Deep Learning

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Deep Learning Buzz



2012: Is Deep Learning a revolution in artificial intelligence?



Accomplishments

Apple's Siri virtual personal assistant

Google's Street View

Google/Facebook/Tweeter/Yahoo Deep Learning Acquisition

Hinton's identification of drug molecule

Hinton's hand writing recognition

Swiss AI Lab's recognition of German traffic sign images beats human experts

Rashid's speech was translated into Chinese by deep learning tools.

3³, **3**³

Who's heard of ...

- Energy Based Models (EBMs)
- Restricted Boltzmann Machines (RBMs)
- Deep Belief Networks
- Auto-encoders

Objectives

- 1. Awareness of new developments in statistical machine learning
- Exposure to Energy Based Models, RBMs and Deep Belief Networks
- Generate some excitement about these new developments

Outline

- Motivating factors for study
- RBMs
- Deep Belief Networks
- Applications



The Toolbox

We often reach for the familiar...

For discriminative tasks we have

- neural networks (~1980's, back-prop)
- SVM (~1990's, Vapnik)



But is there anything better out there???

Challenges with SVM/NN

Potential difficulties with SVM

- Training time for large datasets
- Large number of support vectors for hard classification problems

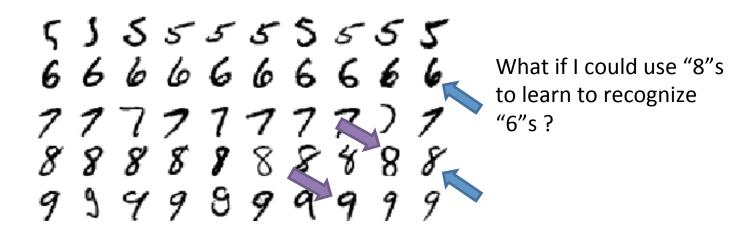
Potential difficulties with NN & back-prop

- Diminishing gradient inhibits multiple layers
- Can get stuck in local minimums
- Training time can be extensive

Challenges with SVM/NN

More general "problems" with NNs and SVM...

- Need labeled data (what about unlabeled data?)
- Amount of information restricted by labels (ie, hard to learn a complex model if we are limited by labels)



How to respond to these challenges

- Try to model the structure of the sensory input (ie, data), but keep the efficiency and simplicity of a gradient method
 - Adjust the weights to maximize the probability that a generative model would have produced the sensory input.
 - Learn p(data) not p(label | data)
- So instead of learning a label, first learn how to generative your data

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- Try to model the structure of the sensory input (ie, data), but keep the efficiency and simplicity of a gradient method
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 - Learn p(data) not p(label | data)
- So instead of learning bel, first learn how to generative your data Immediate benefit in that all data

does not have to be label. Also reduces dependency on label.

Recap

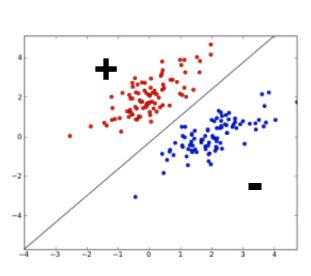


So, we are convinced we ...

- recognize some concerns with "standard" tools and would like what other options are out there
- 2. like the idea of modeling the input first (ie, building a model of our data as oppose to an out right classifier)

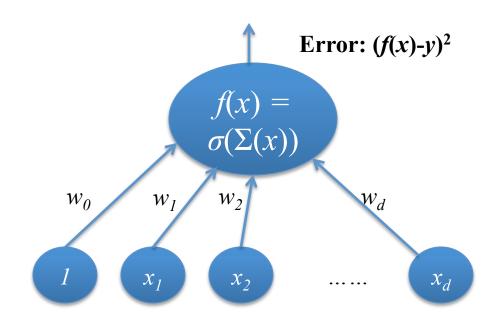
Perceptron

Learning to map input to output / label and is guided by output.



$$f(x) = w_0 + w_1 x_1 + w_2 x_2 + ..., w_d x_d$$

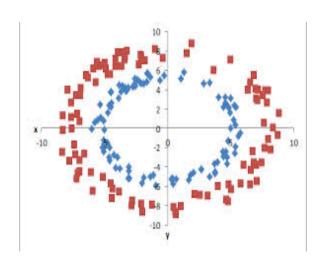
f(x) > 0: positive (1) f(x) < 0: negative (-1)



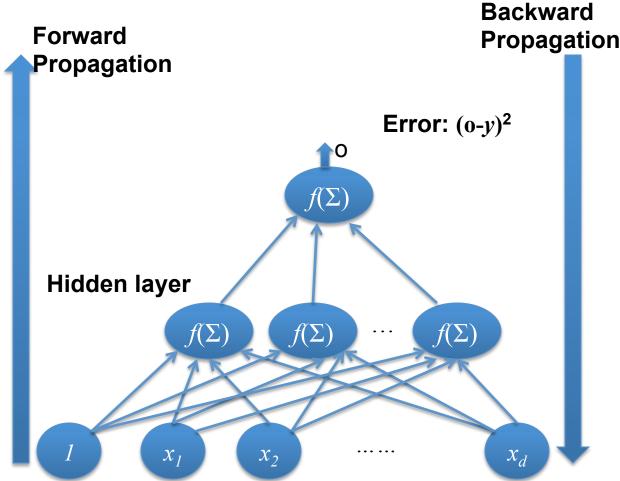
$$w^{new} = w^{cur} - \frac{\partial Error}{\partial w} = w^{cur} - (f(x) - y)x$$

Perceptron – 1950s

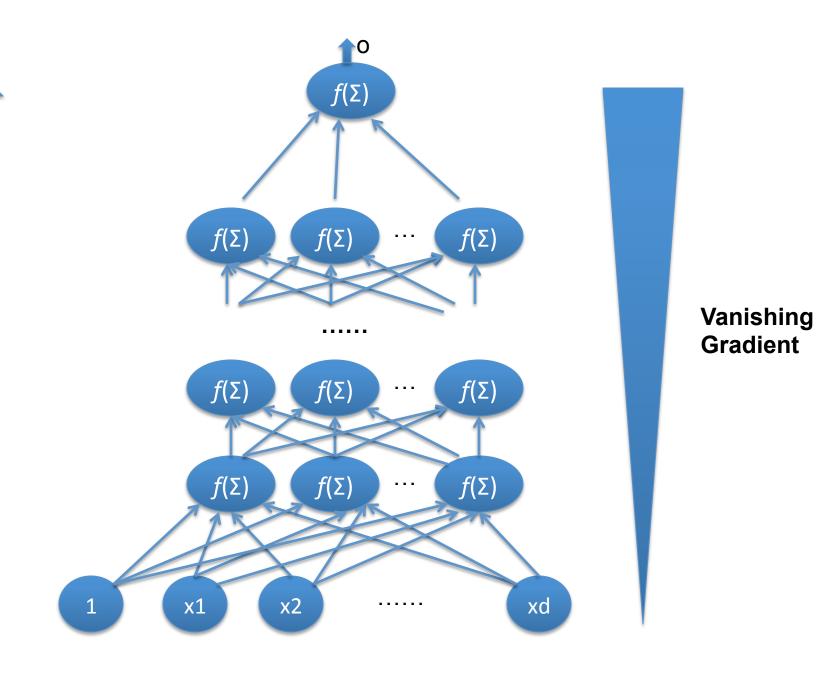
Neural Network



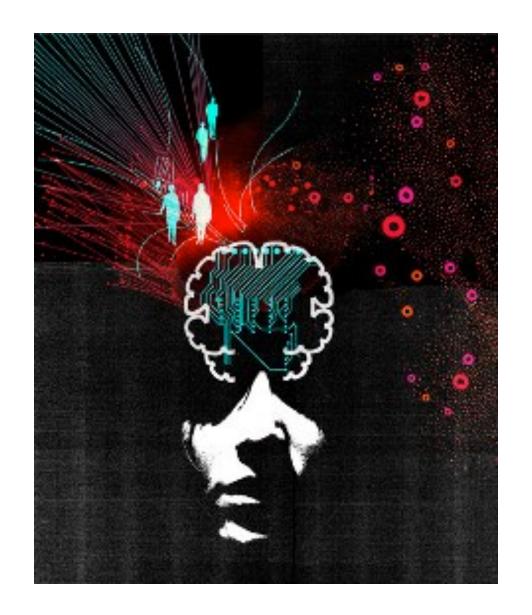




1980s - Neural Network Revolution



How to Construct Deep Networks?



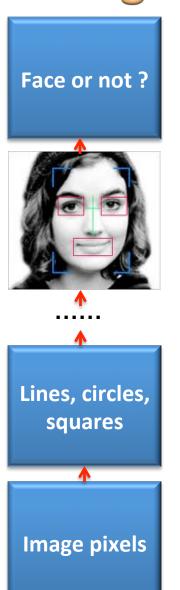




G. Hinton

2006

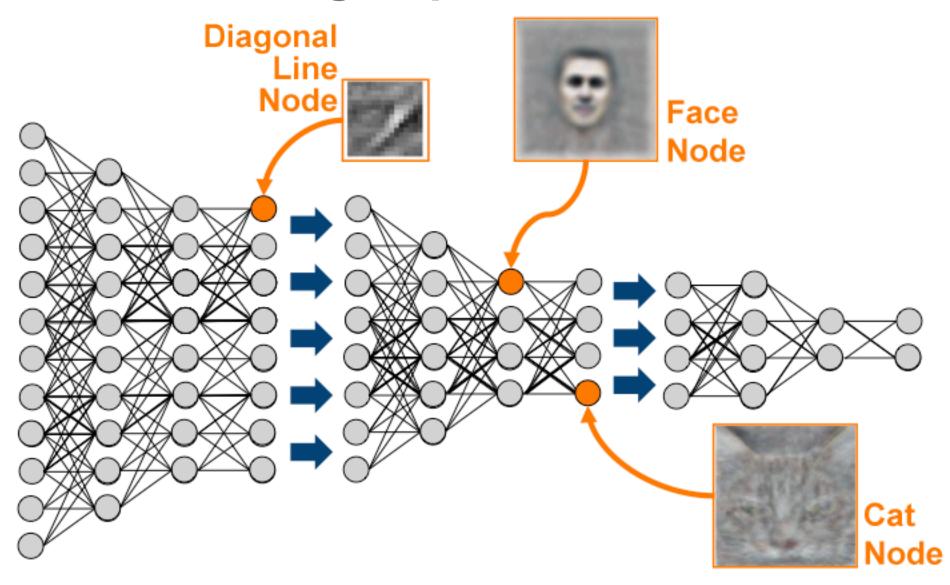
Why Deep Learning? – A Face Recognition Analogy





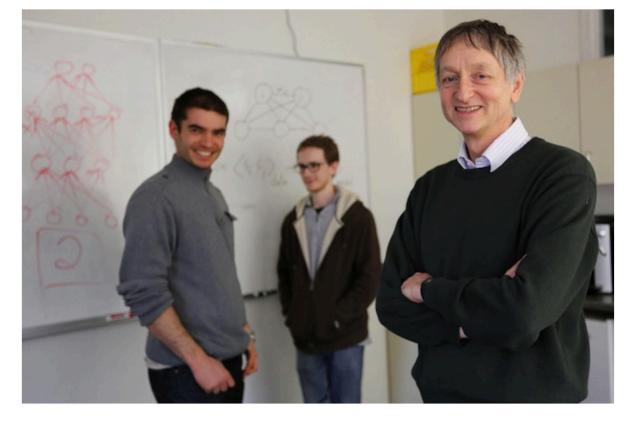
Brain Learning

Learning Representation First



GOOGLE HIRES BRAINS THAT HELPED SUPERCHARGE MACHINE LEARNING

A Deep Learning Success



Geoffrey Hinton (right) Alex Krizhevsky, and Ilya Sutskever (left) will do machine learning work at Google. *Photo: U of T*

Energy Based Models

p(x) – probability of our data; data is represented by feature vector **x**.

 $p(x) = \frac{e^{-E(x)}}{Z}.$

and

$$Z = \sum_{x} e^{-E(x)}$$

Attach an energy function (ie, E(x)) to score a configuration (ie, each possible input x).

We want desirable data to have low energy. Thus, tweak the parameters of E(x) accordingly.

EBMs with Hidden Units

To increase power of EBMs, add hidden variables.

$$P(x) = \sum_{h} P(x,h) = \sum_{h} \frac{e^{-E(x,h)}}{Z}.$$



We can rewrite p(x) in a form similar to the standard EBM,

$$P(x) = \frac{e^{-\mathcal{F}(x)}}{Z} \text{ with } Z = \sum_{x} e^{-\mathcal{F}(x)}.$$
 $\log(P(x)) = -F(x) - \log(Z)$

Tweakin' Parameters

Now we need to adjust the model so it reflects our data, do ML

Likelihood fn

$$L(\theta) = \prod_{i=1}^{n} p(x_i; \theta)$$

• Avg. Log-likelihood fn

$$\ell(\theta) = \frac{1}{n} \log(\Pi_i p(x_i; \theta)) = \frac{1}{n} \sum_i \log(p(x_i; \theta))$$
$$= \frac{1}{n} \sum_i \log \frac{e^{-F(x_i)}}{Z} = \frac{1}{n} \sum_i (-F(x_i) - \log(Z))$$

Tweakin' Parameters

Take the derivative

$$\frac{\partial \ell(\theta)}{\partial \theta_{j}} = \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} - \frac{\partial \log Z}{\partial \theta_{j}} \right) = \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} - \frac{1}{Z} \frac{\partial Z}{\partial \theta_{j}} \right)
= \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} - \frac{1}{Z} \sum_{\hat{x}} e^{-F(\hat{x})} \frac{\partial F(\hat{x})}{\partial \theta_{j}} \right)
= \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} \right) - \sum_{\hat{x}} p(\hat{x}) \frac{\partial F(\hat{x})}{\partial \theta_{j}}
= \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} \right) - E_{p} \left[\frac{\partial F(x)}{\partial \theta_{j}} \right]$$

Tweakin' Parameters

Take the derivative

$$\frac{\partial \ell(\theta)}{\partial \theta_{j}} = \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} - \frac{\partial \log Z}{\partial \theta_{j}} \right) = \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} + \frac{1}{Z} \frac{\partial Z}{\partial \theta_{j}} \right)$$

$$= \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} + \frac{1}{Z} \sum_{\hat{x}} e^{-F(\hat{x})} \frac{\partial F(\hat{x})}{\partial \theta_{j}} \right)$$

$$= \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} \right) + \sum_{\hat{x}} p(\hat{x}) \frac{\partial F(\hat{x})}{\partial \theta_{j}}$$

$$= \frac{1}{n} \sum_{i} \left(\frac{-\partial F(x_{i})}{\partial \theta_{j}} \right) + E_{p} \left[\frac{\partial F(x)}{\partial \theta_{j}} \right]$$

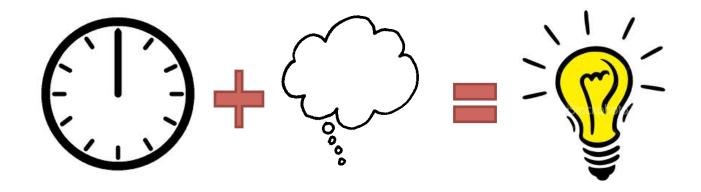
Can think of as an expectation over dataset.

This is an expectation over all possible configurations of input x. ?#@! Grows exponentially as function of the length of input

Restricted Boltzann Machines (RBM)

Transition to RBM

Looks like training a EBM is, in general, a tall task. But after much

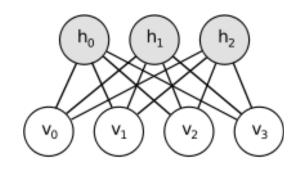


Jump to an end result...

Restricted Boltzmann Machines (RBM)

RBMs

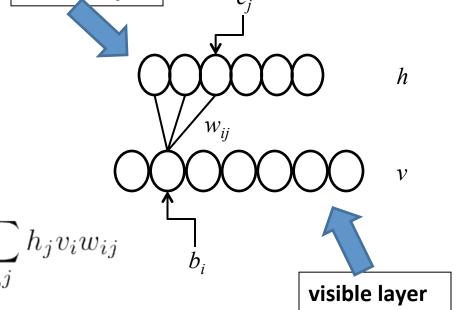
- Represented by a bipartite graph, with symmetric, weighted connections
- One layer has visible nodes and the other hidden (ie, latent) variables.
- Notes are often binary, stochastic units (ie, assume 0 or 1 based on probability)



Unsupervised Restricted Boltzmann Machine (RBM)

hidden layer

- A model for a distribution over two layers of binary nodes
- Probability is defined via an "energy"



$$E(v,h) = -\sum_{i} b_i v_i - \sum_{j} c_j h_j - \sum_{i,j} h_j v_i w_{ij}$$

$$p(v,h) = \frac{e^{-E(v,h)}}{Z}$$

$$p(v,h) = \frac{e^{-E(v,h)}}{Z}$$
 $Z = \sum_{v} \sum_{h} e^{-E(v,h)}$

$$p(v) = \sum_{h} \frac{e^{-E(v,h)}}{Z}$$

What's gained by "Restricted"

1) Conditional probabilities factor nicely

$$P(h|v) = \Pi_i P(h_i|v)$$
 and $P(v|h) = \Pi_i P(v_i|h)$

2) Using binary units, we also can get

$$P(v_j = 1|h) = \sigma(b_j + W'_j h)$$

$$P(h_i = 1|v) = \sigma(c_i + W_j v)$$

So we can get a sample of the visible or hidden nodes easily...

Training a RBM - Maximum Likelihood

$$l(\theta) = \frac{1}{n} \sum_{i} \log(\sum_{h} e^{-E(v_{i},h)}) - \log Z$$

$$p(v) = \sum_{h} \frac{e^{-E(v,h)}}{Z}$$

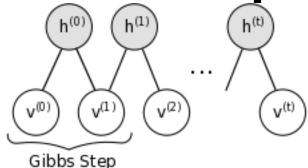
$$\frac{\partial l(\theta)}{\partial \theta_{j}} = \frac{1}{n} \sum_{i} \frac{\sum_{h} e^{-E(v_{i},h)}}{\sum_{h} e^{-E(v_{i},h)}} \frac{-\partial E}{\partial \theta_{j}} - \frac{1}{Z} \sum_{v} \sum_{h} e^{-E(v,h)} \frac{-\partial E}{\partial \theta_{j}}$$

$$= \frac{1}{n} \sum_{i} \sum_{h} \frac{p(v_{i},h)}{p(v_{i})} \left(\frac{-\partial E}{\partial \theta_{j}}\right) - E\left[\frac{-\partial E}{\partial \theta_{j}}\right]_{p^{\infty}}$$

$$= \frac{1}{n} \sum_{i} \sum_{h} p(h|v_{i}) \left(\frac{-\partial E}{\partial \theta_{j}}\right) - E\left[\frac{-\partial E}{\partial \theta_{j}}\right]_{p^{\infty}}$$

$$= E\left[\frac{-\partial E}{\partial \theta_{j}}\right]_{p^{0}} - E\left[\frac{-\partial E}{\partial \theta_{j}}\right]_{p^{\infty}}$$

Gibbs Sampling



Can sample from p(v,h) by repeatedly sampling from v and h using the eqns. for p(v|h) and p(h|v).

As $t \to \infty$, $(v^{(t)}, h^{(t)})$ converge to samples of p(v,h).

But... hard to know when equilibrium has been reach, can be computationally expensive

Training a RBM - Contrastive Divergence based on Gibbs Sampling

Instead of attempting to sample from joint distribution p(v,h) (i.e. $p\infty$), sample from $p^1(v,h)$.

$$\Delta\theta_{j} \propto E \left[\frac{-\partial E}{\partial \theta_{j}} \right]_{p^{0}} - E \left[\frac{-\partial E}{\partial \theta_{j}} \right]_{p^{\infty}}$$

$$\Delta\theta_{j} \propto E \left[\frac{-\partial E}{\partial \theta_{j}} \right]_{p^{0}} - E \left[\frac{-\partial E}{\partial \theta_{j}} \right]_{p^{1}}$$

Learning Rule

Recall energy function

$$E(v,h) = -\sum_{i} b_{i}v_{i} - \sum_{j} c_{j}h_{j} - \sum_{i,j} v_{i}h_{j}w_{i,j}$$

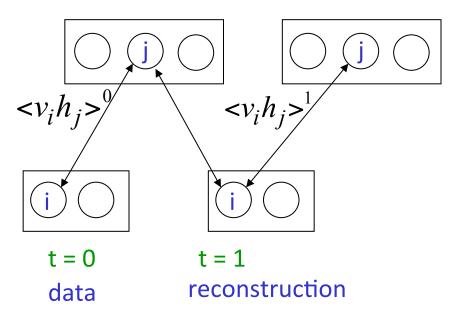
Calculating derivatives...

$$\frac{\partial E(v,h)}{\partial w_{i,j}} = v_i h_j \qquad \qquad \frac{\partial E(v,h)}{\partial b_i} = v_i$$

$$\frac{\partial E(v,h)}{\partial c_j} = h_j$$

So,
$$\Delta w_{i,j} \propto \epsilon (\langle v_i h_j \rangle^0 - \langle v_i h_j \rangle^\infty)$$

A quick way to learn an RBM



Start with a training vector on the visible units.

Update all the hidden units in parallel

Update the all the visible units in parallel to get a "reconstruction".

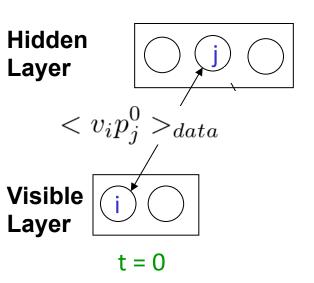
Update the hidden units again.

$$\Delta w_{ij} = \varepsilon \left(\langle v_i h_j \rangle^0 - \langle v_i h_j \rangle^1 \right)$$

This is not following the gradient of the log likelihood. But it works well. It is approximately following the gradient of another objective function (Carreira-Perpinan & Hinton, 2005).

Training a RBM via Contrastive Divergence

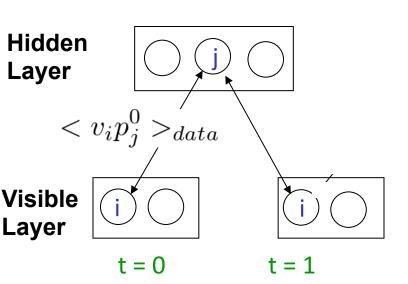
Gradient of the likelihood with respect to $w_{ij} \approx$ the difference between interaction of v_i and h_j at time 0 and at time 1.



$$p_j^{(0)} = \sigma(\sum_i v_i w_{ij} + c_j)$$

Training a RBM via Contrastive Divergence

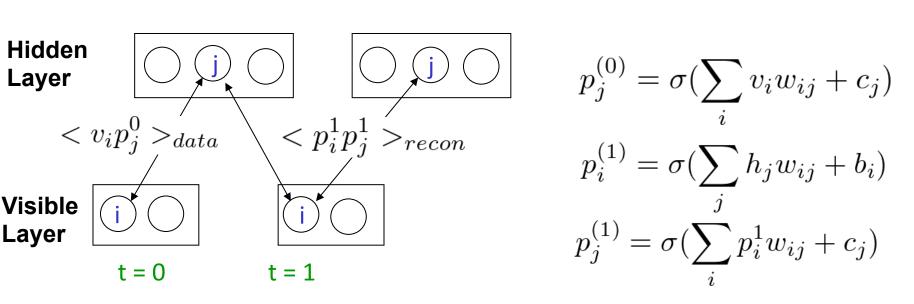
Gradient of the likelihood with respect to $w_{ij} \approx$ the difference between interaction of v_i and h_j at time 0 and at time 1.



$$p_j^{(0)} = \sigma(\sum_i v_i w_{ij} + c_j)$$
$$p_i^{(1)} = \sigma(\sum_j h_j w_{ij} + b_i)$$

Training a RBM via Contrastive Divergence

Gradient of the likelihood with respect to $w_{ij} \approx$ the difference between interaction of v_i and h_j at time 0 and at time 1.



σ: sigmoid function

$$\Delta w_{i,j} = \langle v_i p_i^0 \rangle - \langle p_i^1 p_i^1 \rangle$$

Hinton, Neural Computation (2002)

Challenges with RBMs

A number of choices to be made

- Types of nodes, learning weight, initial values, batch sizes, etc.
- Care should be taken to avoid over-fitting

A RBM "manual" is available on line...

http://www.cs.utoronto.ca/~hinton/absps/guideTR.pdf

Software package: Pylearn2:

http://deeplearning.net/software/pylearn2/

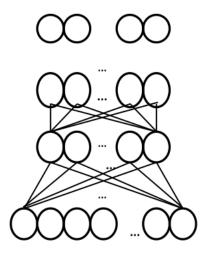
On both GPU and CPU

GPU Implementation

Calculations need for training and classification made use of CUDAMat and GPUs



Train with over one million parameters in about an hour



Why ???

Okay, we can model p(x).

But how to...

- 1. Find p(label|x). We want a classifier!
- 2. Improve the model for p(x).

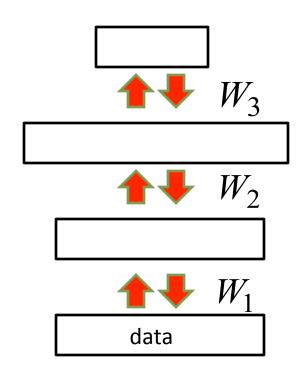


Deep Belief Nets

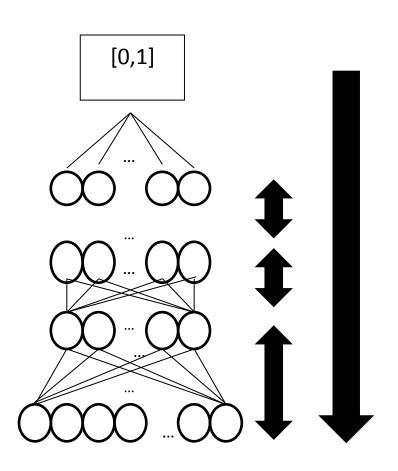
RBMs are typically used in stack

- Train them up one layer at a time
- Hidden units become visible units to the next layer up

If your goal is a discriminator, you train a classifier on the top level representation of your input.



Training a Deep Network



- 1. Weights are learned layer by layer via unsupervised learning.
- 2. Final layer is learned as a supervised neural network.
- 3. All weights are finetuned using <u>supervised</u> <u>back propagation</u>.

Why stack them up? Why does this work?

This is a good question, with a long complicated answer.

Basically, doing so can improve a lower variation bound on the probability of training data under the model.

Hinton, Osindero, & The, 2006

How to generate from the model

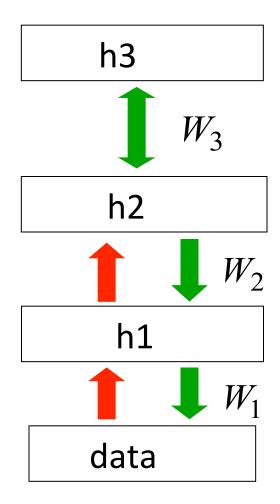
Bonus when we modeling plx), we modeling plx), we modeling plx), we modeling plx), we model believes in model believes in

To generate data:

Get an equilibrium sample from the top-level RBM by performing alternating Gibbs sampling for a long time.

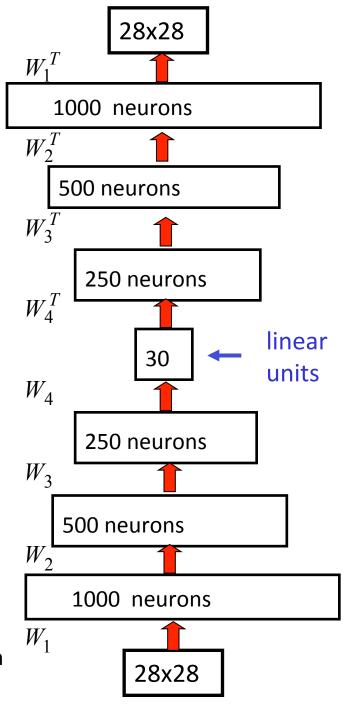
Perform a top-down pass to get states for all the other layers.

So the lower level bottom-up connections are not part of the generative model. They are just used for inference.



Deep Autoencoders

- They always looked like a really nice way to do nonlinear dimensionality reduction:
 - But it is very difficult to optimize deep autoencoders using backpropagation.
- We now have a much better way to optimize them:
 - First train a stack of 4RBM's
 - Then "unroll" them.
 - Then fine-tune with backprop.



Hinton & Salakhutdinov, 2006; slide form Hinton UCL tutorial

Some Applications

We will look at two applications done by Hinton's Lab

- A model for digit recognition
- Cluster/search documents



Applications: A model of digit recognition

- Classify digits (0-9)
- Input is a 28x28 image from MNIST (training 60k, test 10k examples)

Applications: A model of digit recognition

This is work from Hinton et al., 2006

The top two layers form an associative memory whose energy landscape models the low dimensional manifolds of the digits.

The energy valleys have names

The model learns to generate combinations of labels and images.

To perform recognition we start with a neutral state of the label units and do an up-pass from the image followed by a few iterations of the top-level associative memory.

Matlab/Octave code available at http://www.cs.utoronto.ca/~hinton/

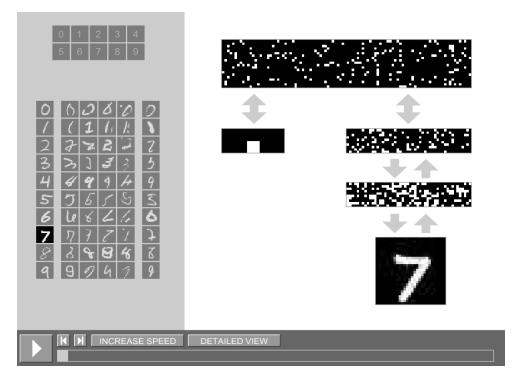
2000 top-level neurons 10 label 500 neurons neurons 500 neurons 28 x 28 pixel image

Slide modified from Hinton, 2007

Model in action

Hinton has provided an excellent way to view the model in

action...



http://www.cs.toronto.edu/~hinton/digits.html

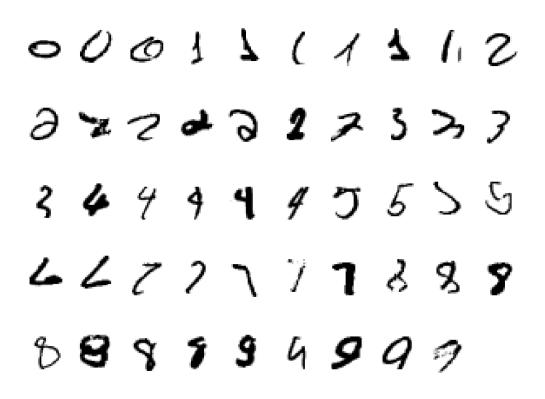
More Digits

Samples generated by letting the associative memory run with one label clamped. There are 1000 iterations of alternating Gibbs sampling between samples.

Slide from Hinton, 2007

Even More Digits

Examples of correctly recognized handwritten digits that the neural network had never seen before



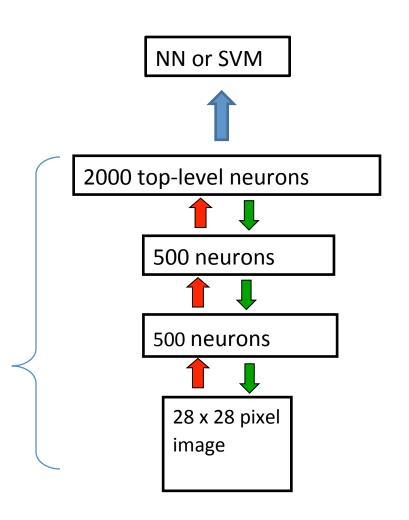
Slide from Hinton, 2007

Extensions

Do classification.

One way (probably no the best), train generative model with labeled/unlabeled data

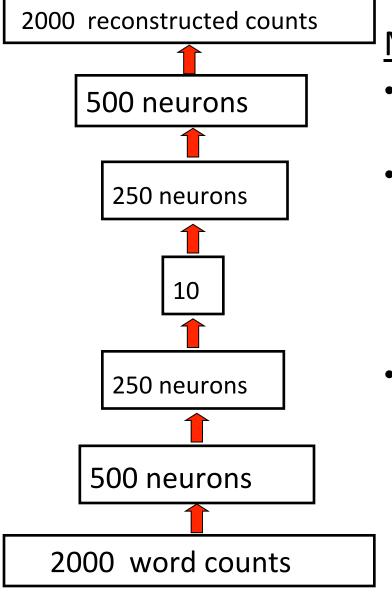
Then train a NN on higher dimensional representation.



Applications: Classifying text documents

- A document can be characterized by the frequency of words that appear (ie, word counts for some dictionary become feature vector)
- Goals...
 - 1. Group/cluster similar documents
 - 2. Find similar documents

How to compress the count vector

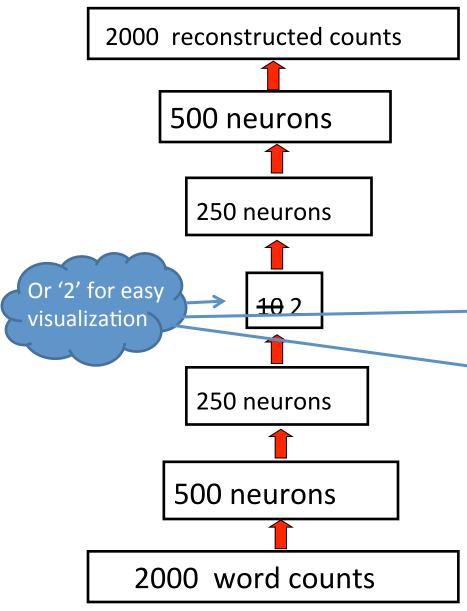


Multi-layer auto-encoder

- Train a model to reproduce its input vector as its output
- This setup forces as much information as possible be compressed and passed thru the 10 numbers in the central bottleneck.
- These 10 numbers are then a good way to compare documents.

Slide modified from Hinton, 2007

How to compress the count vector



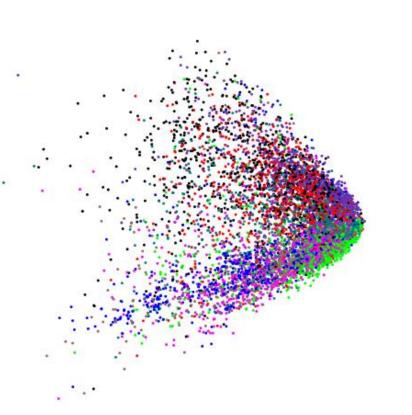
Multi-layer auto-encoder

- Train a model to reproduce its input vector as its output
- This setup forces as much information as possible be compressed and passed thru
 the 19 2 numbers in the central bottleneck.
- These 10 2 numbers are then a good way to compare documents.

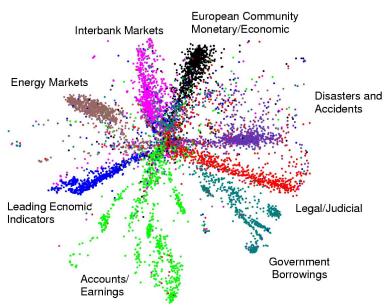
Slide modified from Hinton, 2007

Clusters

LSA 2-D Topic Space

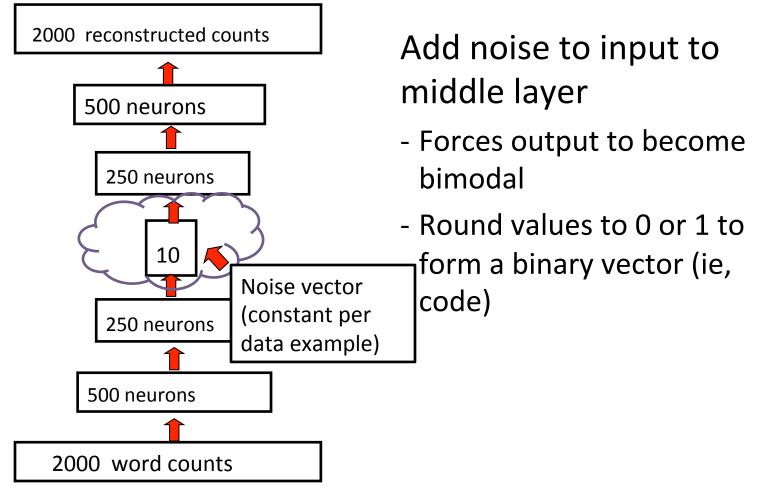


Autoencoder 2-D Topic Space



Images from Hinton, 2007

Search

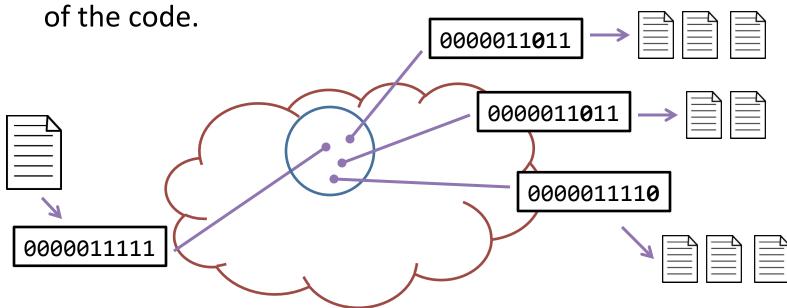


Hinton, 2007

Search

Use the binary codes as a key/hash documents

To find a similar document, calculate binary code and then retrieve documents that correspond to small deviations



A summary of functions of deep learning – a universal learner

- Classification
- Regression
- Clustering
- Autoencoding
- Compression
- Dimension reduction
- Data generation
- Modeling distribution
- Feature abstraction
- Flexible training and architecture
- Unsupervised, supervised, and semi-supervised learning
- Suitable for big data



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