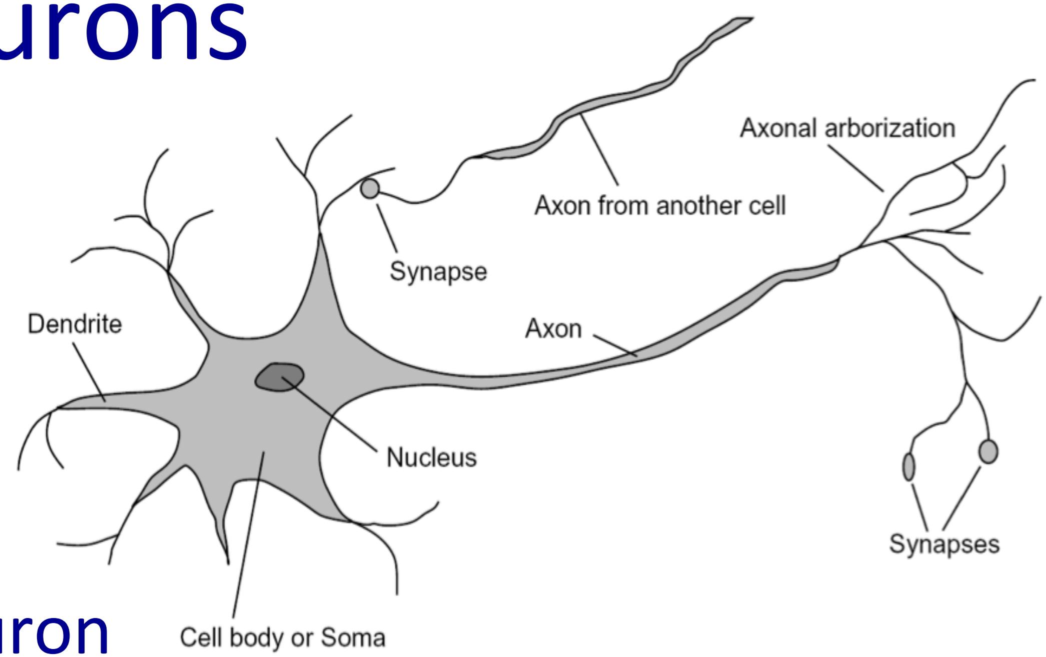
Neural Networks

Instructor: Alan Ritter

Many Slides from Carlos Guestrin and Richard Socher

Human Neurons



- Switching time
  - ~ 0.001 second
- Number of neurons
  - 10^{10}
- Connections per neuron
  - $10^{4\text{-}5}$
- Scene recognition time
  - 0.1 seconds
- Number of cycles per scene recognition?
  - 100 → much parallel computation!

How to Extend Linear Models to Learn Nonlinear Functions?

» Transform the input (e.g. kernel methods)

$$x \to \phi(x)$$

» Q: how do we decide on the right representation?

-Very high-dimensional representation?

How to Extend Linear Models to Learn Nonlinear Functions?

» Transform the input (e.g. kernel methods)

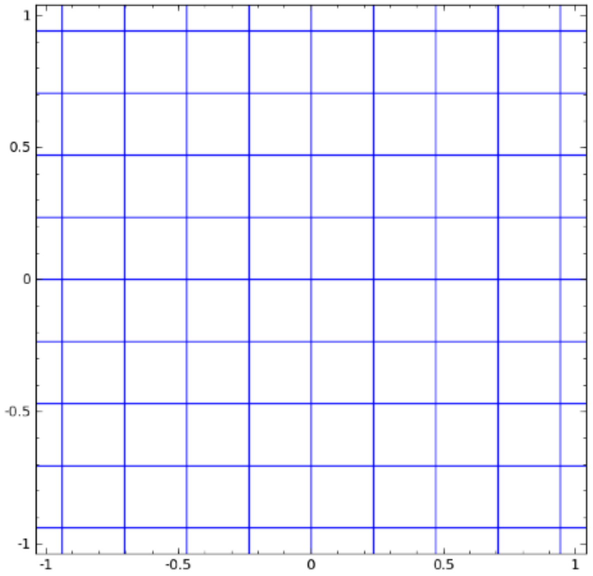
$$x \rightarrow \phi(x)$$

» Q: how do we decide on the right representation?

-Very high-dimensional representation?

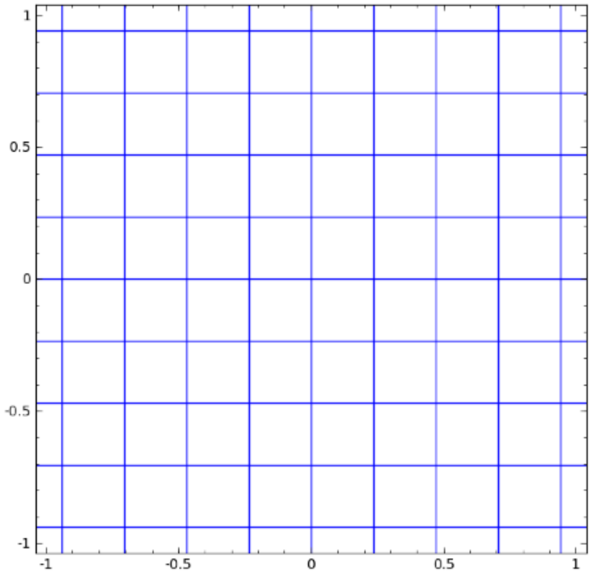
-Neural Networks: Let's learn the representation!

Neural Networks



Neural Networks

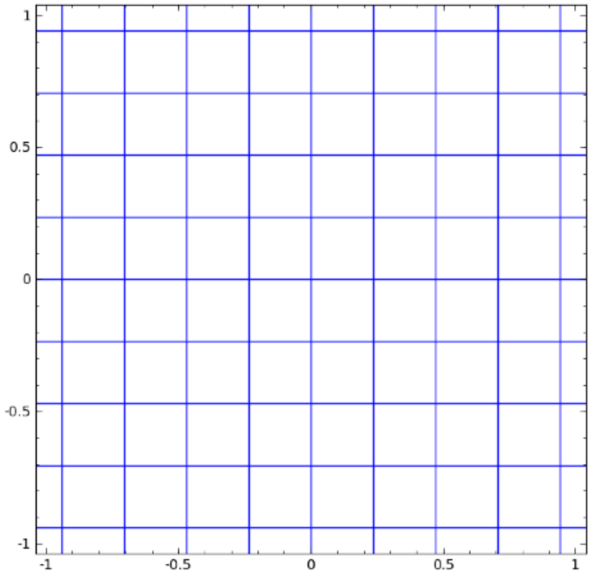
Linear model: $y = \mathbf{w} \cdot \mathbf{x} + b$



Neural Networks

Linear model: $y = \mathbf{w} \cdot \mathbf{x} + b$

$$y = g(\mathbf{w} \cdot \mathbf{x} + b)$$



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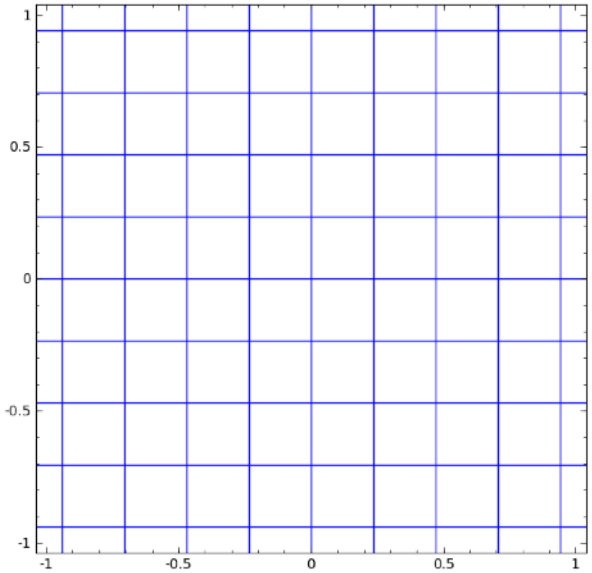
Nonlinear transformation



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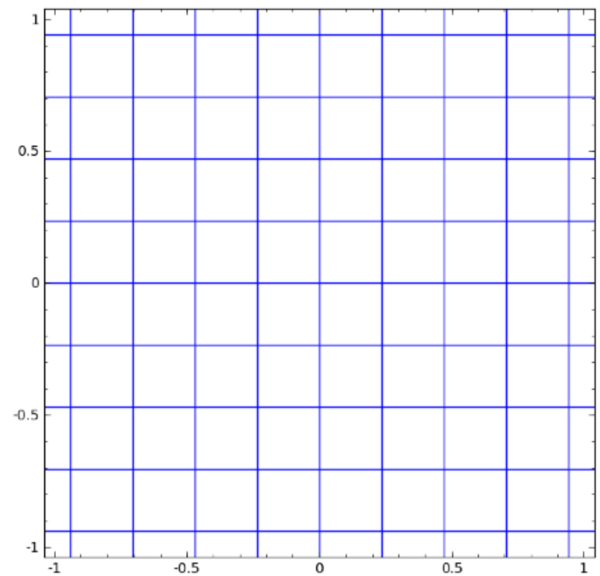
Nonlinear transformation

Warp space



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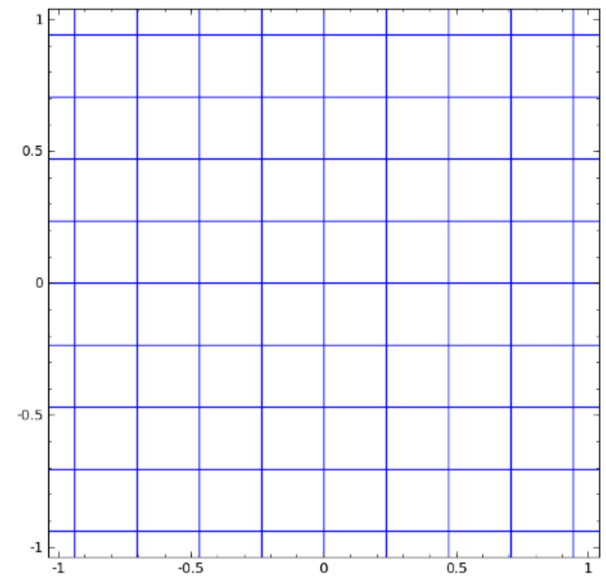
Nonlinear transformation　Warp space　Shift



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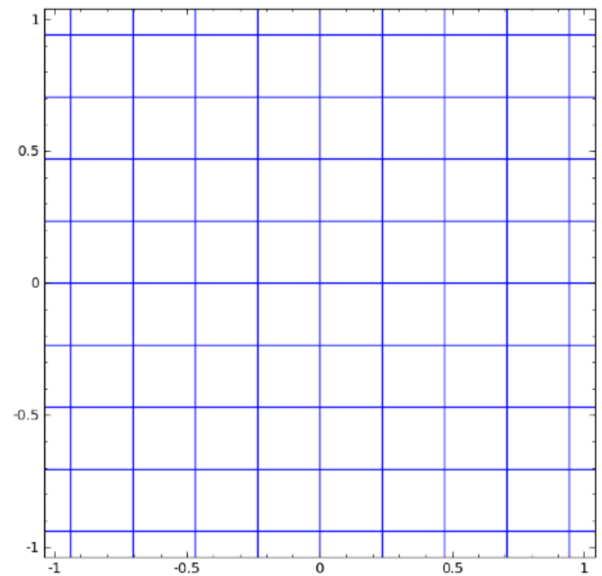
Nonlinear transformation

Warp space

Shift



Taken from http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

Neural Networks

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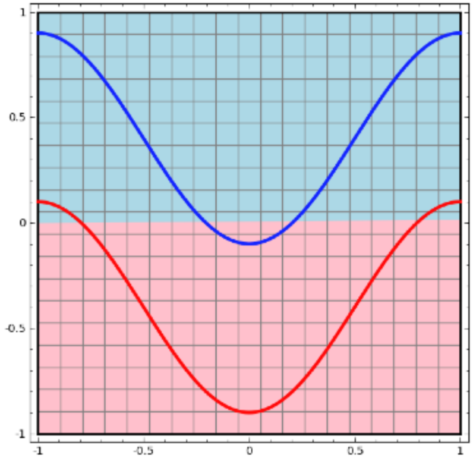
Neural Networks

Linear classifier



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Neural Networks

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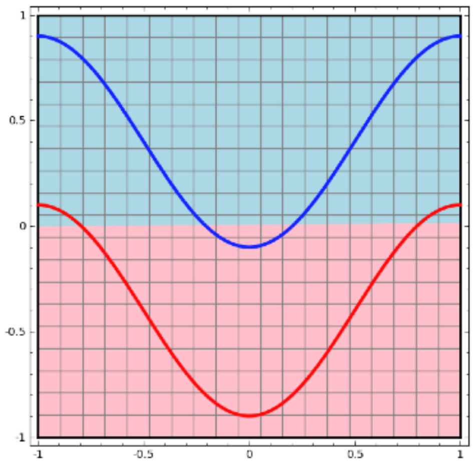
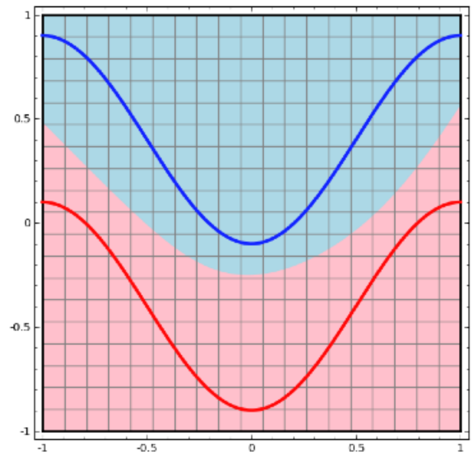


Neural network



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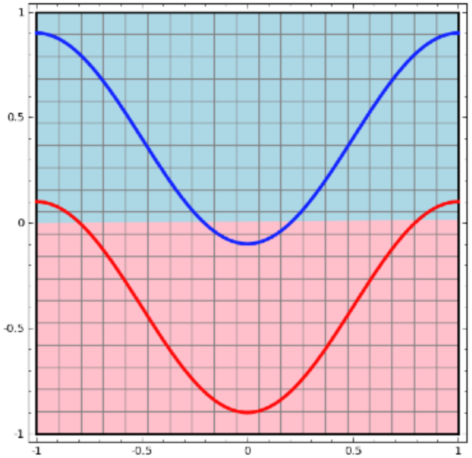
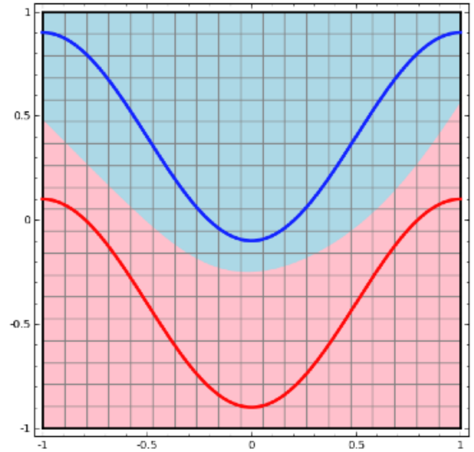
Neural Networks

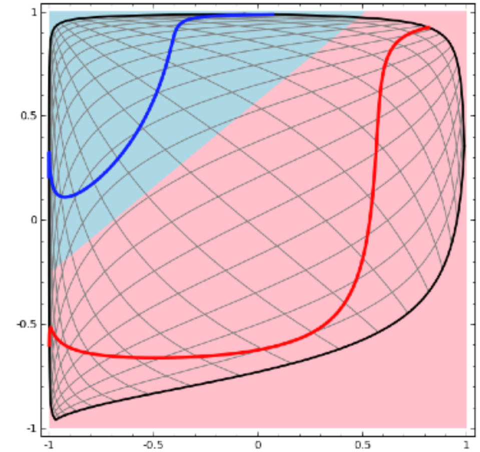
Linear classifier



Neural network



…possible because we transformed the space!



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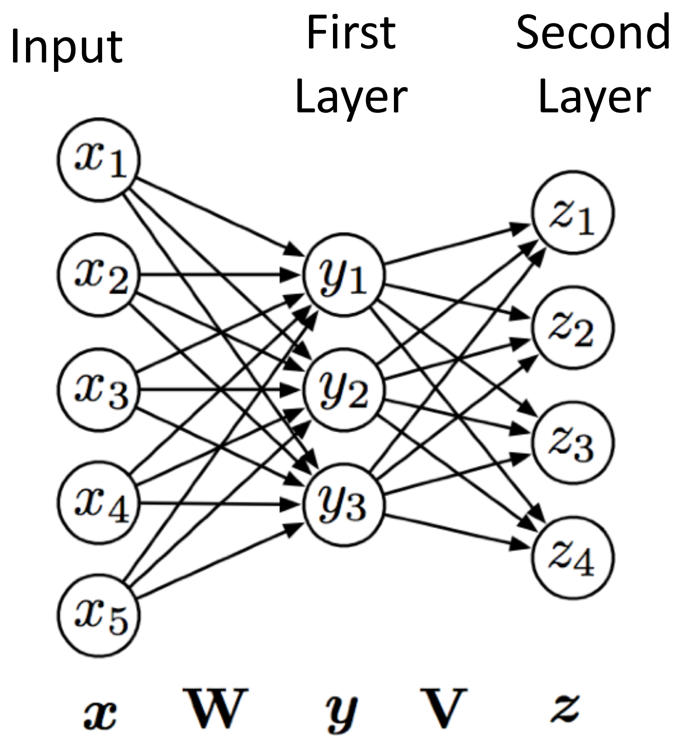
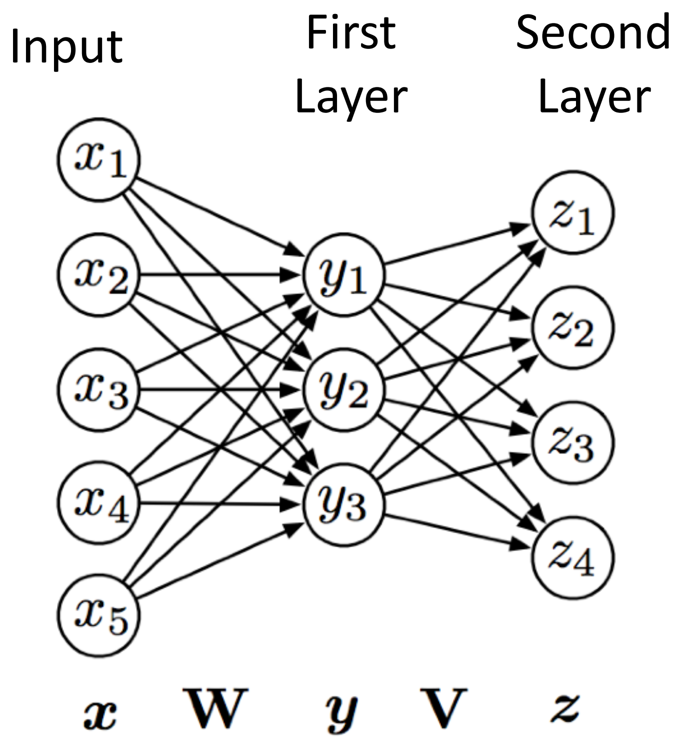
Deep Neural Networks



$$\boldsymbol{y} = g(\mathbf{W}\boldsymbol{x} + \boldsymbol{b})$$

Adopted from Chris Dyer

Deep Neural Networks



$$\boldsymbol{y} = g(\mathbf{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\mathbf{z} = g(\mathbf{V}\mathbf{y} + \mathbf{c})$$

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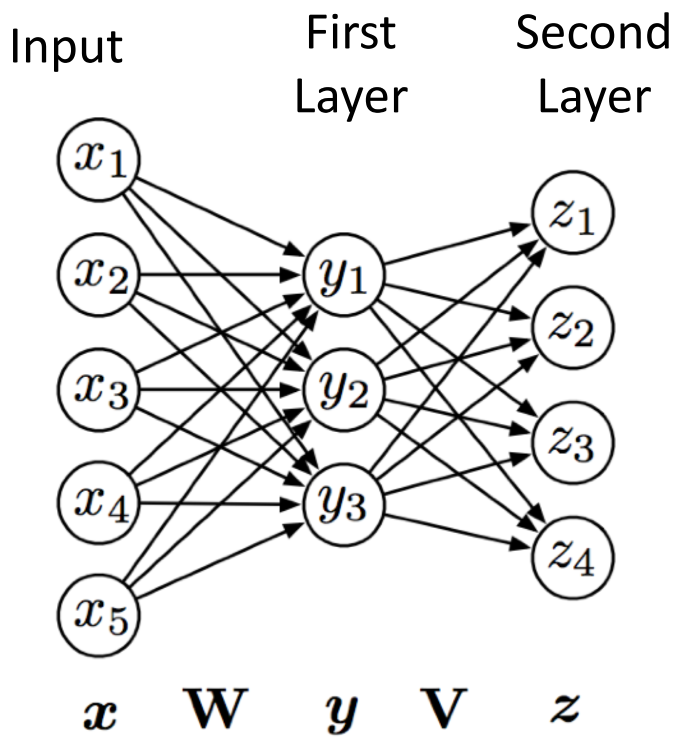
Deep Neural Networks



$$\boldsymbol{y} = g(\mathbf{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\mathbf{z} = g(\mathbf{V}\mathbf{y} + \mathbf{c})$$

$$\mathbf{z} = g(\mathbf{V}\underbrace{g(\mathbf{W}\mathbf{x} + \mathbf{b})}_{\text{output of first layer}} + \mathbf{c})$$

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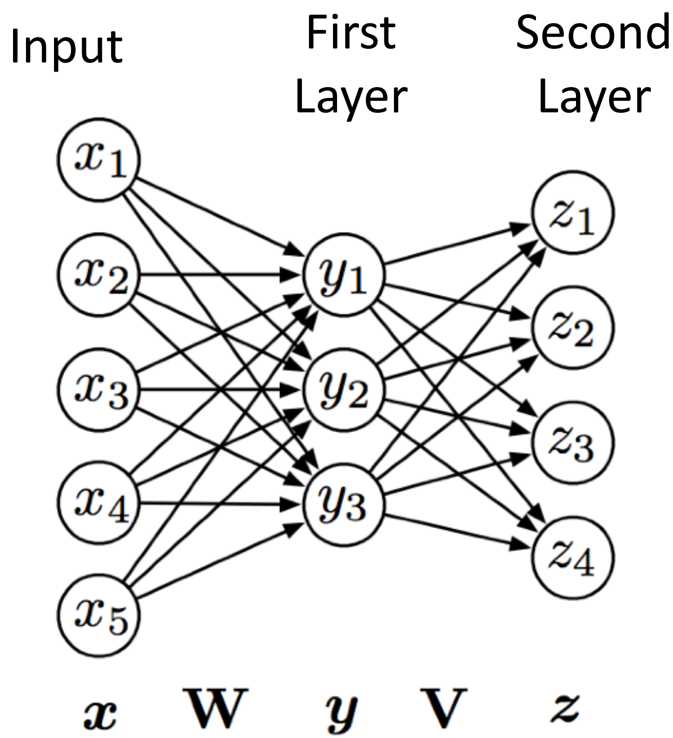
Deep Neural Networks



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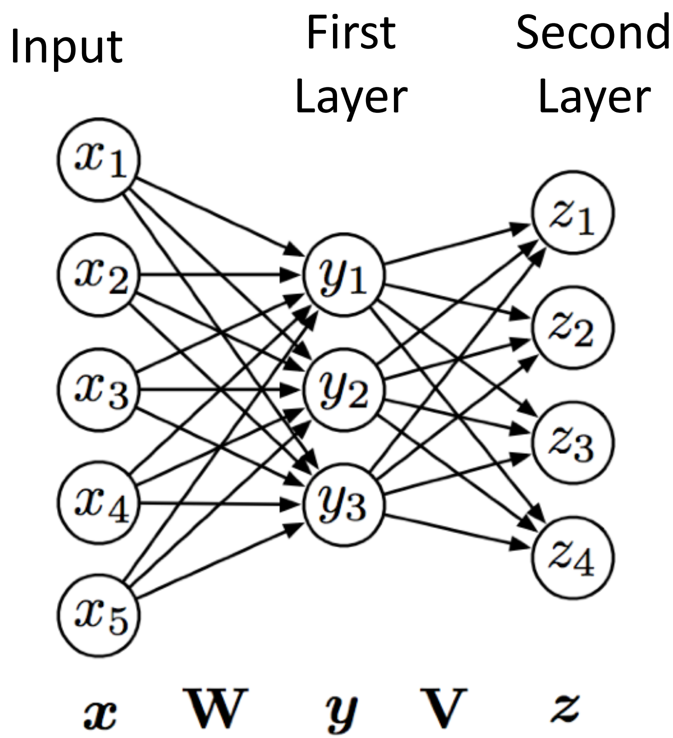
"Feedforward" computation (not recurrent)

Adopted from Chris Dyer

Deep Neural Networks



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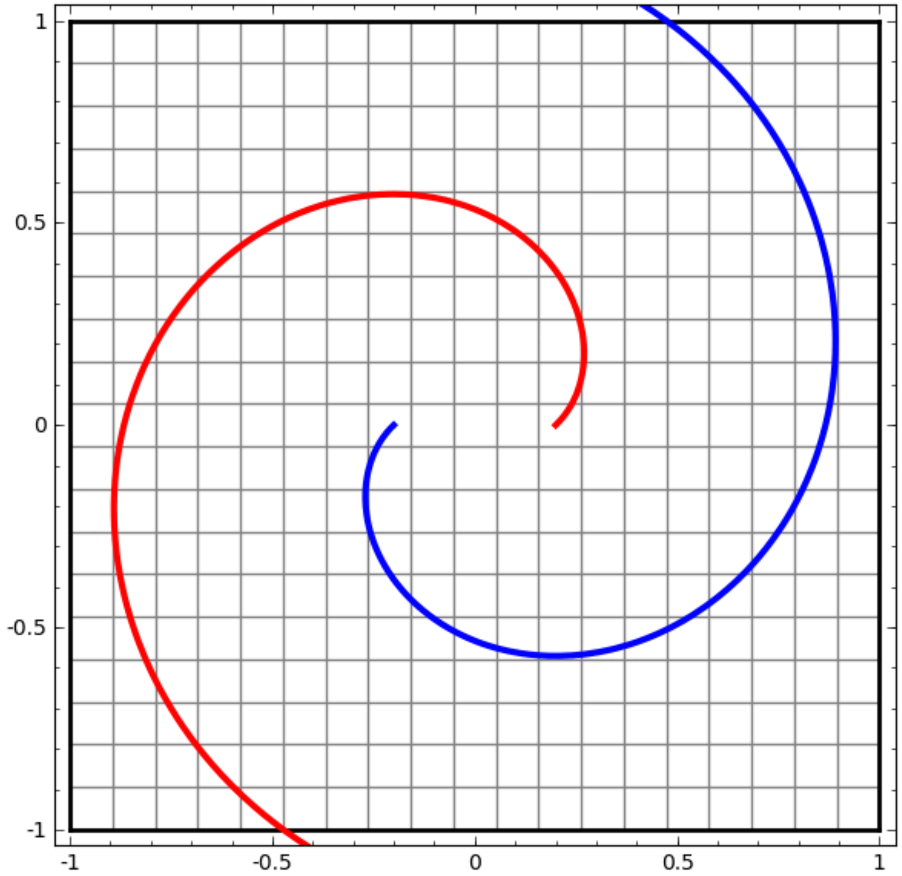
"Feedforward" computation (not recurrent)

Check: what happens if no nonlinearity? More powerful than basic linear models?

$$\mathbf{z} = \mathbf{V}(\mathbf{W}\mathbf{x} + \mathbf{b}) + \mathbf{c}$$

Adopted from Chris Dyer

Deep Neural Networks



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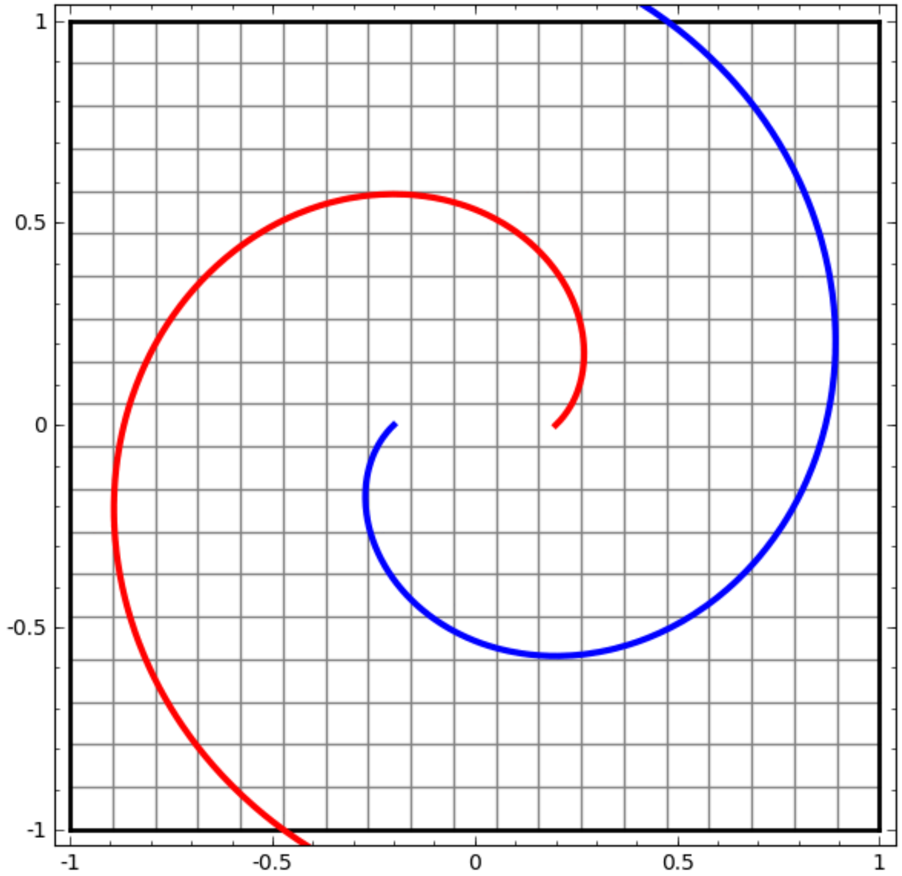

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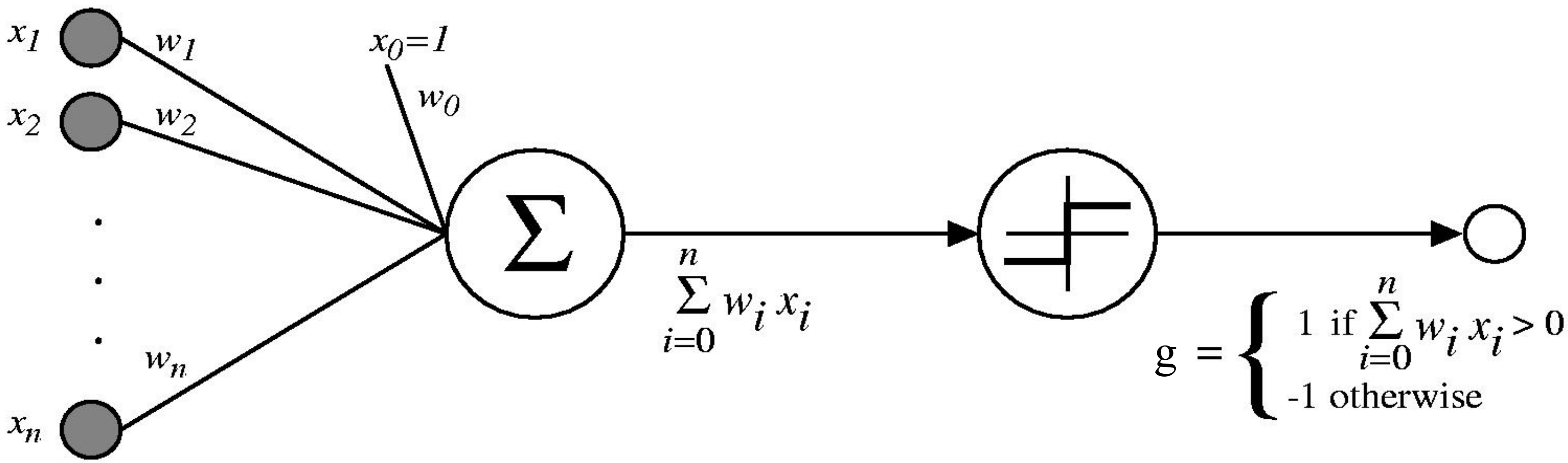
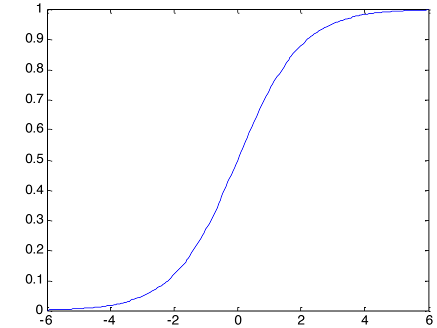
Perceptron as a Neural Network



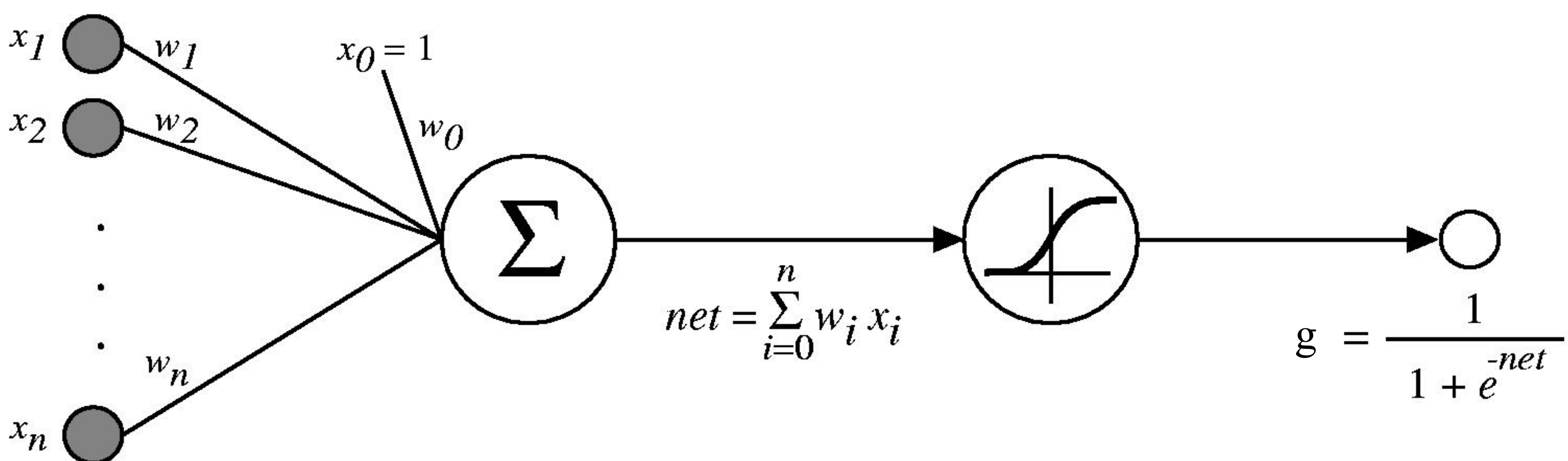
This is one neuron:

- Input edges $x_1 \ldots x_n$, along with basis
- The sum is represented graphically
- Sum passed through an activation function g

Sigmoid Neuron



$$g(w_0 + \sum_i w_i x_i) = \frac{1}{1 + e^{-(w_0 + \sum_i w_i x_i)}}$$



Just change g!

- Why would be want to do this?
- Notice new output range [0,1]. What was it before?
- Look familiar?

Optimizing a neuron

$$\frac{\partial}{\partial x} f(g(x)) = f'(g(x))g'(x)$$

We train to minimize sum-squared error

$$\ell(W) = \frac{1}{2}\sum_j [y^j - g(w_0 + \sum_i w_i x_i^j)]^2$$

$$\frac{\partial l}{\partial w_i} = -\sum_j [y_j - g(w_0 + \sum_i w_i x_i^j)] \frac{\partial}{\partial w_i} g(w_0 + \sum_i w_i x_i^j)$$

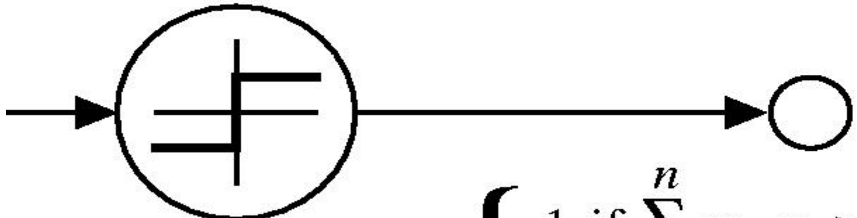
$$\frac{\partial}{\partial w_i} g(w_0 + \sum_i w_i x_i^j) = x_i^j g'(w_0 + \sum_i w_i x_i^j)$$

$$\boxed{\frac{\partial \ell(W)}{\partial w_i} = -\sum_j [y^j - g(w_0 + \sum_i w_i x_i^j)] \; x_i^j \; g'(w_0 + \sum_i w_i x_i^j)}$$

Solution just depends on g’: derivative of activation function!

Re-deriving the perceptron update

$$\frac{\partial \ell(W)}{\partial w_i} = -\sum_j [y^j - g(w_0 + \sum_i w_i x_i^j)]\ x_i^j\ g'(w_0 + \sum_i w_i x_i^j)$$



$$g = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ -1 \text{ otherwise} \end{cases}$$

$$\frac{\partial \ell(W)}{\partial w_i} = -\sum_j [y^j - g(w_0 + \sum_i w_i x_i^j)]\ x_i^j$$

For a specific, incorrect example:

- $w = w + y^*x$ (our familiar update!)

Re-deriving the perceptron update

$$\frac{\partial \ell(W)}{\partial w_i} = -\sum_j [y^j - g(w_0 + \sum_i w_i x_i^j)] \; x_i^j \; g'(w_0 + \sum_i w_i x_i^j)$$

=0
everywhere :(

$$g = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ \text{-1 otherwise} \end{cases}$$

$$\frac{\partial \ell(W)}{\partial w_i} = -\sum_j [y^j - g(w_0 + \sum_i w_i x_i^j)] \; x_i^j$$

For a specific, incorrect example:

- $w = w + y*x$ (our familiar update!)

Sigmoid units: have to differentiate g

$$\frac{\partial \ell(W)}{\partial w_i} = -\sum_j [y^j - g(w_0 + \sum_i w_i x_i^j)]\ x_i^j\ g'(w_0 + \sum_i w_i x_i^j)$$

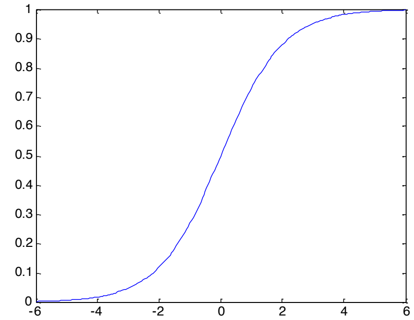
$$g(x) = \frac{1}{1+e^{-x}} \qquad g'(x) = g(x)(1-g(x))$$

$$\boxed{w_i \leftarrow w_i + \eta \sum_j x_i^j \delta^j}$$

$$\delta^j = [y^j - g(w_0 + \sum_i w_i x_i^j)] g^j (1 - g^j)$$

$$g^j = g(w_0 + \sum_i w_i x_i^j)$$

Aside: Comparison to logistic regression



- P(Y|X) represented by:

$$P(Y = 1 \mid x, W) = \frac{1}{1 + e^{-(w_0 + \sum_i w_i x_i)}}$$
$$= g(w_0 + \sum_i w_i x_i)$$

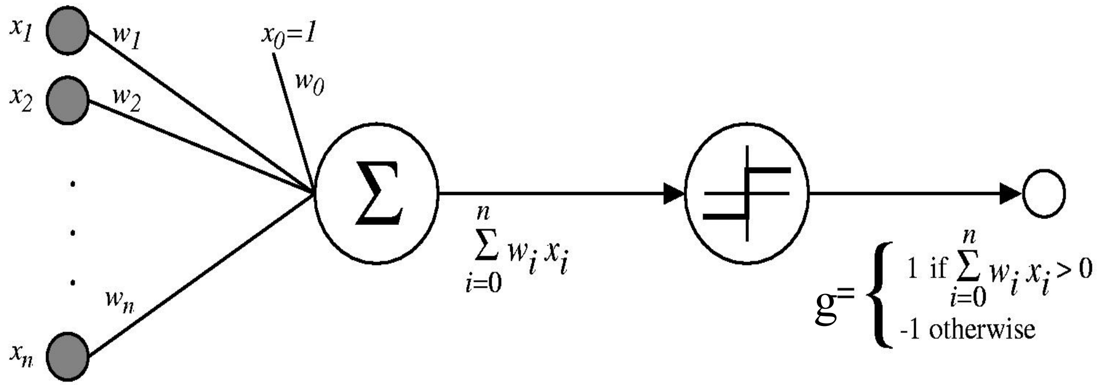
- Learning rule – MLE:

$$\frac{\partial \ell(W)}{\partial w_i} = \sum_j x_i^j [y^j - P(Y^j = 1 \mid x^j, W)]$$
$$= \sum_j x_i^j [y^j - g(w_0 + \sum_i w_i x_i^j)]$$

$$w_i \leftarrow w_i + \eta \sum_j x_i^j \delta^j$$

$$\delta^j = y^j - g(w_0 + \sum_i w_i x_i^j)$$

Perceptron, linear classification, Boolean functions: $x_i \in \{0,1\}$



- Can learn $x_1 \vee x_2$?
  - $-0.5 + x_1 + x_2$
- Can learn $x_1 \wedge x_2$?
  - $-1.5 + x_1 + x_2$
- Can learn any conjunction or disjunction?
  - $-0.5 + x_1 + \ldots + x_n$
  - $(n-0.5) + x_1 + \ldots + x_n$
- Can learn majority?
  - $(-0.5*n) + x_1 + \ldots + x_n$
- What are we missing? The dreaded XOR!, etc.

Going beyond linear classification

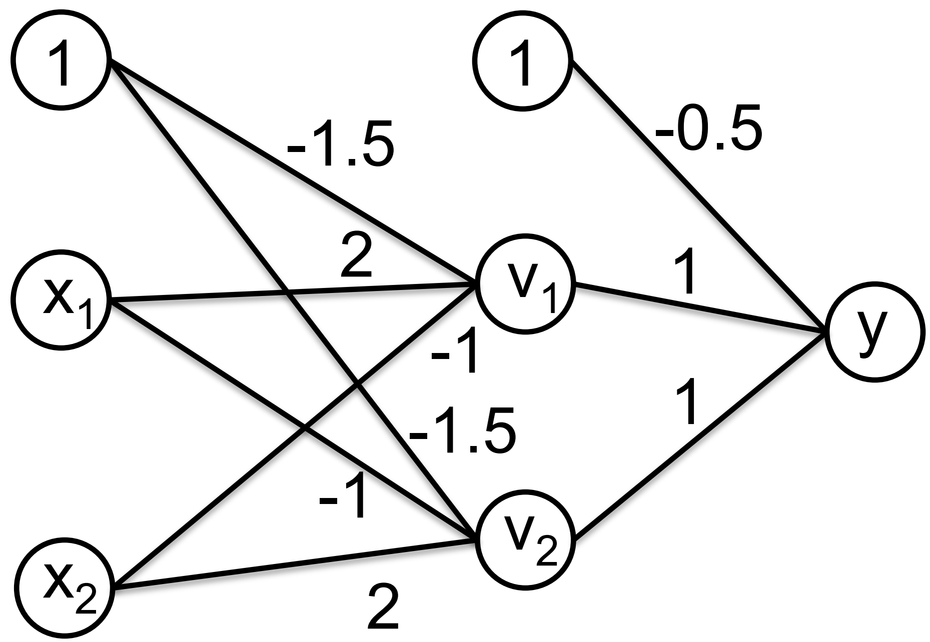
Solving the XOR problem

$y = x_1 \text{ XOR } x_2 = (x_1 \wedge \neg x_2) \vee (x_2 \wedge \neg x_1)$

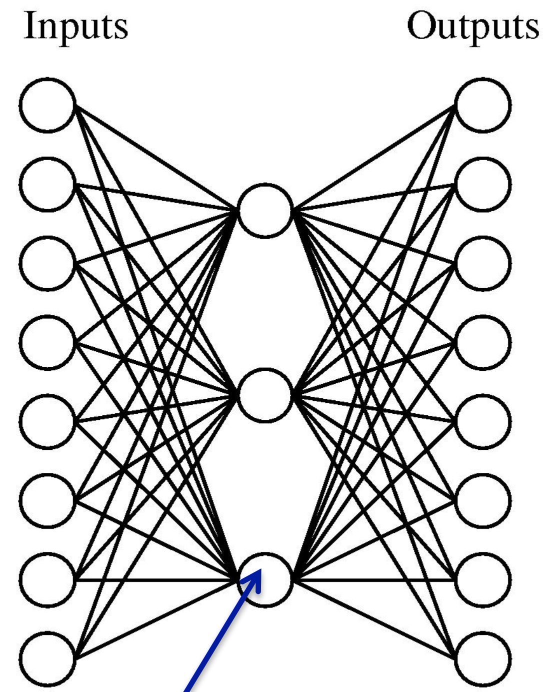
$v_1 = (x_1 \wedge \neg x_2)$
$\quad = -1.5 + 2x_1 - x_2$

$v_2 = (x_2 \wedge \neg x_1)$
$\quad = -1.5 + 2x_2 - x_1$

$y = v_1 \vee v_2$
$\quad = -0.5 + v_1 + v_2$



Hidden layer



- Single unit:

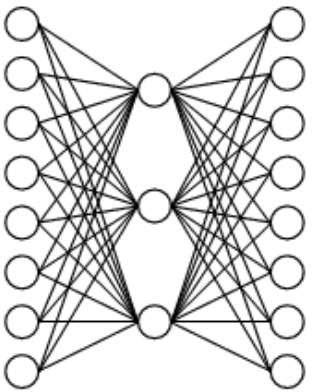
$$out(\mathbf{x}) \;=\; g(w_0 + \sum_i w_i x_i)$$

- 1-hidden layer:

$$out(\mathbf{x}) \;=\; g\left(w_0 + \sum_k w_k g(w_0^k + \sum_i w_i^k x_i)\right)$$

- No longer convex function!

Example data for NN with hidden layer

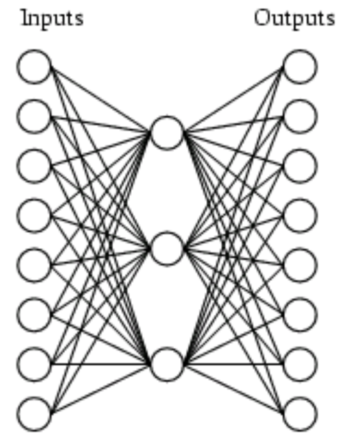


A target function:

Input		Output
10000000	$\rightarrow$	10000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	00000001

Can this be learned??

Example data for NN with hidden layer



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Input		Output
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01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	00000001

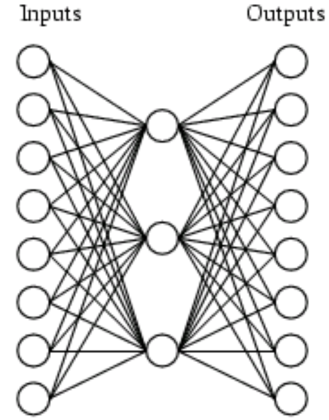
Autoencoder
(kind of unsupervised learning)

Dimensionality Reduction

Can this be learned??

Learned weights for hidden layer

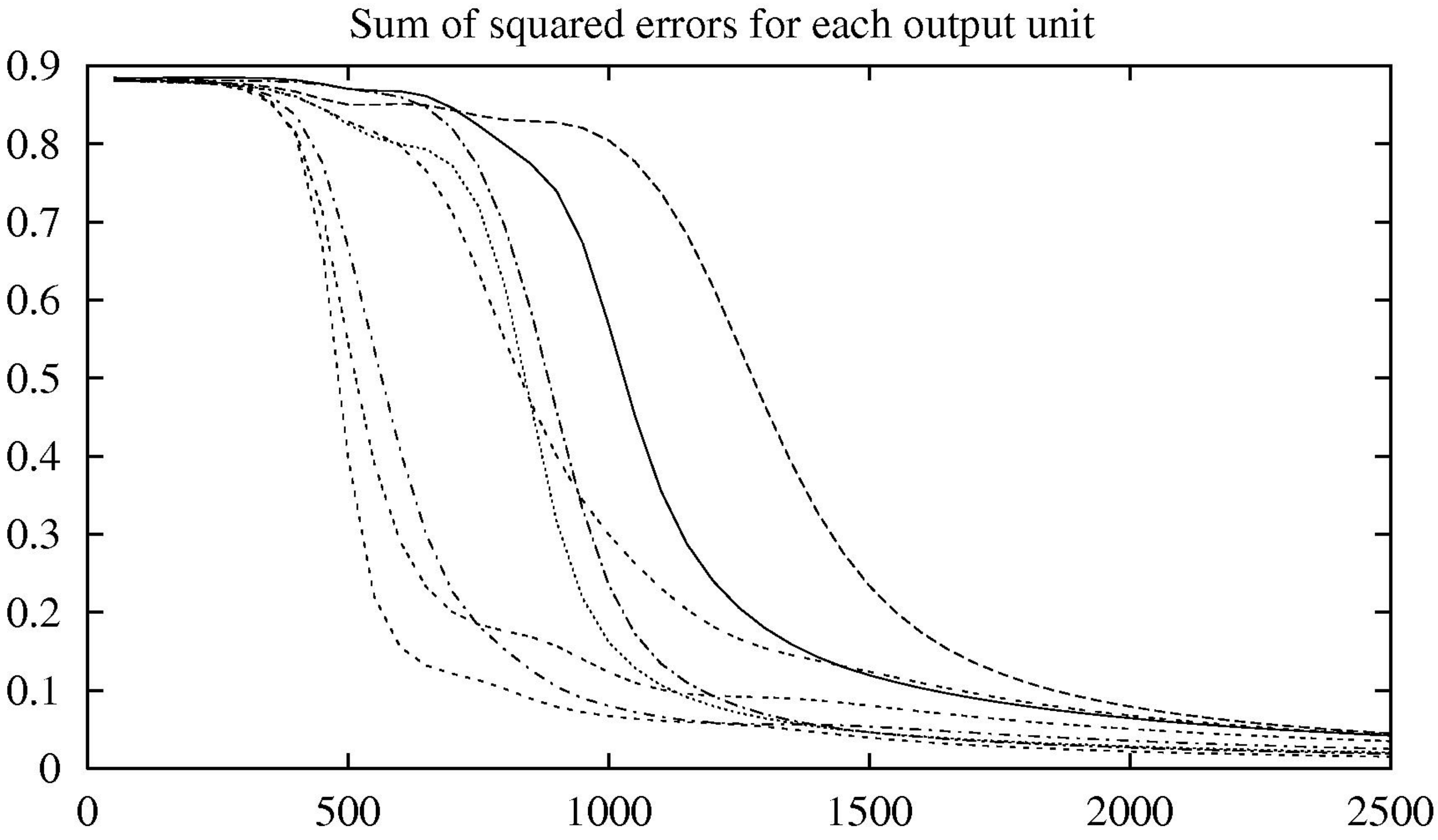
A network:



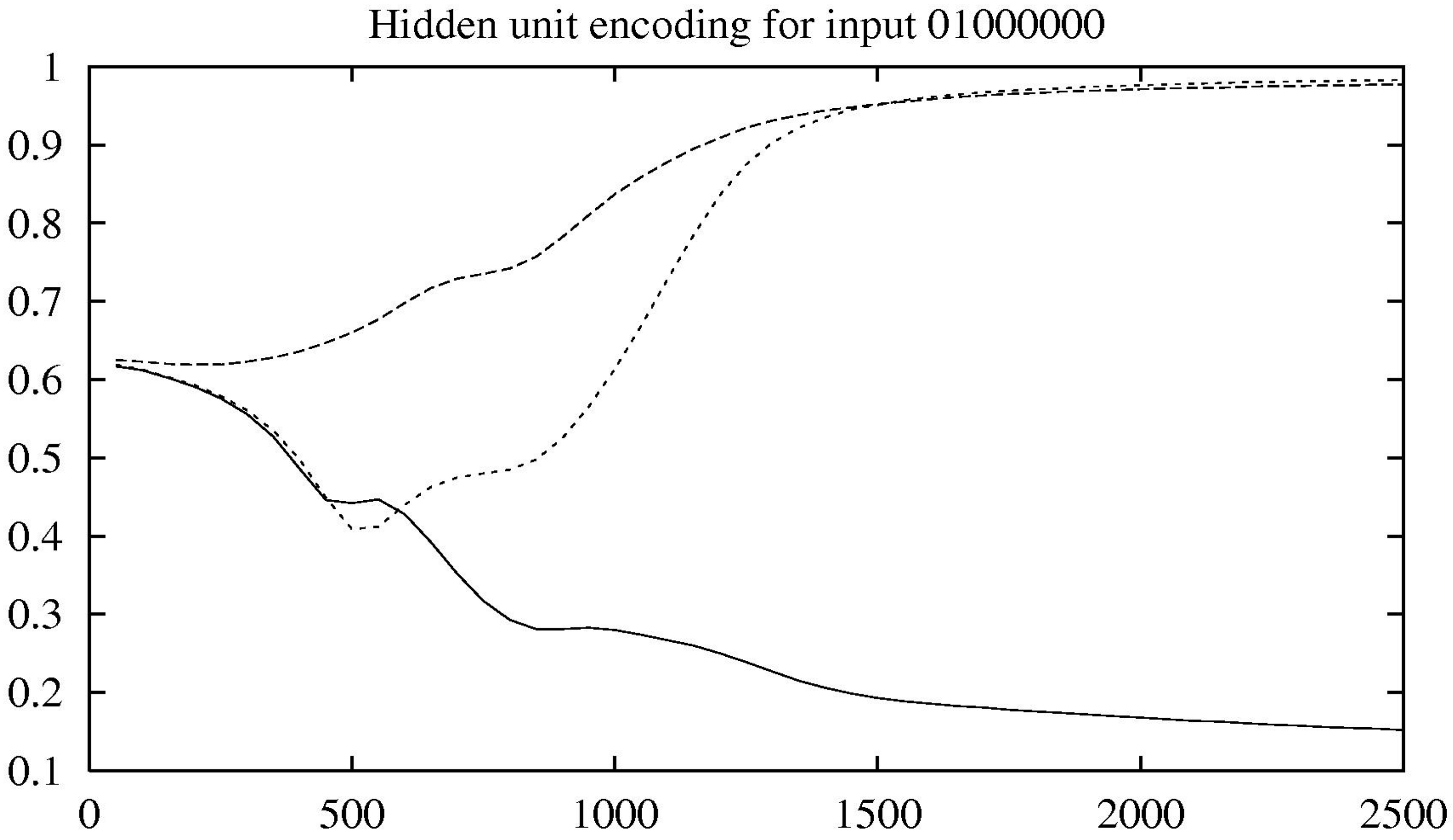
Learned hidden layer representation:

Input		Hidden Values				Output
10000000	$\rightarrow$	.89	.04	.08	$\rightarrow$	10000000
01000000	$\rightarrow$	.01	.11	.88	$\rightarrow$	01000000
00100000	$\rightarrow$	.01	.97	.27	$\rightarrow$	00100000
00010000	$\rightarrow$	.99	.97	.71	$\rightarrow$	00010000
00001000	$\rightarrow$	.03	.05	.02	$\rightarrow$	00001000
00000100	$\rightarrow$	.22	.99	.99	$\rightarrow$	00000100
00000010	$\rightarrow$	.80	.01	.98	$\rightarrow$	00000010
00000001	$\rightarrow$	.60	.94	.01	$\rightarrow$	00000001

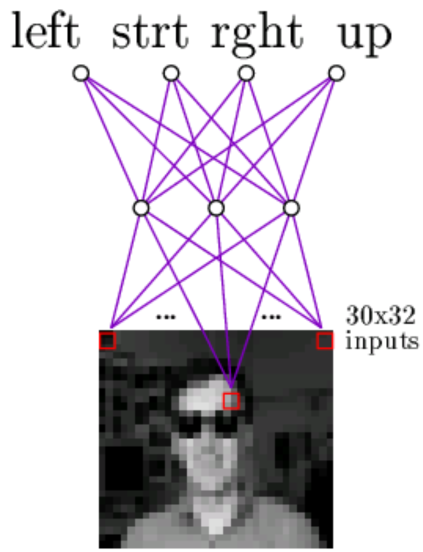
Learning the weights



Learning an encoding



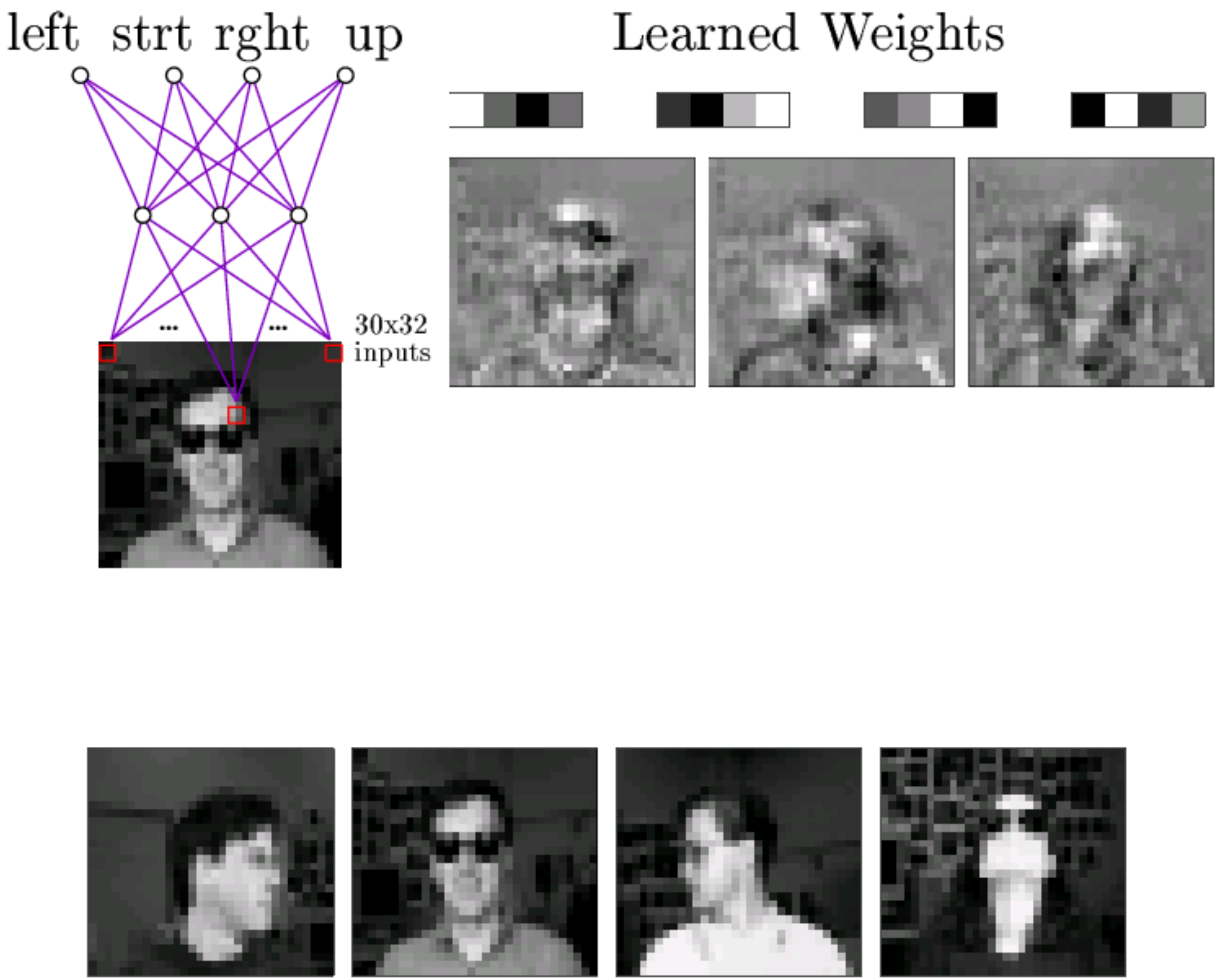
NN for images




Typical input images

90% accurate learning head pose, and recognizing 1-of-20 faces

Weights in NN for images



Typical input images

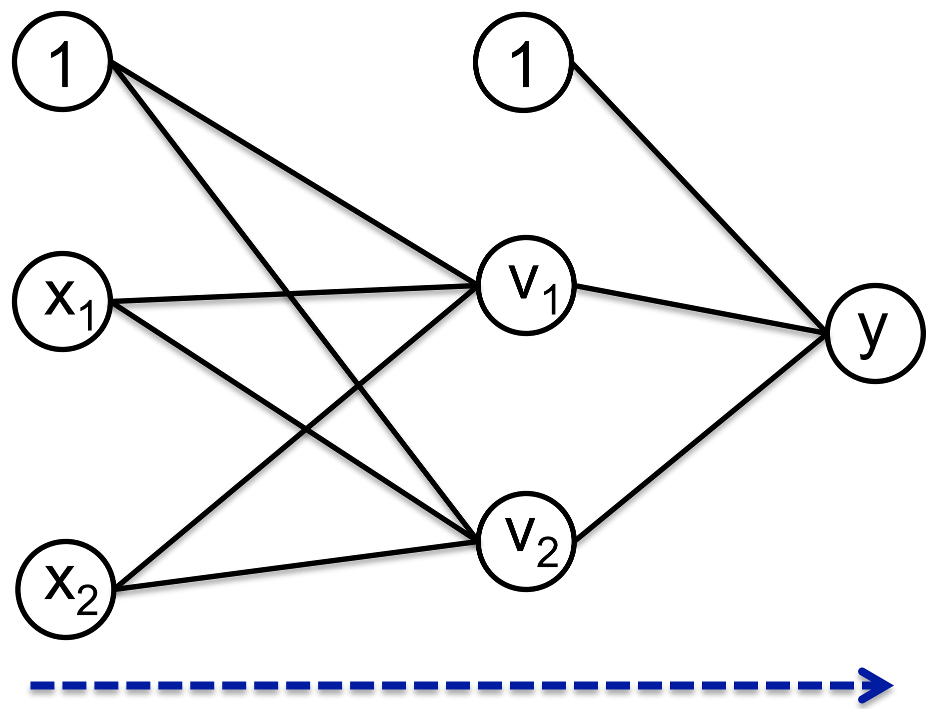
Forward propagation

1-hidden layer:

$$out(\mathbf{x}) \;=\; g\left(w_0 + \sum_k w_k g(w_0^k + \sum_i w_i^k x_i)\right)$$

Compute values left to right

1. Inputs: $x_1, \ldots, x_n$
2. Hidden: $v_1, \ldots, v_n$
3. Output: y



Forward propagation

1-hidden layer:

k sums over hidden layer

i sums over input layer

$$out(\mathbf{x}) = g\left(w_0 + \sum_k w_k g(w_0^k + \sum_i w_i^k x_i)\right)$$

Compute values left to right

1. Inputs: $x_1, \ldots, x_n$
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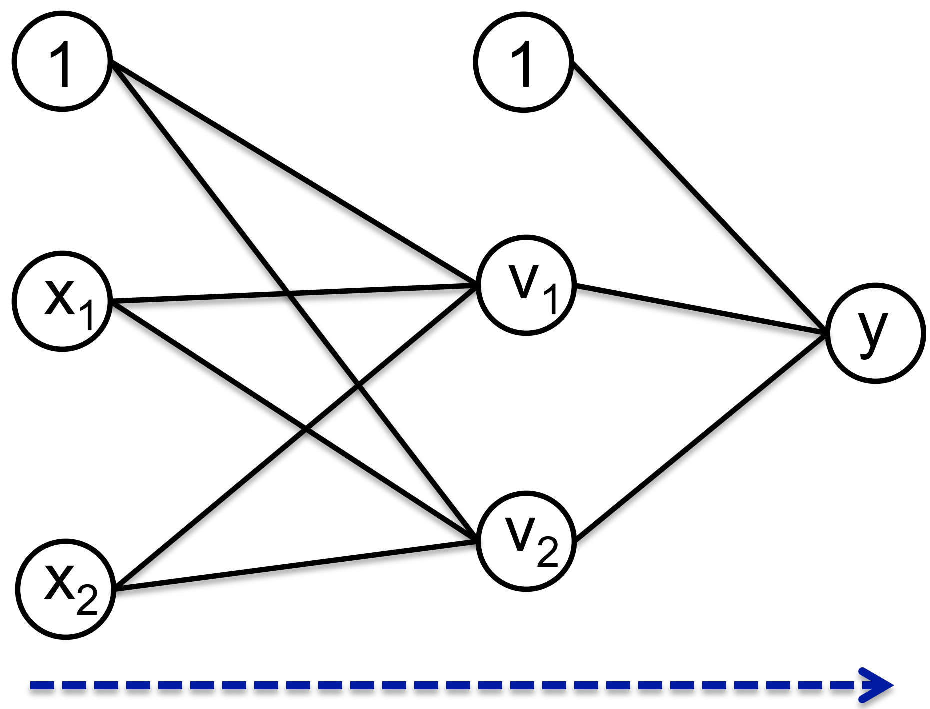


Gradient descent for 1-hidden layer

$$\boxed{\frac{\partial \ell(W)}{\partial w_k}}$$

Dropped w_0 to make derivation simpler

$$\ell(W) = \frac{1}{2}\sum_j [y^j - out(\mathbf{x}^j)]^2$$

$$out(\mathbf{x}) = g\left(\sum_{k'} w_{k'} g(\sum_{i'} w_{i'}^{k'} x_{i'})\right)$$

$$\boxed{v_k^j = g\left(\sum_{i'} w_{i'}^{k'} x_{i'}\right)}$$

$$\frac{\partial \ell(W)}{\partial w_k} = \sum_{j=1}^{m} -[y^j - out(\mathbf{x}^j)]\frac{\partial out(\mathbf{x}^j)}{\partial w_k}$$

$$out(x) = g\left(\sum_{k'} w_{k'} v_{k'}^j\right)$$

$$\frac{\partial out(\mathbf{x})}{\partial w_k} = v_k^j g'\left(\sum_{k'} w_{k'} v_{k'}^j\right)$$

Gradient for last layer same as the single node case, but with hidden nodes v as input!

Gradient descent for 1-hidden layer

$$\boxed{\frac{\partial \ell(W)}{\partial w_i^k}}$$

Dropped w_0 to make derivation simpler

$$\boxed{\frac{\partial}{\partial x} f(g(x)) = f'(g(x))g'(x)}$$

$$\ell(W) = \frac{1}{2}\sum_j [y^j - out(\mathbf{x}^j)]^2$$

$$out(\mathbf{x}) = g\left(\sum_{k'} w_{k'} g(\sum_{i'} w_{i'}^{k'} x_{i'})\right)$$

$$\frac{\partial \ell(W)}{\partial w_i^k} = \sum_{j=1}^{m} -[y - out(\mathbf{x}^j)]\frac{\partial out(\mathbf{x}^j)}{\partial w_i^k}$$

$$\frac{\partial out(\mathbf{x})}{\partial w_i^k} = g'\left(\sum_{k'} w_{k'} g(\sum_{i'} w_{i'}^{k'} x_{i'})\right) \frac{\partial}{\partial w_i^k} g\left(\sum_{i'} w_{i'}^{k'} x_{i'}\right) w_k$$

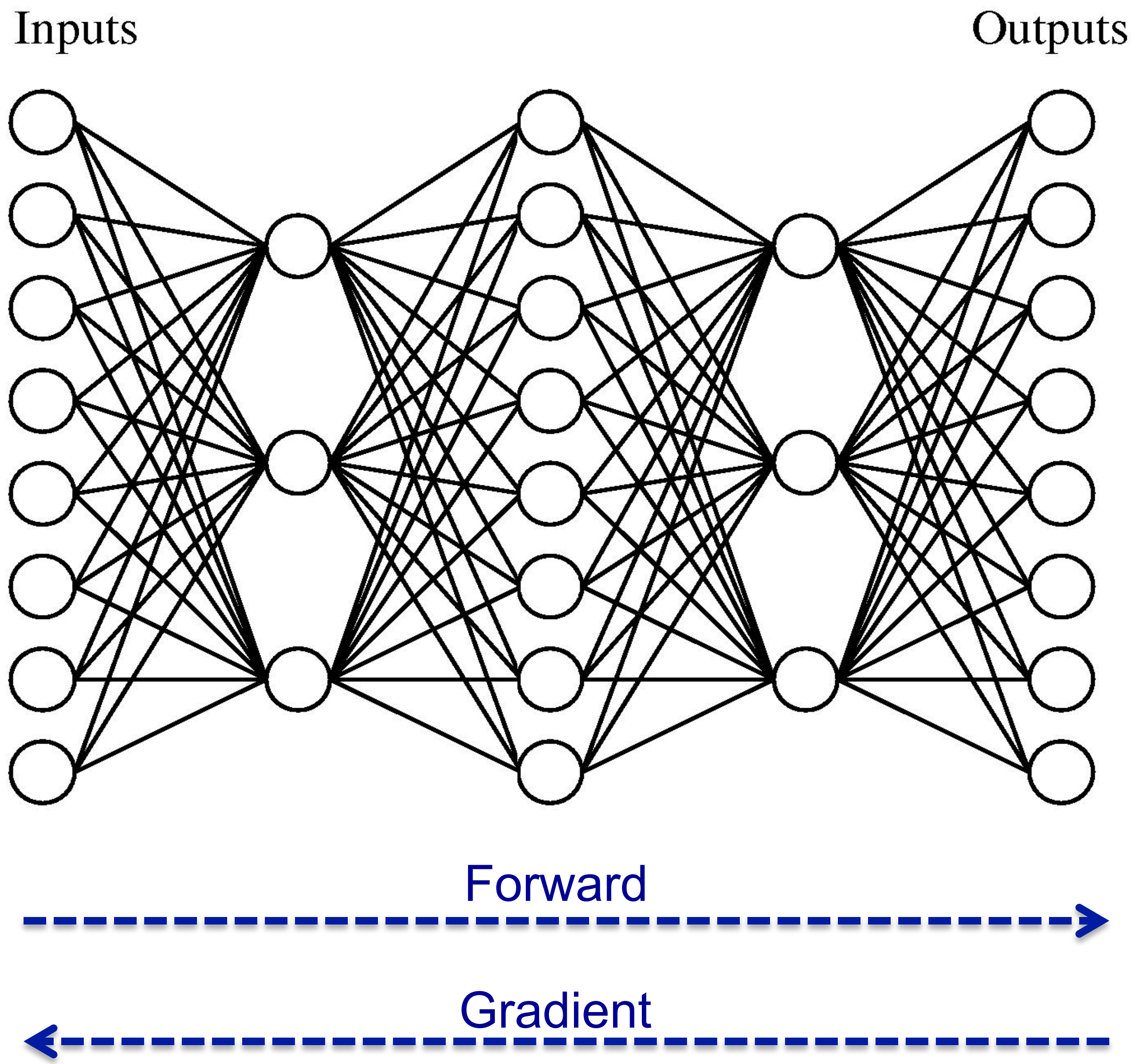
For hidden layer, two parts:

- Normal update for single neuron
- Recursive computation of gradient on output layer

Multilayer neural networks

Inference and Learning:

- Forward pass: left to right, each hidden layer in turn
- Gradient computation: right to left, propagating gradient for each node



Forward propagation – prediction

- Recursive algorithm
- Start from input layer
- Output of node V_k with parents $U_1, U_2, \ldots$:

$$\boxed{V_k \; = \; g\left(\sum_i w_i^k U_i\right)}$$

Back-propagation – learning

- Just gradient descent!!!
- Recursive algorithm for computing gradient
- For each example
  - Perform forward propagation
  - Start from output layer
    - Compute gradient of node V_k with parents $U_1, U_2, \ldots$
    - Update weight w_i^k
    - Repeat (move to preceding layer)

Back-propagation – pseudocode

Initialize all weights to small random numbers

- Until convergence, do:
  - For each training example x,y:
    1. Forward propagation, compute node values V_k
    2. For each output unit o (with labeled output y):

       $$\delta_o = V_o(1-V_o)(y-V_o)$$

    3. For each hidden unit h:

       $$\delta_h = V_h(1-V_h) \sum_{k \text{ in } output(h)} w_{h,k}\delta_k$$

    4. Update each network weight $w_{i,j}$ from node i to node j

       $$w_{i,j} = w_{i,j} + \eta\delta_j x_{i,j}$$

Convergence of backprop

- Perceptron leads to convex optimization
  - Gradient descent reaches **global minima**
- Multilayer neural nets **not convex**
  - Gradient descent gets stuck in local minima
  - Selecting number of hidden units and layers = fuzzy process
  - NNs have made a HUGE comeback in the last few years!!!
    - Neural nets are back with a new name!!!!
      - Deep belief networks
      - Huge error reduction when trained with lots of data on GPUs

Weight Initialization

» Don’t just initialize weights to 0!
- (like we did with linear models)
- Bad local optima

» Initial weights = 0
- => all hidden units = 0
- => Gradient on output layer will be 0
- => Gradients of weights on each hidden unit will be the same.
- => Values of hidden units always the same

Breadth vs. Depth

» 2 layer networks can represent any function

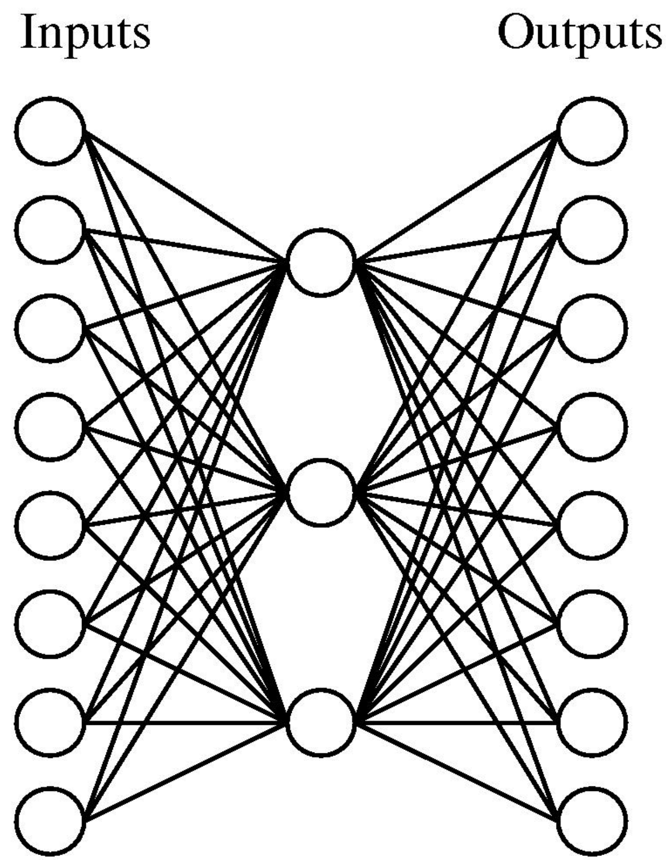
» But, can require exponentially many hidden units

» Analogy to circuit complexity

- Parity function
- Easy to define O(log(D)) depth circuit
- Exponential # of gates required for constant depth

Overfitting in NNs

- Are NNs likely to overfit?
  – Yes, they can represent arbitrary functions!!!
- Avoiding overfitting?
  – More training data
  – Fewer hidden nodes / better topology
  – Regularization
  – Early stopping



Disadvantages of Neural Networks

» Lots of hyperparameters!

- Learning rate
- Early stopping
- How many hidden units?
- How many layers?
- …

Disadvantages of Neural Networks

» Vanishing Gradients

- gradients shrink during backprop
- At beginning of deep network, changing one weight doesn’t have much effect on the output
- Derivatives are small

Computation Graphs

- » Arbitrary graphs of function composition
- » Choose whatever activation functions
- » Choose any loss function
- » Computing gradients is all very mechanical
- » Also automatically parallelize on GPUs

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TensorFlow

Computation Graphs

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TensorFlow

theano

Keras == simple
10 lines of code

```
input_encoder = Sequential()
input_encoder.add(Embedding(input_dim=vocab_size, output_dim=64))
input_encoder.add(LSTM(64))

question_encoder = Sequential()
question_encoder.add(Embedding(input_dim=vocab_size, output_dim=64))
question_encoder.add(LSTM(64))

model = Sequential()
model.add(Merge([input_encoder, question_encoder], mode='concat'))
model.add(Dense(128))
model.add(Activation('softmax'))
```

Computation Graphs

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theano

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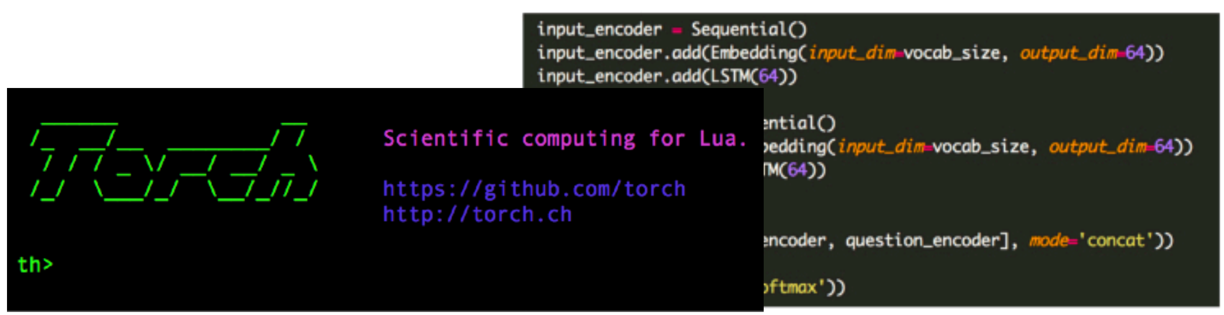

Computation Graphs

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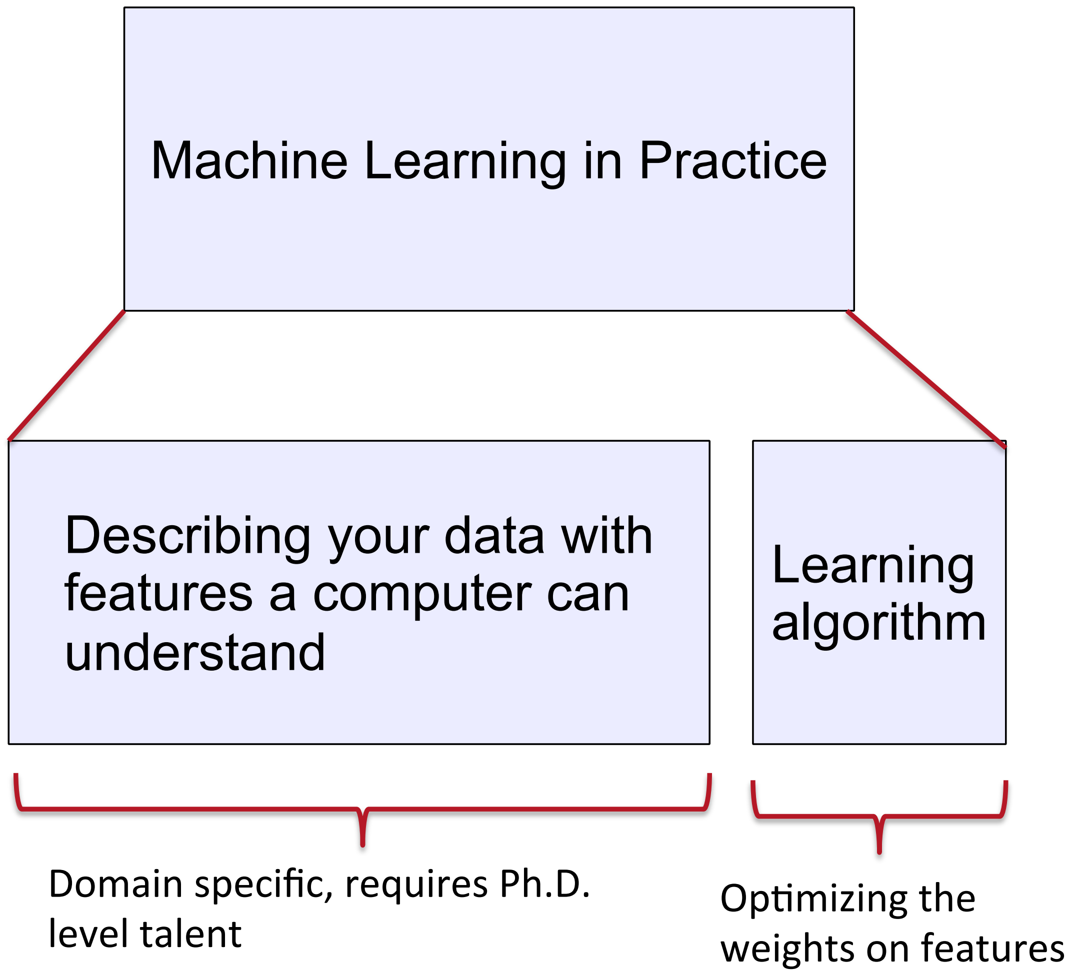
Machine Learning vs Deep Learning



Reasons for Exploring Deep Learning

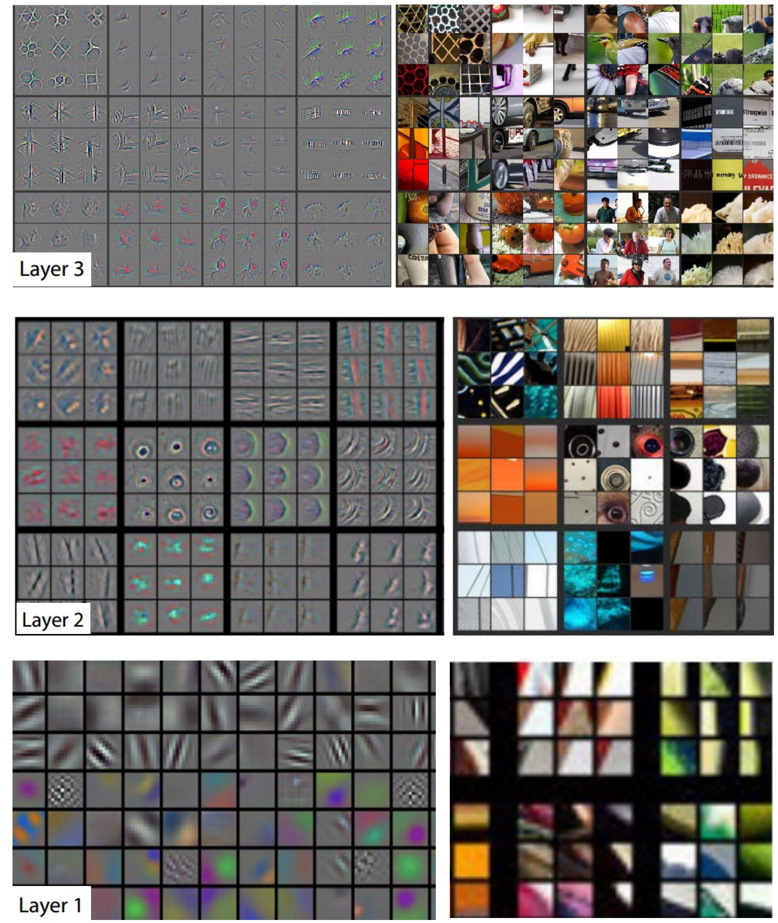
- In 2006 **deep** learning techniques started outperforming other machine learning techniques. Why now?

- DL techniques benefit more from a lot of data
- Faster machines and multicore CPU/GPU help DL
- New models, algorithms, ideas

→ **Improved performance** (first in speech and vision, then NLP)

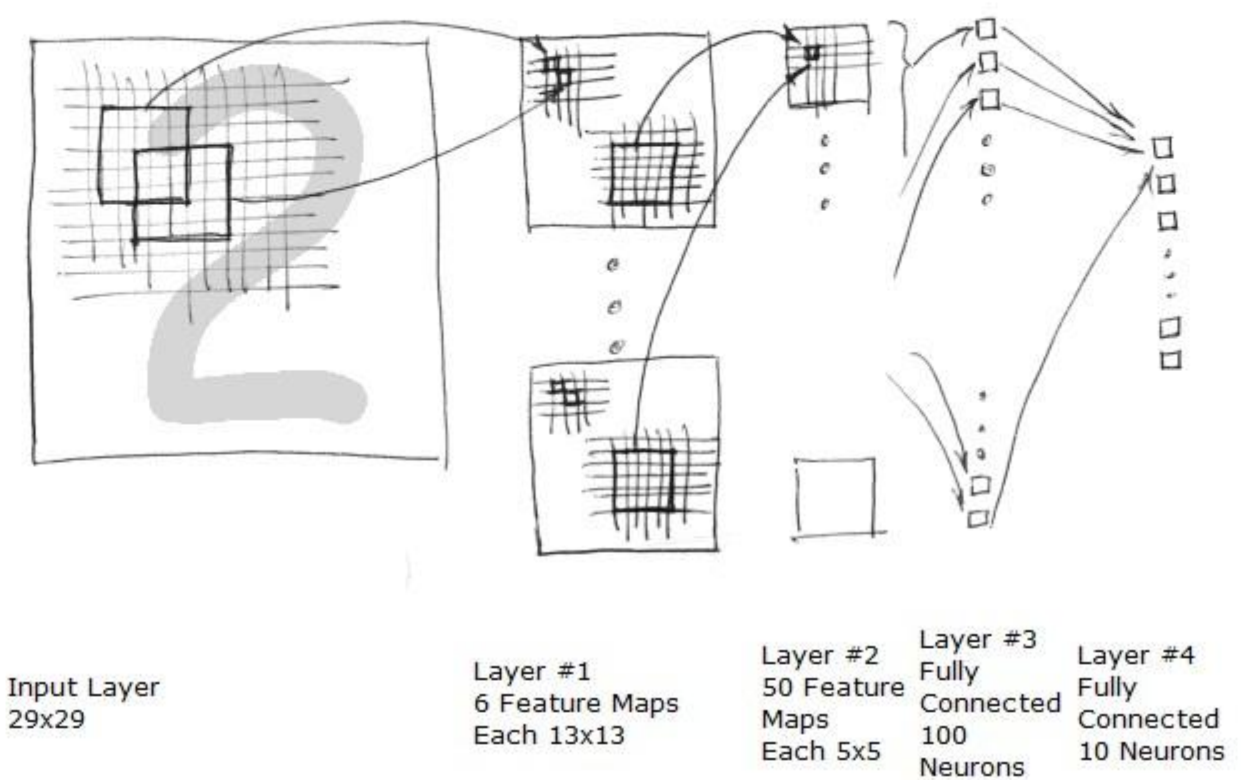
Deep Learning for Computer Vision

- Most deep learning groups have (until recently) largely focused on computer vision
- Break through paper: ImageNet Classification with Deep Convolutional Neural Networks by Krizhevsky et al. 2012



Zeiler and Fergus (2013)

Convolutional Neural Networks



AlexNet

ImageNet Classification with Deep Convolutional Neural Networks

Alex Krizhevsky
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Ilya Sutskever
University of Toronto
ilya@cs.utoronto.ca

Geoffrey E. Hinton
University of Toronto
hinton@cs.utoronto.ca

AlexNet

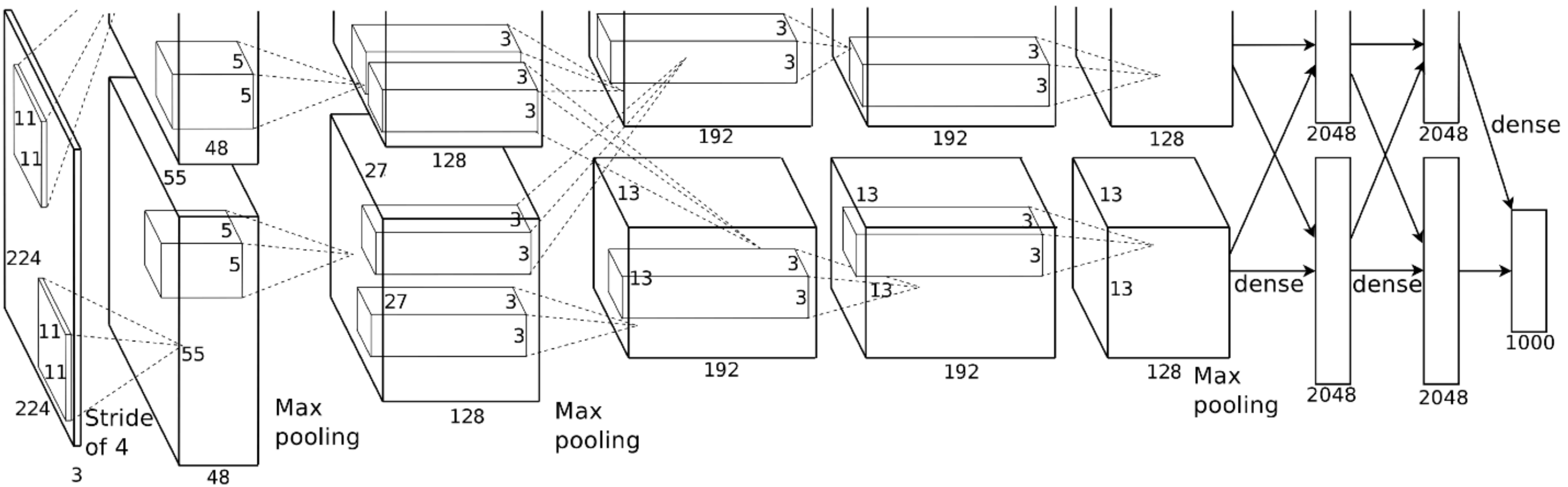
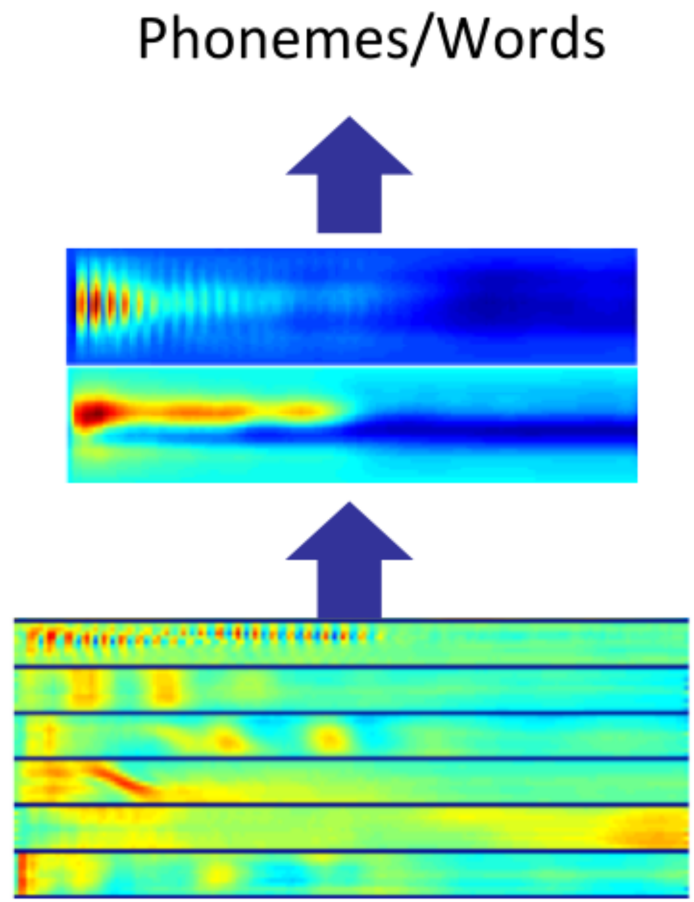


Figure 2: An illustration of the architecture of our CNN, explicitly showing the delineation of responsibilities between the two GPUs. One GPU runs the layer-parts at the top of the figure while the other runs the layer-parts at the bottom. The GPUs communicate only at certain layers. The network's input is 150,528-dimensional, and the number of neurons in the network's remaining layers is given by 253,440–186,624–64,896–64,896–43,264–4096–4096–1000.

Deep Learning for Speech

- The first breakthrough results of "deep learning" on large datasets happened in speech recognition
- Context-Dependent Pre-trained Deep Neural Networks for Large Vocabulary Speech Recognition Dahl et al. (2010)



Acoustic model	Recog \ WER	RT03S FSH	Hub5 SWB
Traditional features	1-pass −adapt	**27.4**	**23.6**
Deep Learning	1-pass −adapt	**18.5** (−33%)	**16.1** (−32%)

Machine Translation

- Many levels of translation have been tried in the past:

- Traditional MT systems are very large complex systems

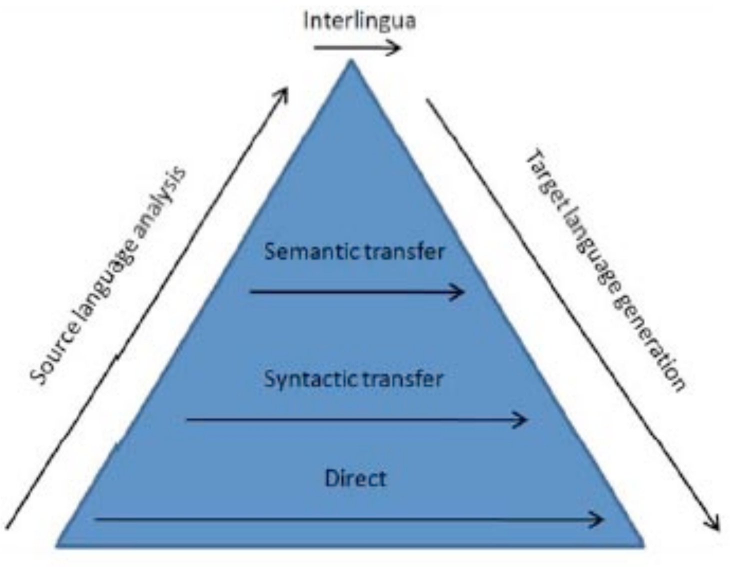
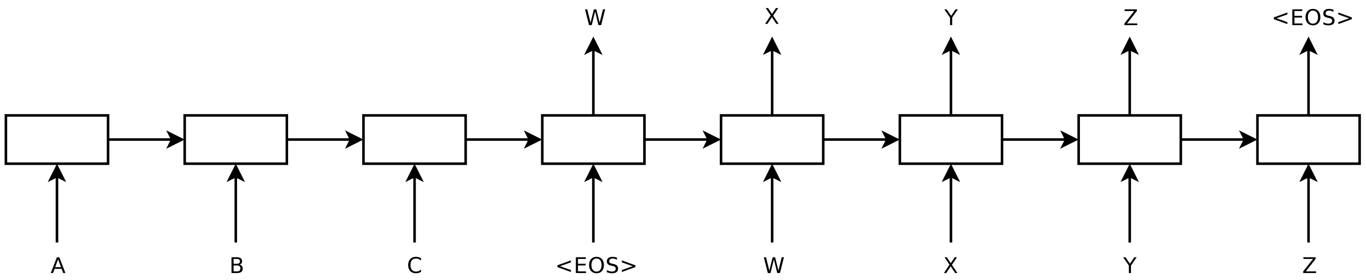


Figure 1: The Vauquois triangle

- What do you think is the interlingua for the DL approach to translation?

Machine Translation

- Source sentence mapped to vector, then output sentence generated.



- Sequence to Sequence Learning with Neural Networks by Sutskever et al. 2014

What you need to know about neural networks

- Perceptron:
  - Relationship to general neurons
- Multilayer neural nets
  - Representation
  - Derivation of backprop
  - Learning rule
- Overfitting