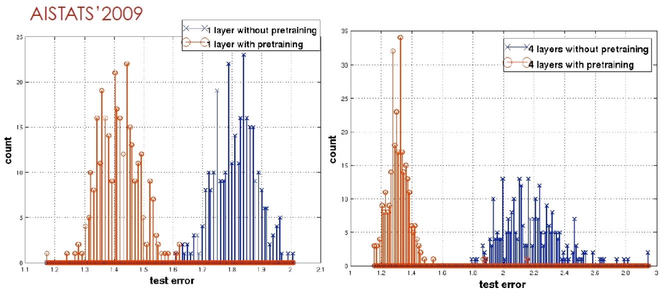
G. E. Hinton, S Osindero, YW Teh, A fast learning algorithm for deep belief nets, Neural Computation, 2006

Deep Belief Networks: Object Parts



Convolutional deep belief networks for scalable unsupervised learning of hierarchical representations. Honglak Lee, Roger Grosse, Rajesh Ranganath, and Andrew Y. Ng

Effect of Unsupervised Pre-training



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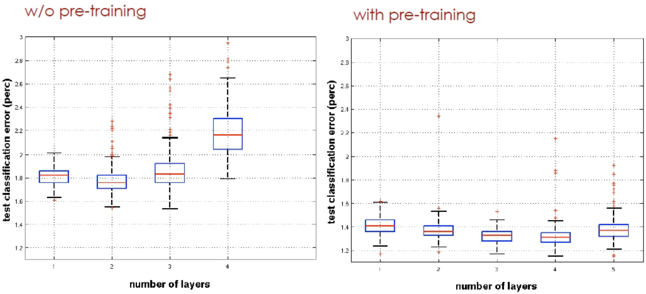

Why does Unsupervised Pre-training work?

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Autoencoders

- Main idea
- Sparse Autoencoders
- Denoising Autoencoders
- Pretraining using Autoencoders