Machine Learning

4771

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Topic 4

- Tutorial: Matlab
- Perceptron, Online & Stochastic Gradient Descent
- Convergence Guarantee
- Perceptron vs. Linear Regression
- Multi-Layer Neural Networks
- Back-Propagation
- Demo: LeNet
- Deep Learning

Tutorial: Matlab

- Matlab is the most popular language for machine learning
- See www.cs.columbia.edu->computing->Software->Matlab
- Online info to get started is available at:
  http://www.cs.columbia.edu/~jebara/tutorials.html
- Matlab tutorials
- List of Matlab function calls
- Example code: for homework #1 will use polyreg.m

- General: help, lookfor, 1:N, rand, zeros, A', reshape, size
- Math: max, min, cov, mean, norm, inv, pinv, det, sort, eye
- Control: if, for, while, end, %, function, return, clear
- Display: figure, clf, axis, close, plot, subplot, hold on, fprintf
- Input/Output: load, save, ginput, print,

- BBS and TA's are also helpful

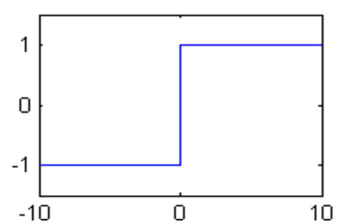
Perceptron (another Neuron)

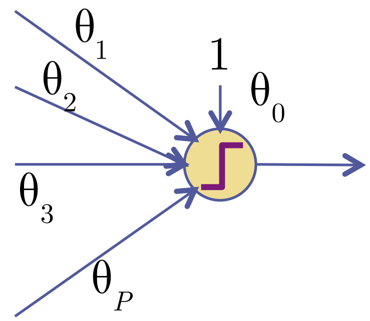
- Classification scenario once again but consider +1, -1 labels

$$\mathcal{X} = \left\{ \left(x_1, y_1\right), \left(x_2, y_2\right), \ldots, \left(x_N, y_N\right) \right\} \quad x \in \mathbb{R}^D \quad y \in \left\{-1, 1\right\}$$

- A better choice for a classification squashing function is

$$g\left(z\right) = \begin{cases} -1 \text{ when } z < 0 \\ +1 \text{ when } z \geq 0 \end{cases}$$





- And a better choice is classification loss

$$L\left(y, f\left(\mathbf{x};\theta\right)\right) = \text{step}\left(-yf\left(\mathbf{x};\theta\right)\right)$$

- Actually with above g(z) any loss is like classification loss

$$R\left(\theta\right) = \tfrac{1}{4N}\sum\nolimits_{i=1}^{N}\left(y - g\left(\theta^T x_i\right)\right)^2 \equiv \tfrac{1}{N}\sum\nolimits_{i=1}^{N} \text{step}\left(-y_i \theta^T x_i\right)$$

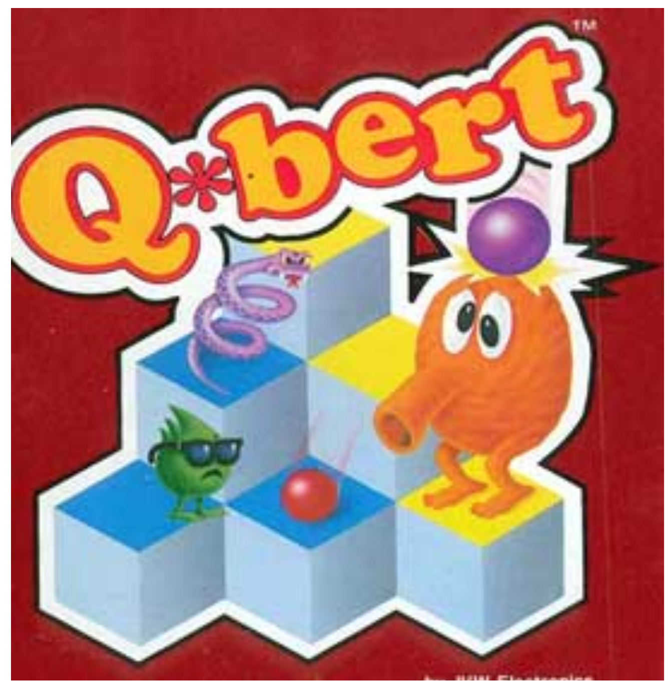
- What does this $R(\theta)$ function look like?

Perceptron & Classification Loss

- Classification loss for the Risk leads to hard minimization
- What does this R(θ) function look like?

$$R(\theta) = \frac{1}{N}\sum_{i=1}^{N} \mathrm{step}\left(-y_i \theta^T x_i\right)$$

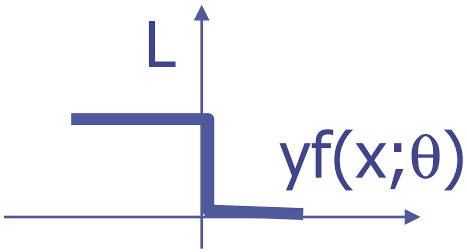
- Qbert-like, can't do gradient descent since the gradient is zero except at edges when a label flips



Perceptron & Perceptron Loss

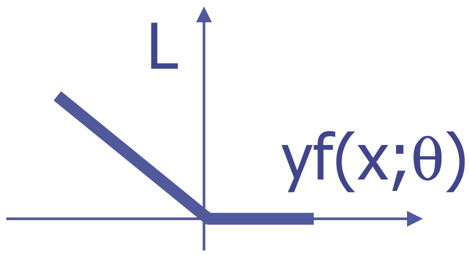
- Instead of Classification Loss

$$R(\theta) = \tfrac{1}{N}\sum_{i=1}^{N} \mathrm{step}\left(-y_i \theta^T x_i\right)$$



- Consider Perceptron Loss:

$$R^{per}(\theta) = -\tfrac{1}{N}\sum_{i \in misclassified} y_i \left(\theta^T x_i\right)$$



- Instead of staircase-shaped R get smooth piece-wise linear R

- Get reasonable gradients for gradient descent

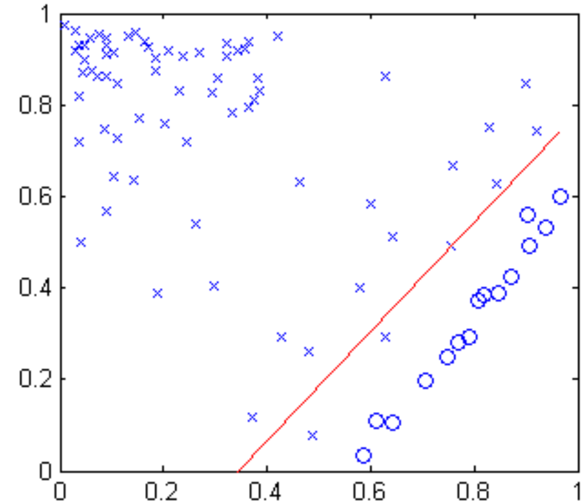
$$\nabla_\theta R^{per}(\theta) = -\tfrac{1}{N}\sum_{i \in misclassified} y_i \mathbf{x}_i$$

$$\theta^{t+1} = \theta^t - \eta \nabla_\theta R^{per}\Big|_{\theta^t} = \theta^t + \eta \tfrac{1}{N}\sum_{i \in misclassified} y_i \mathbf{x}_i$$

Perceptron vs. Linear Regression

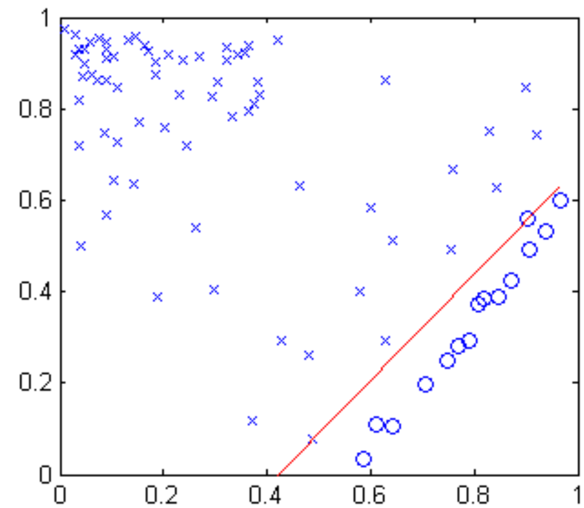
- Linear regression gets close but doesn't do perfectly

  classification error = 2
  squared error = 0.139



- Perceptron gets zero error

  classification error = 0
  perceptron err = 0



Stochastic Gradient Descent

- Gradient Descent vs. Stochastic Gradient Descent

- Instead of computing the average gradient for all points and then taking a step

$$\nabla_\theta R^{per}\left(\theta\right) = -\frac{1}{N}\sum_{i \in misclassified} y_i \mathbf{x}_i$$

- Update the gradient for each mis-classified point by itself

$$\nabla_\theta R^{per}\left(\theta\right) = -y_i \mathbf{x}_i$$ if i mis-classified

- Also, set η to 1 without loss of generality

$$\theta^{t+1} = \theta^t - \eta \nabla_\theta R^{per}\Big|_{\theta^t} = \theta^t + y_i \mathbf{x}_i$$ if i mis-classified

Online Perceptron

- Apply stochastic gradient descent to a perceptron
- Get the "online perceptron" algorithm:

$$
\begin{array}{l}
initialize\ t = 0\ and\ \theta^0 = \vec{0} \\
while\ not\ converged\ \{ \\
\quad pick\ i \in \left\{1,\ldots,N\right\} \\
\quad if\left(y_i x_i^T \theta^t \leq 0\right) \quad \{\ \theta^{t+1} = \theta^t + y_i x_i \\
\qquad\qquad\qquad\qquad\qquad\quad\ t = t+1 \qquad\qquad \}\ \}
\end{array}
$$

- Either pick i randomly or use a "for i=1 to N" loop
- If the algorithm stops, we have a theta that separates data
- The total number of mistakes we made along the way is t

Online Perceptron Theorem

Theorem: the online perceptron algorithm converges to zero error in finite t if we assume

1) all data inside a sphere of radius r: $\left\|\mathbf{x}_i\right\| \leq r \quad \forall i$
2) data is separable with margin γ: $y_i \left(\theta^*\right)^T \mathbf{x}_i \geq \gamma \quad \forall i$

Proof:

- Part 1) Look at inner product of current θ^t with θ^*

  assume we just updated a mistake on point i:

$$\left(\theta^*\right)^T \theta^t = \left(\theta^*\right)^T \theta^{t-1} + y_i \left(\theta^*\right)^T \mathbf{x}_i \geq \left(\theta^*\right)^T \theta^{t-1} + \gamma$$

  after applying t such updates, we must get:

$$\left(\theta^*\right)^T \theta^t = \left(\theta^*\right)^T \theta^t \geq t\gamma$$

Online Perceptron Proof

- Part 1) $\left(\theta^*\right)^T \theta^t = \left(\theta^*\right)^T \theta^t \geq t\gamma$

- Part 2) $\left\|\theta^t\right\|^2 = \left\|\theta^{t-1} + y_i \mathbf{x}_i\right\|^2 = \left\|\theta^{t-1}\right\|^2 + 2y_i \left(\theta^{t-1}\right)^T \mathbf{x}_i + \left\|\mathbf{x}_i\right\|^2$

$$\leq \left\|\theta^{t-1}\right\|^2 + \left\|\mathbf{x}_i\right\|^2$$

$$\leq \left\|\theta^{t-1}\right\|^2 + r^2$$

$$\leq tr^2$$

since only update mistakes middle term is negative

- Part 3) Angle between optimal & current solution

$$\cos\left(\theta^*, \theta^t\right) = \frac{\left(\theta^*\right)^T \theta^t}{\left\|\theta^t\right\|\left\|\theta^*\right\|} \geq \frac{t\gamma}{\left\|\theta^t\right\|\left\|\theta^*\right\|} \geq \frac{t\gamma}{\sqrt{tr^2}\left\|\theta^*\right\|}$$

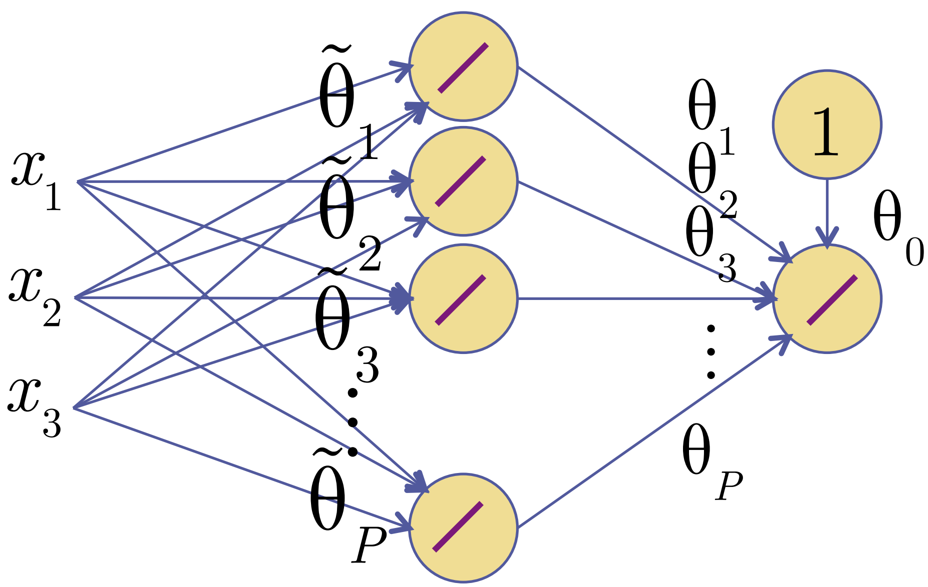
apply part 1 then part 2

- Since $\cos \leq 1 \Rightarrow \frac{t\gamma}{\sqrt{tr^2}\left\|\theta^*\right\|} \leq 1 \Rightarrow t \leq \frac{r^2}{\gamma^2}\left\|\theta^*\right\|^2$

...so t is finite!

Multi-Layer Neural Networks

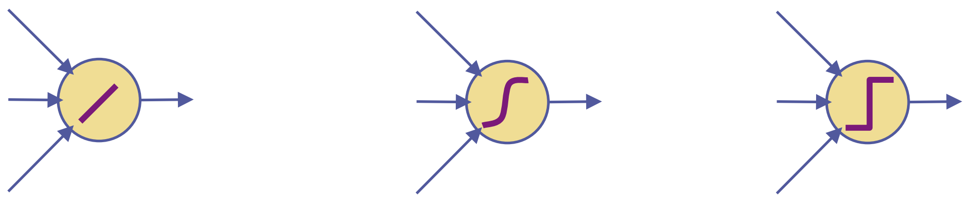
- What if we consider cascading multiple layers of network?
- Each output layer is input to the next layer
- Each layer has its own weights parameters
- Eg: each layer has linear nodes (not perceptron/logistic)



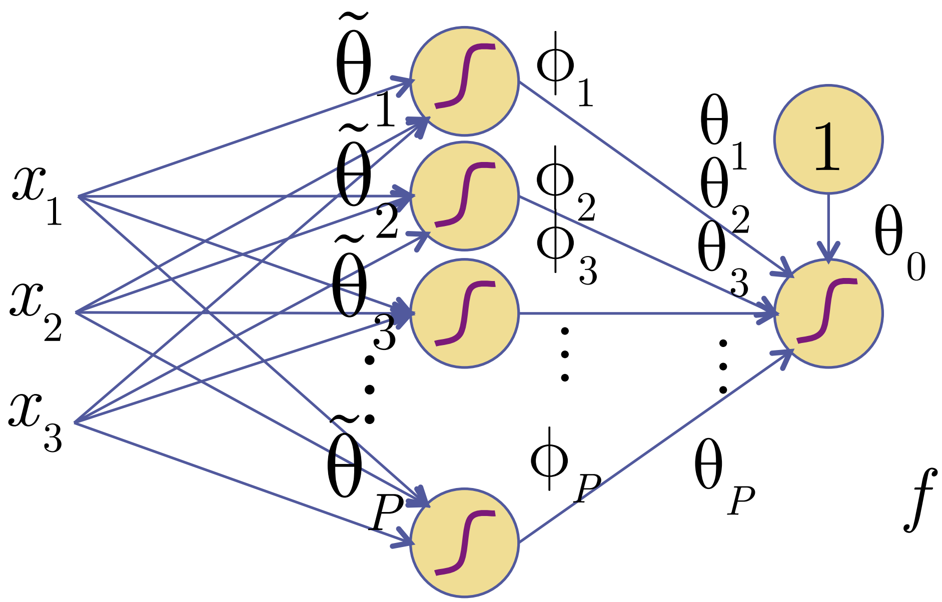
- Above Neural Net has 2 layers. What does this give?

Multi-Layer Neural Networks

- Need to introduce non-linearities between layers
- Avoids previous redundant linear layer problem



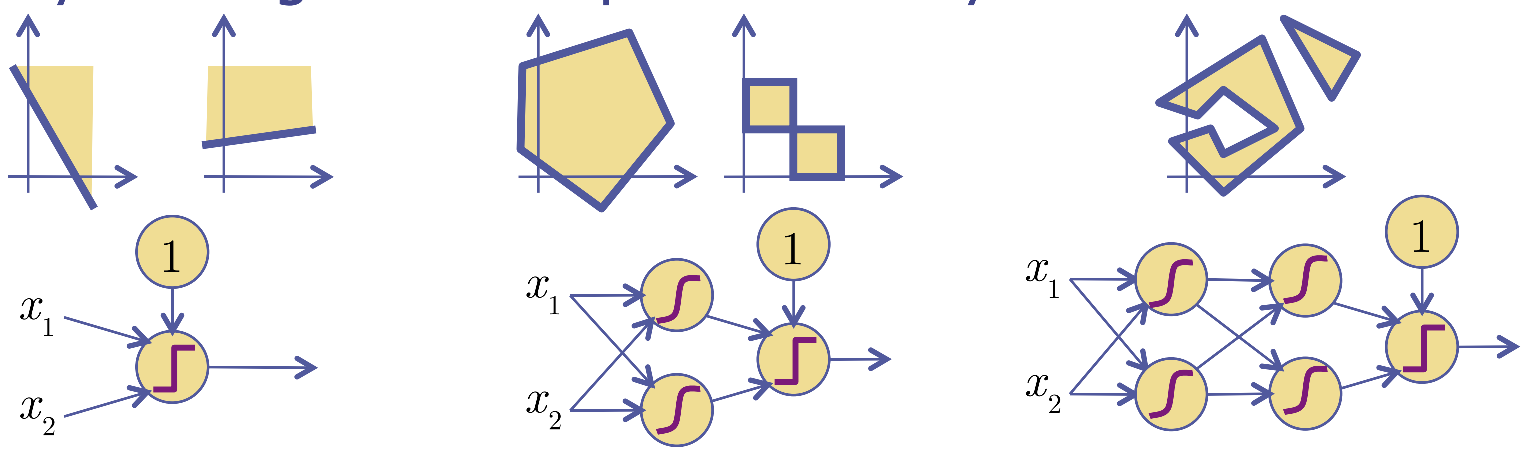
- Neural network can adjust the basis functions themselves…



$$f(\mathbf{x}) = g\left(\sum_{i=1}^{P} \theta_i g\left(\tilde{\theta}_i^T \mathbf{x}\right)\right)$$

Multi-Layer Neural Networks

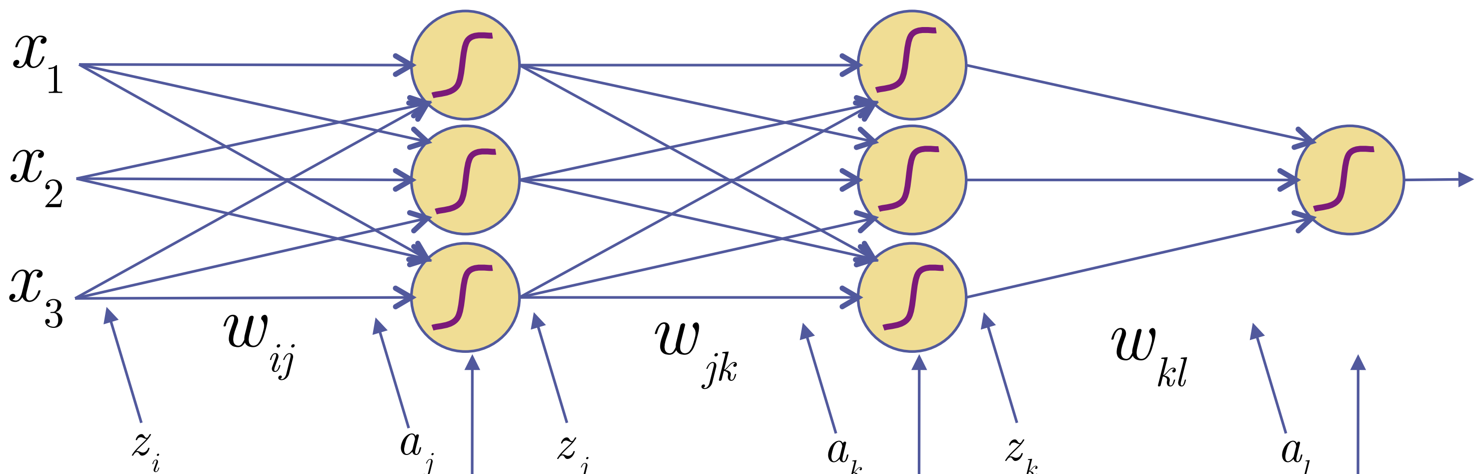
- Multi-Layer Network can handle more complex decisions
- 1-layer: is linear, can't handle XOR
- Each layer adds more flexibility (but more parameters!)
- Each node splits its input space with linear hyperplane
- 2-layer: if last layer is AND operation, get convex hull
- 2-layer: can do almost anything multi-layer can
  by fanning out the inputs at 2nd layer



- Note: Without loss of generality, we can omit the 1 and θ_0

Back-Propagation

- Gradient descent on squared loss is done layer by layer
- Layers: input, hidden, output. Parameters: $\theta = \left\{ w_{ij}, w_{jk}, w_{kl} \right\}$



$$a_j = \sum_i w_{ij} z_i \qquad a_k = \sum_j w_{jk} z_j \qquad a_l = \sum_k w_{kl} z_k$$

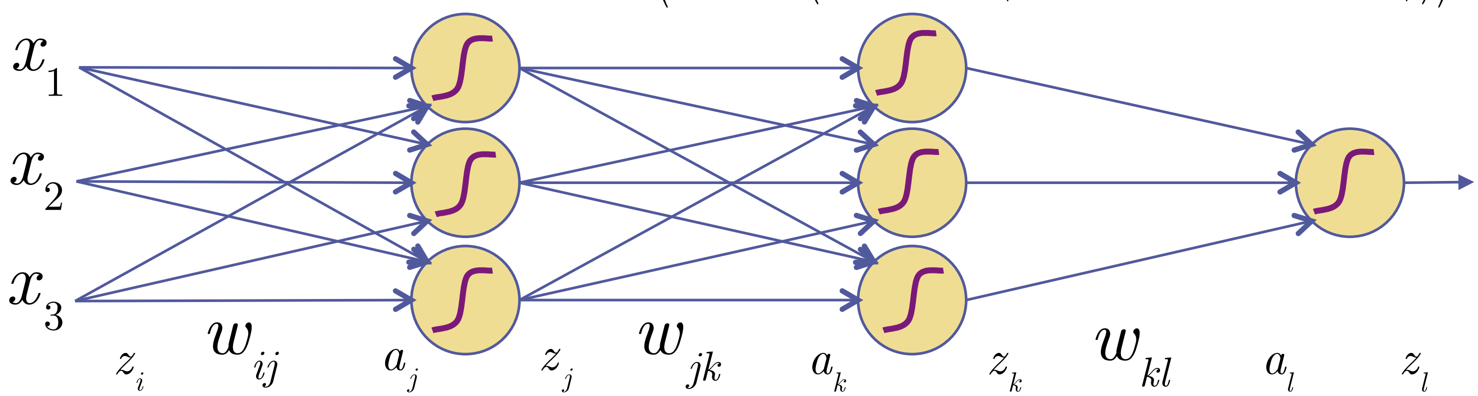
$$z_j = g(a_j) \qquad z_k = g(a_k) \qquad z_l = g(a_l)$$

- Each input x_n for n=1..N generates its own a's and z's
- Back-Propagation: Splits layer into its inputs & outputs
- Get gradient on output…back-track chain rule until input

Back-Propagation

- Cost function: $R(\theta) = \frac{1}{N}\sum_{n=1}^{N} L\left(y^n - f\left(x^n\right)\right)$

$$= \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl}\, g\left(\sum_j w_{jk}\, g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$$



- First compute output layer derivative:

$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right)$$

Chain Rule

$$define \;\; L^n := \frac{1}{2}\left(y^n - f\left(x^n\right)\right)^2$$

Back-Propagation

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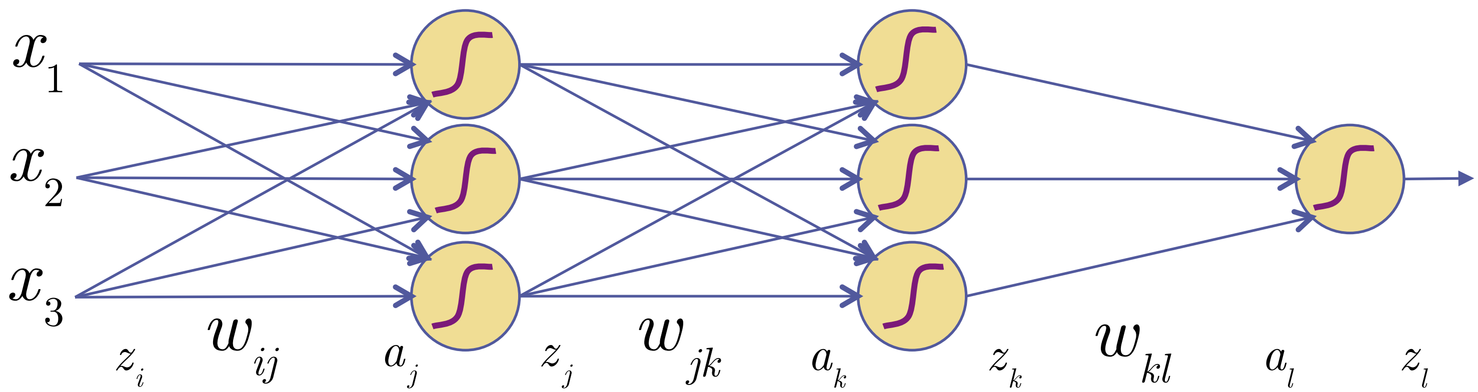

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$$= \frac{1}{N}\sum_n \left[\frac{\partial \frac{1}{2}\left(y^n - g\left(a_l^n\right)\right)^2}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right)$$

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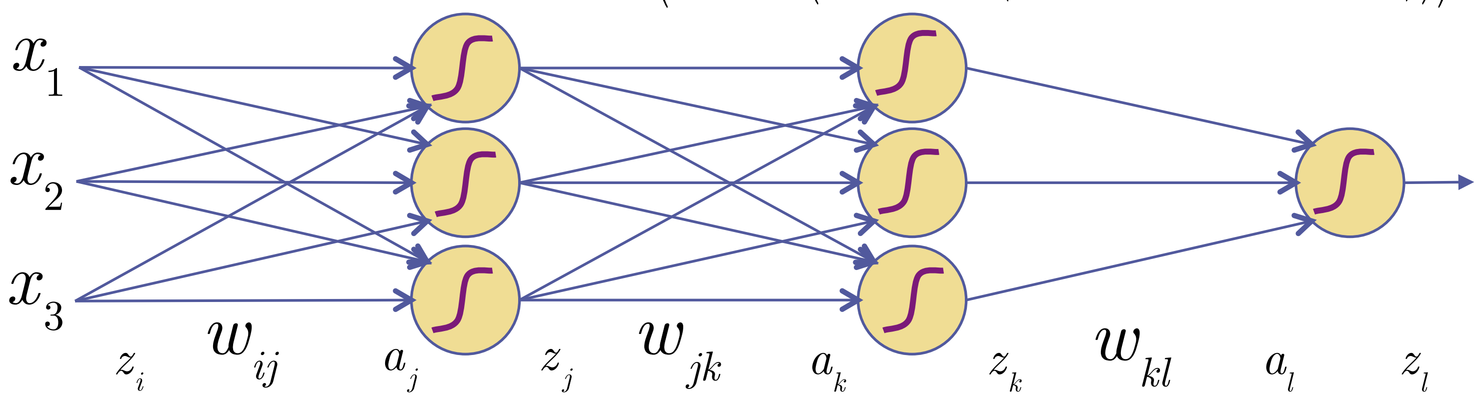

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Back-Propagation

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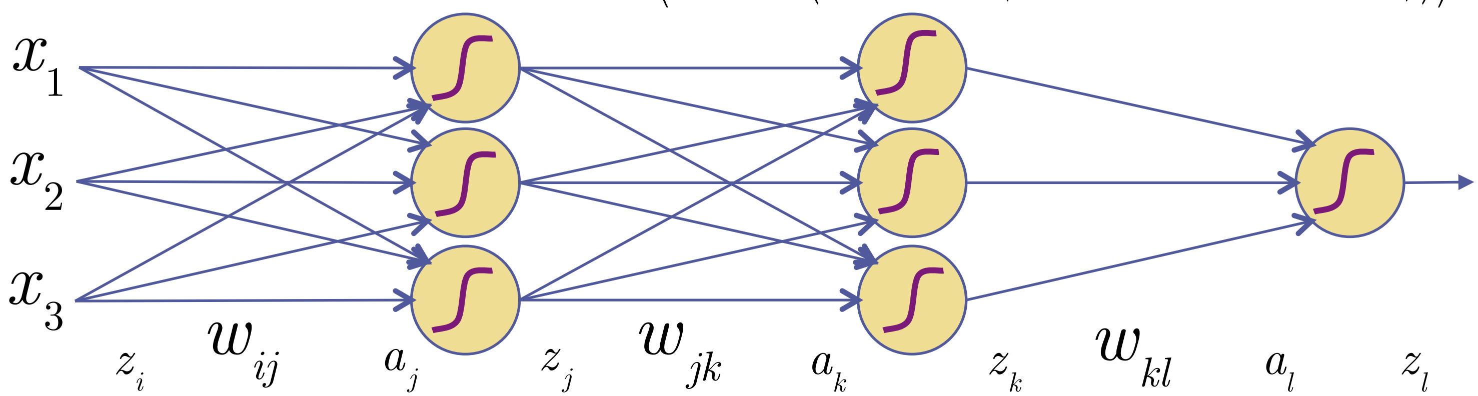

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$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right)$$

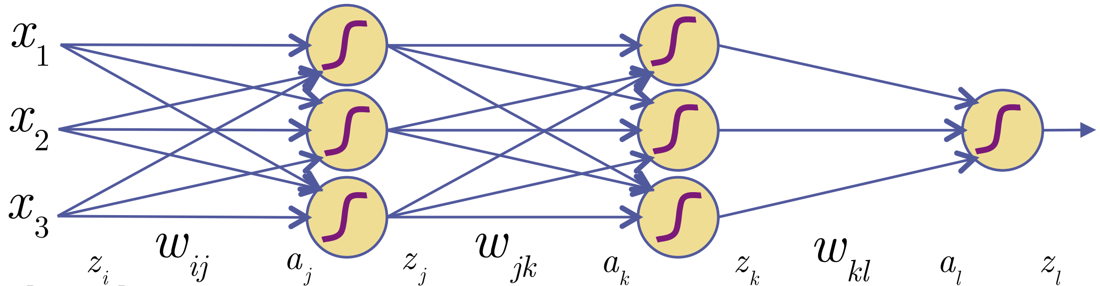
Chain Rule

Define as δ

$$= \frac{1}{N}\sum_n \left[\frac{\partial \frac{1}{2}\left(y^n - g\left(a_l^n\right)\right)^2}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right) = \frac{1}{N}\sum_n \left[-\left(y^n - z_l^n\right) g'\left(a_l^n\right)\right]\left(z_k^n\right) = \frac{1}{N}\sum_n \delta_l^n z_k^n$$

Back-Propagation

- Cost function: $R(\theta) = \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$



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- Next, hidden layer derivative:

$$\frac{\partial R}{\partial w_{jk}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_k^n}\right]\left(\frac{\partial a_k^n}{\partial w_{jk}}\right)$$

Back-Propagation

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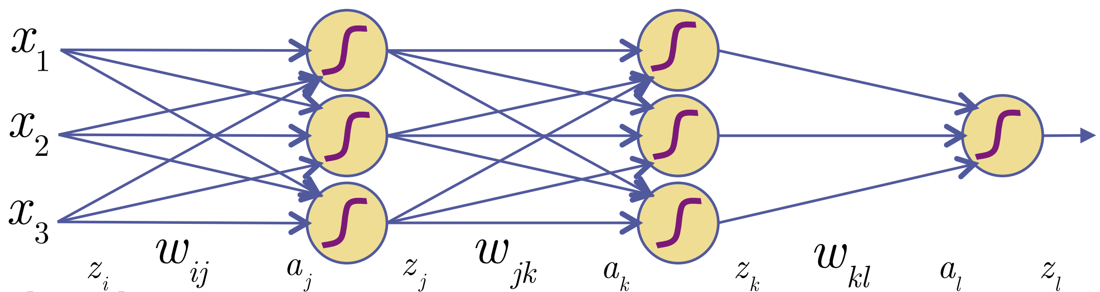

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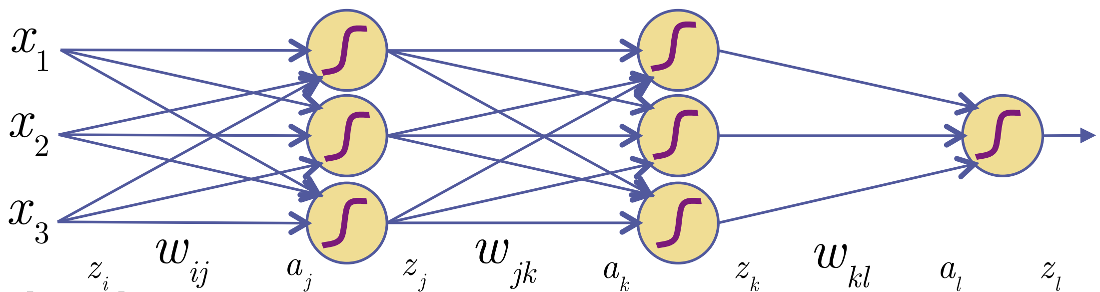
Multivariate Chain Rule

Back-Propagation

- Cost function: $R(\theta) = \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$



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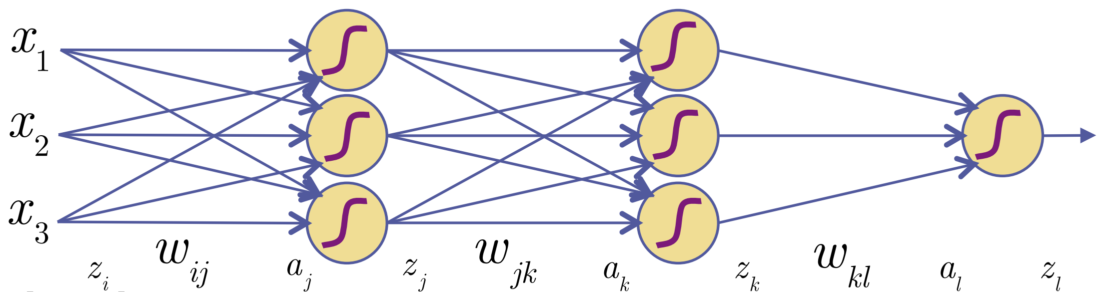
Multivariate Chain Rule

$$= \frac{1}{N}\sum_n \left[\sum_l \delta_l^n \frac{\partial a_l^n}{\partial a_k^n}\right]\left(z_j^n\right)$$

Back-Propagation

- Cost function: $R(\theta) = \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$



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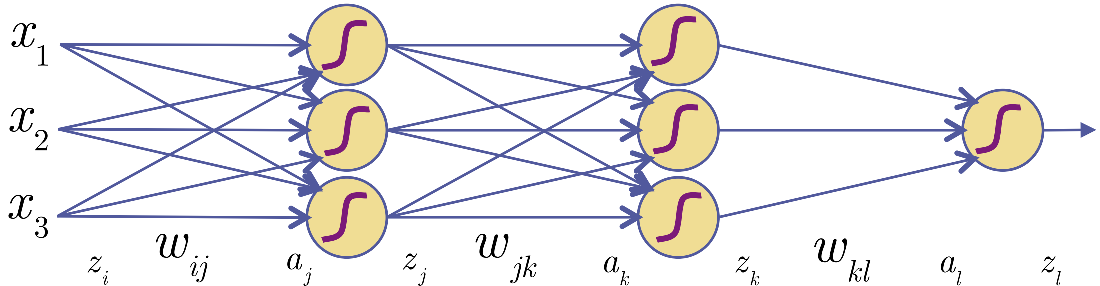
Multivariate Chain Rule

$$= \frac{1}{N}\sum_n \left[\sum_l \delta_l^n \frac{\partial a_l^n}{\partial a_k^n}\right]\left(z_j^n\right)$$

Recall $a_l = \sum_k w_{kl} g\left(a_k\right)$

Back-Propagation

- Cost function: $R(\theta) = \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$



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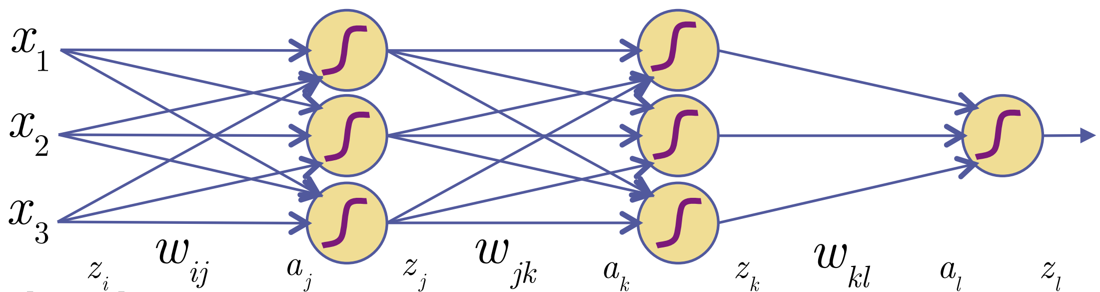
Multivariate Chain Rule

$$= \frac{1}{N}\sum_n \left[\sum_l \delta_l^n \frac{\partial a_l^n}{\partial a_k^n}\right]\left(z_j^n\right) = \frac{1}{N}\sum_n \left[\sum_l \delta_l^n w_{kl} g'\left(a_k^n\right)\right]\left(z_j^n\right)$$

Recall $a_l = \sum_k w_{kl} g\left(a_k\right)$

Back-Propagation

- Cost function: $R(\theta) = \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$



$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right) = \frac{1}{N}\sum_n \left[-\left(y^n - z_l^n\right) g'\left(a_l^n\right)\right]\left(z_k^n\right) = \frac{1}{N}\sum_n \delta_l^n z_k^n$$

- Next, hidden layer derivative:

$$\frac{\partial R}{\partial w_{jk}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_k^n}\right]\left(\frac{\partial a_k^n}{\partial w_{jk}}\right) = \frac{1}{N}\sum_n \left[\sum_l \frac{\partial L^n}{\partial a_l^n}\frac{\partial a_l^n}{\partial a_k^n}\right]\left(\frac{\partial a_k^n}{\partial w_{jk}}\right)$$

Multivariate Chain Rule

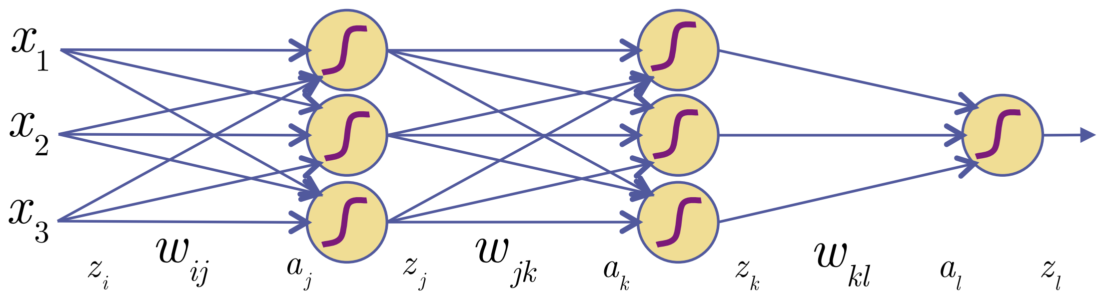
$$= \frac{1}{N}\sum_n \left[\sum_l \delta_l^n \frac{\partial a_l^n}{\partial a_k^n}\right]\left(z_j^n\right) = \frac{1}{N}\sum_n \left[\sum_l \delta_l^n w_{kl} g'\left(a_k^n\right)\right]\left(z_j^n\right) = \frac{1}{N}\sum_n \delta_k^n z_j^n$$

Recall $a_l = \sum_k w_{kl} g\left(a_k\right)$

Define as δ

Back-Propagation

- Cost function: $R(\theta) = \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$



$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right) = \frac{1}{N}\sum_n \left[-\left(y^n - z_l^n\right) g'\left(a_l^n\right)\right]\left(z_k^n\right) = \frac{1}{N}\sum_n \delta_l^n z_k^n$$

$$\frac{\partial R}{\partial w_{jk}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_k^n}\right]\left(\frac{\partial a_k^n}{\partial w_{jk}}\right) = \frac{1}{N}\sum_n \left[\sum_l \delta_l^n w_{kl} g'\left(a_k^n\right)\right]\left(z_j^n\right) = \frac{1}{N}\sum_n \delta_k^n z_j^n$$

- Any previous (input) layer derivative: repeat the formula!

$$\frac{\partial R}{\partial w_{ij}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_j^n}\right]\left(\frac{\partial a_j^n}{\partial w_{ij}}\right) = \frac{1}{N}\sum_n \left[\sum_k \frac{\partial L^n}{\partial a_k^n}\frac{\partial a_k^n}{\partial a_j^n}\right]\left(\frac{\partial a_j^n}{\partial w_{ij}}\right) = \frac{1}{N}\sum_n \left[\sum_k \delta_k^n w_{jk} g'\left(a_j^n\right)\right]\left(z_i^n\right) = \frac{1}{N}\sum_n \delta_j^n z_i^n$$

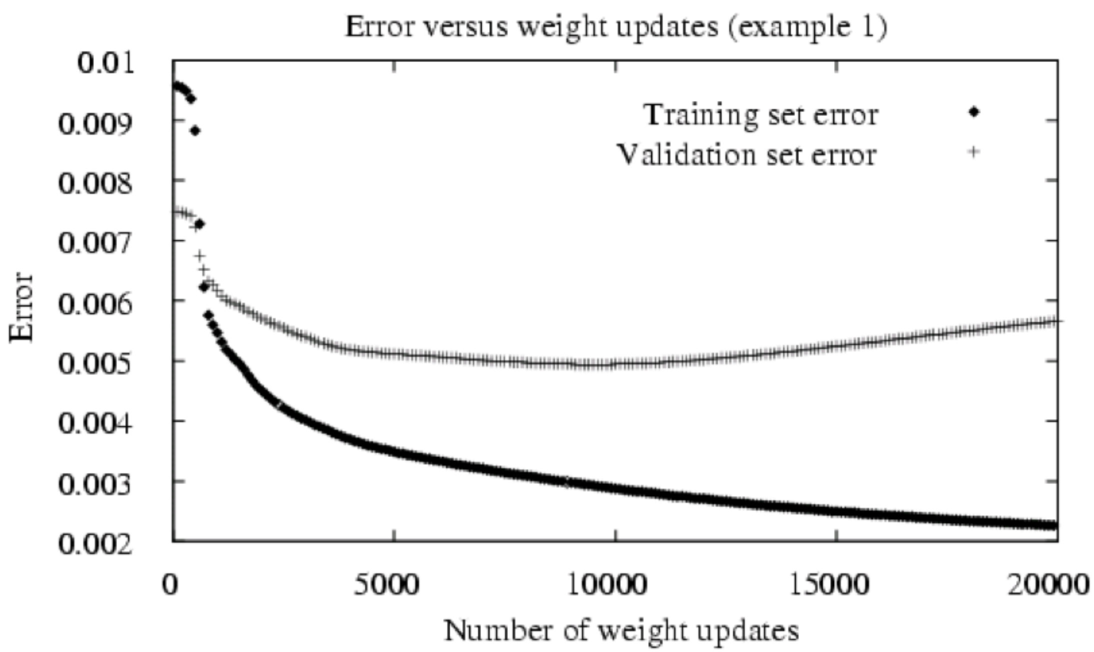
- What is this last z?

Back-Propagation

- Again, take small step in direction opposite to gradient

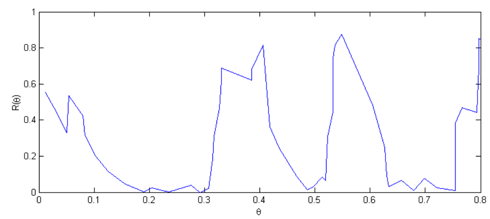
$$w_{ij}^{t+1} = w_{ij}^{t} - \eta \frac{\partial R}{\partial w_{ij}} \qquad w_{jk}^{t+1} = w_{jk}^{t} - \eta \frac{\partial R}{\partial w_{jk}} \qquad w_{kl}^{t+1} = w_{kl}^{t} - \eta \frac{\partial R}{\partial w_{kl}}$$

- Early stop before when error bottoms out on validation set



Neural Networks Demo

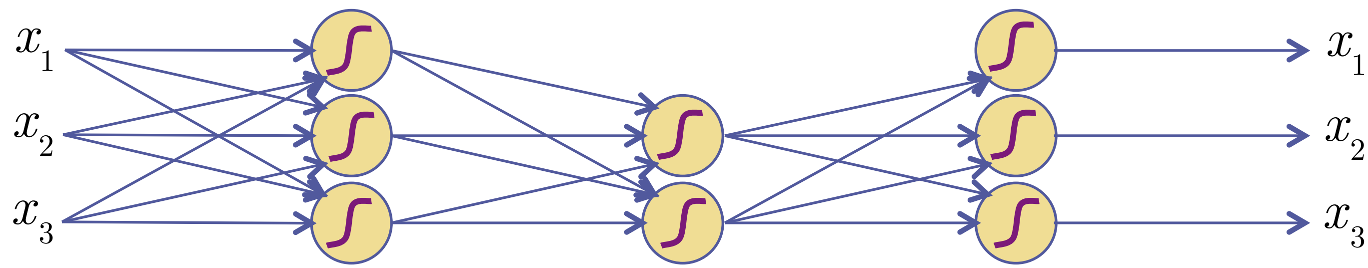
- Again, take small step in direction opposite to gradient
- Digits Demo: LeNet… http://yann.lecun.com
- Problems with back-prop
  is that MLP over-fits…



- Other problems: hard to interpret, black-box
- What are the hidden inner layers doing?

Auto-Encoders

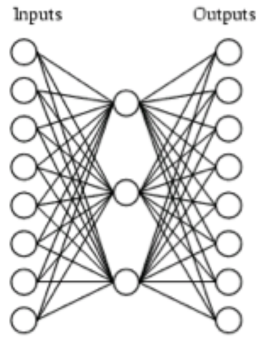
- Make the neural net reconstruct the input vector



- Set the target **y** vector to be the **x** vector again
- But, it gets narrow in the middle!
- So, there is some information "compression"
- This leads to better generalization

- This is unsupervised learning since we only use the **x** data

Auto-Encoders



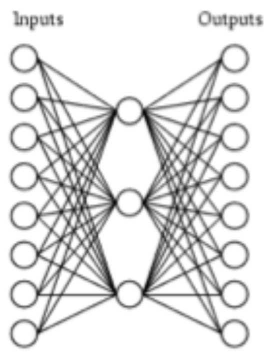
A target function:

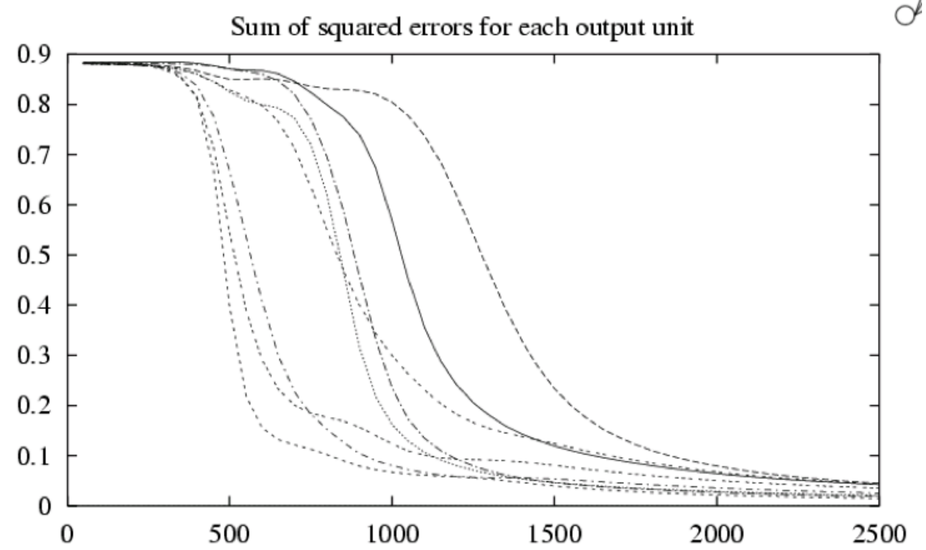
Input		Output
10000000	→	10000000
01000000	→	01000000
00100000	→	00100000
00010000	→	00010000
00001000	→	00001000
00000100	→	00000100
00000010	→	00000010
00000001	→	00000001

Can this be learned??

Auto-Encoders

A network:



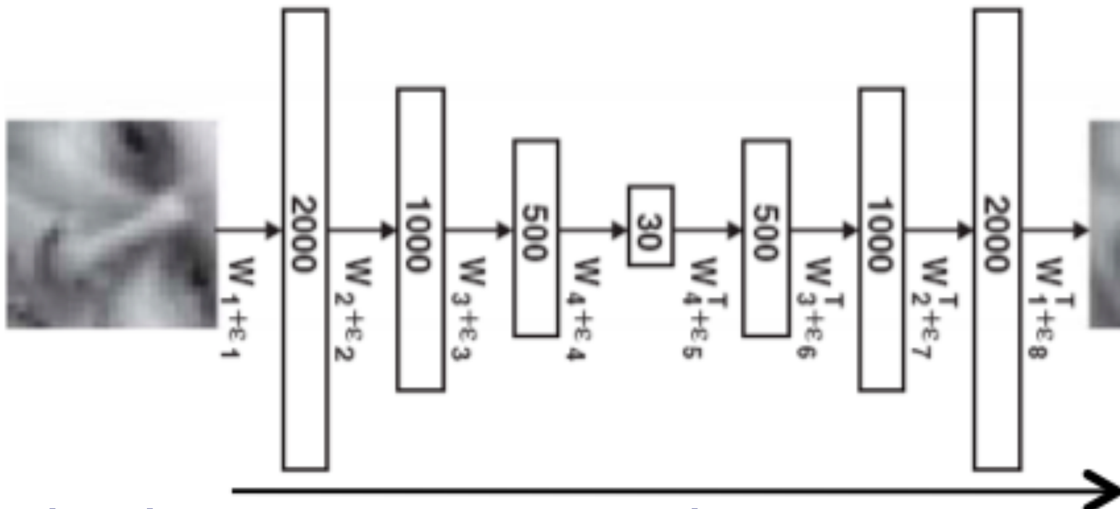


Learned hidden layer representation:

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

Deep Learning

- We can stack several independently trained auto-encoders

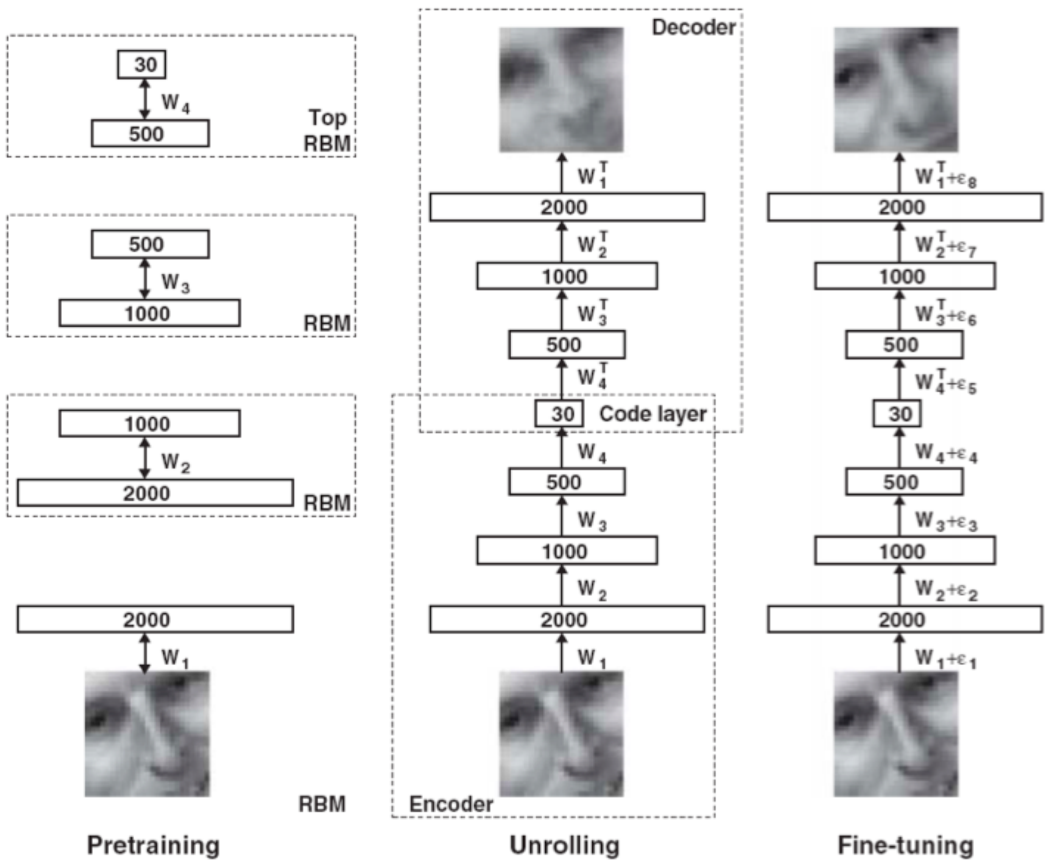


- Using back-propagation, we do *pre-training*
- Train Net 1 to go from 2000 inputs to 1000 to 2000 inputs
- Train Net 2 to go from 1000 hidden values to 500 to 1000
- Train Net 3 to go from 500 hidden to 30 to 500

- Then, do *unrolling* - link up the learned networks as above

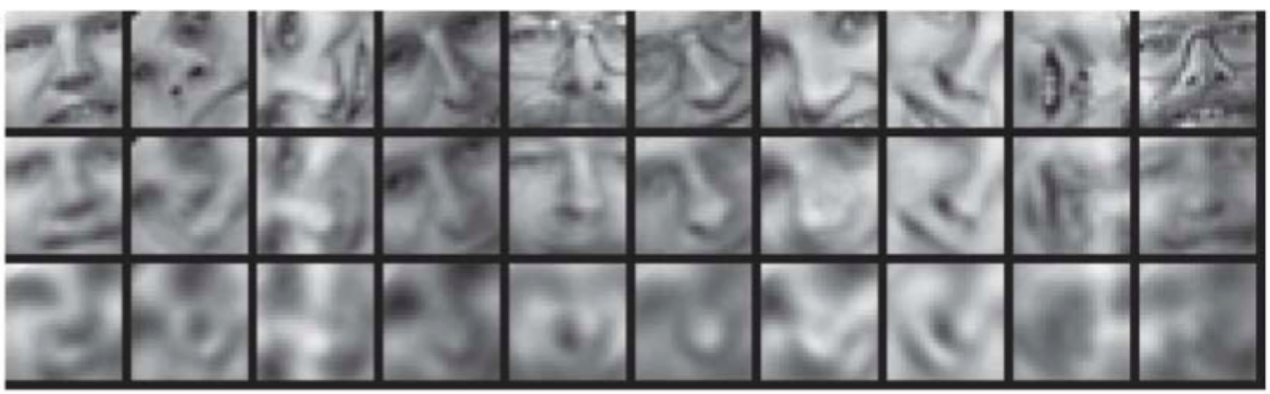
Deep Learning

•Then do *fine-tuning* of the overall neural network by running back-propagation on the whole thing to reconstruct **x** from **x**



Deep Learning

- Does good reconstruction!
- Beats PCA on images of unaligned faces.
- PCA is better when face images are aligned…
- We will cover PCA in a few lectures…

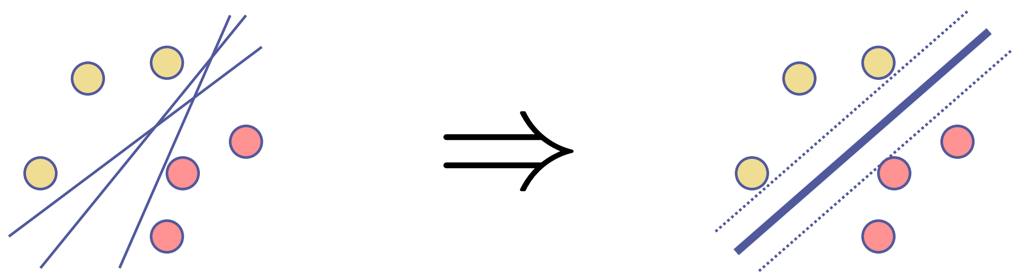


Minimum Training Error?

- Is minimizing Empricial Risk the right thing?
- Are Perceptrons and Neural Networks
  giving the best classifier?

- We are getting: minimum training error
  not minimum testing error

- Perceptrons are giving a bunch of solutions:



... a solution with *guarantees* → SVMs