Machine Learning

4771

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Topic 4

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

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

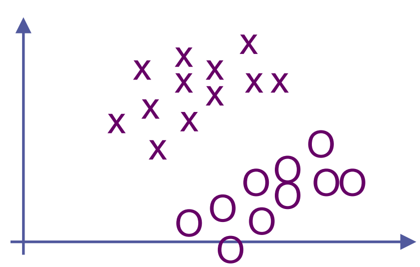
Classification vs. Regression

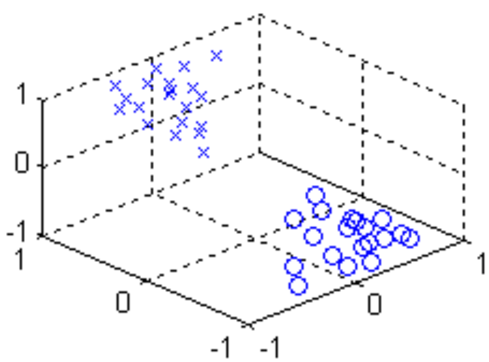
- Classification is another important learning problem

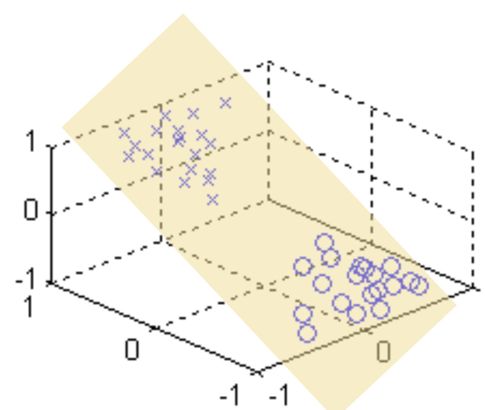
Regression $\mathcal{X} = \left\{ \left(x_1, y_1\right), \left(x_2, y_2\right), \ldots, \left(x_N, y_N\right) \right\} \quad x \in \mathbb{R}^D \quad y \in \mathbb{R}^1$

Classification $\mathcal{X} = \left\{ \left(x_1, y_1\right), \left(x_2, y_2\right), \ldots, \left(x_N, y_N\right) \right\} \quad x \in \mathbb{R}^D \quad y \in \left\{0, 1\right\}$

- E.g. Given x = [tumor size, tumor density]
  Predict y in {benign,malignant}
- Could convert this into a least squares regression problem
- Why is regression & squared error bad for classification?





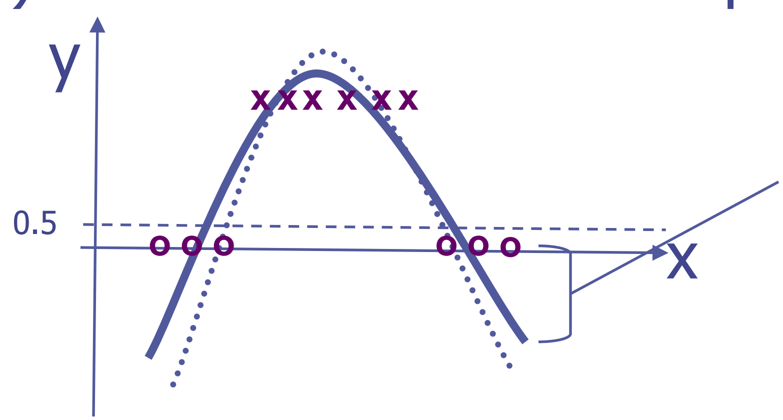


Classification vs. Regression

a) Classification needs binary answers like {0,1}
b) Least squares is an unfair measure of risk here
   e.g. Why penalize a correct but large positive y answer?
   e.g. Why penalize a correct but large negative y answer?

•It's not enough to convert regression output into a decision
$f(x)>0.5 \rightarrow$ Class 1 $\qquad$ $f(x)<0.5 \rightarrow$ Class 0

•If $f(x)=-3.8$ the class=0 but squared error penalizes it…

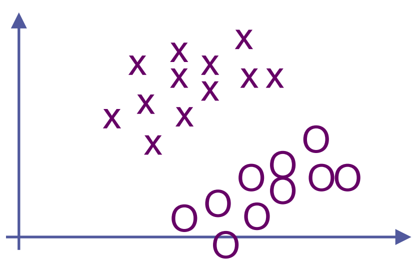


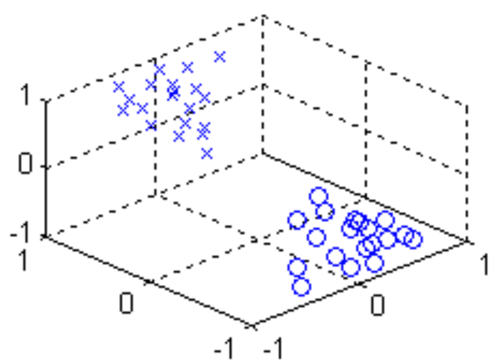
We pay a hefty squared error loss here even if we got the correct classification result. The thick solid line model makes two mistakes while the dashed model is perfect

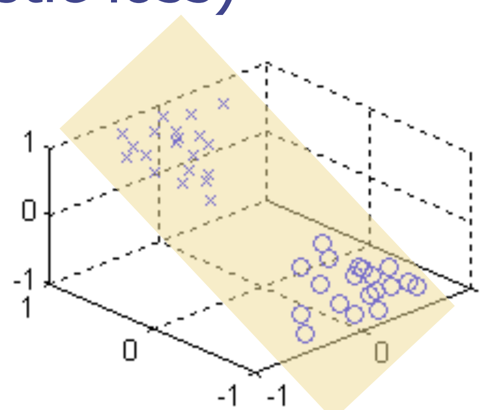
Classification vs. Regression

Let's consider the following four steps to improve from naïve regression to get better classification learning:

1) Fix functions f(x) to give binary output (logistic neuron)
2) Fix our definition of the Risk we will minimize so that we get good classification accuracy (logistic loss)







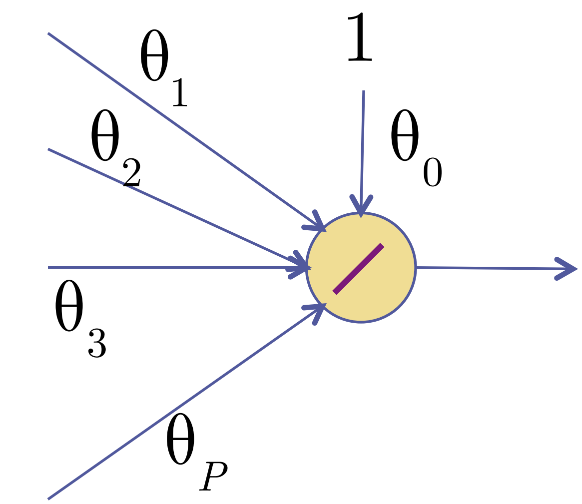
3) Make an even better fix on f(x) to binarize (perceptron)
4) Make an even better risk (perceptron loss)

Logistic Neuron (McCullough-Pitts)

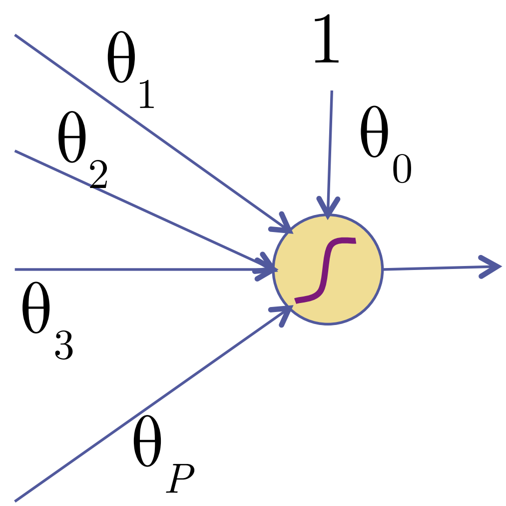
- To output binary, use squashing function g().

$$f\left(\mathbf{x};\theta\right) = \theta^T\mathbf{x}$$

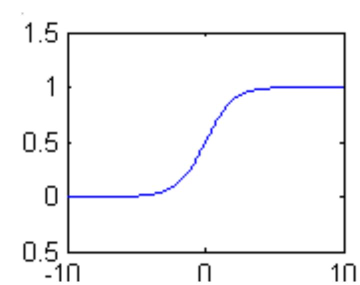
$$f\left(\mathbf{x};\theta\right) = g\left(\theta^T\mathbf{x}\right)$$
$$g\left(z\right) = \left(1+\exp\left(-z\right)\right)^{-1}$$



Linear neuron



Logistic Neuron



- This squashing is called sigmoid or logistic function

Logistic Neuron

- With logistic squashing function, minimizing R(θ) is harder

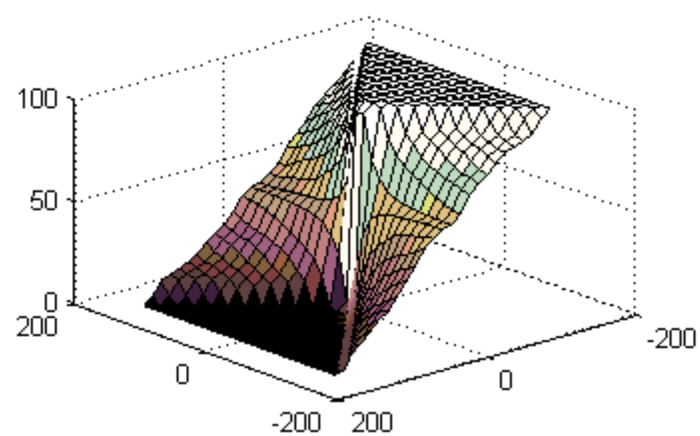
$$R(\theta) = \frac{1}{2N}\sum_{i=1}^{N}\left(y_i - g\left(\theta^T x_i\right)\right)^2$$

$$\nabla_\theta R = \frac{1}{2N}\sum_{i=1}^{N} 2\left(y_i - g\left(\theta^T x_i\right)\right)\left(-1\right) g'\left(\theta^T x_i\right) x_i = 0$$

where…

$$g\left(z\right) = \left(1 + \exp\left(-z\right)\right)^{-1} \qquad g'\left(z\right) = g\left(z\right)\left(1 - g\left(z\right)\right)$$

- Can't minimize risk directly
- Can't solve for best theta directly!



Gradient Descent

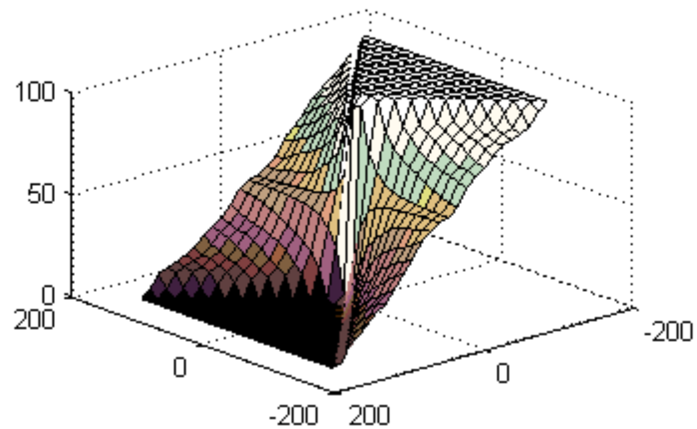
- Useful when we can't the minimum solution in closed form
- Gradient points in direction of fastest increase
- Take step in the opposite direction!

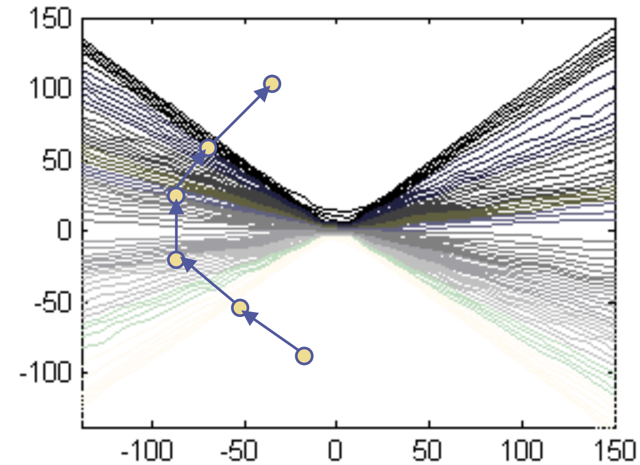
- Gradient Descent Algorithm

1) Chose scalar step size η and theshold ε
2) Set counter t = 0
3) Initialize θ^t = small random vector
4) Update $\theta^{t+1} = \theta^t - \eta \nabla_\theta R \Big|_{\theta^t}$
5) Increment t=t+1
6) If $R\left(\theta^t\right) \leq R\left(\theta^{t-1}\right) - \varepsilon$ *go to 4*

- For appropriate η guaranteed to converge to local minimum

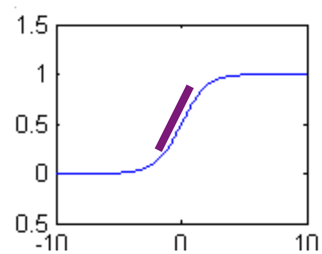
Logistic Neuron Gradient Descent

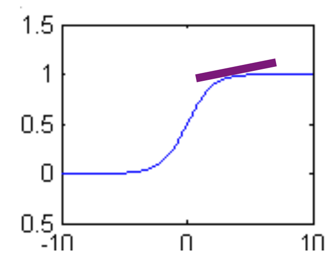




- Need to pick the step size scalar well (each step reduces R)
- Too small → slow, too large → unstable
- Need to avoid flat regions in the space (slow)

- Make sure we are in linear regime of squashing function as in the left panel here





Logistic Regression

- We have done fix 1) Squashing Function with a g() that makes the output {0,1} but we're still using squared loss which is really meant only for regression

$$f\left(\mathbf{x};\theta\right) = \left(1 + \exp\left(-\theta^T \mathbf{x}\right)\right)^{-1}$$

$$L\left(y, f\left(\mathbf{x};\theta\right)\right) = \tfrac{1}{2}\left(y - f\left(\mathbf{x};\theta\right)\right)^2$$

- Next, let's do fix 2) and use Logistic Loss

$$f\left(\mathbf{x};\theta\right) = \left(1 + \exp\left(-\theta^T \mathbf{x}\right)\right)^{-1}$$

$$L\left(y, f\left(\mathbf{x};\theta\right)\right) = y_i \log\left(f\left(\mathbf{x};\theta\right)\right) + \left(1 - y_i\right)\log\left(1 - f\left(\mathbf{x};\theta\right)\right)$$

- The resulting method is called Logistic Regression.
- Use gradient descent on the following risk:

$$R\left(\theta\right) = \tfrac{1}{N}\sum_{i=1}^{N} y_i \log\left(f\left(\mathbf{x};\theta\right)\right) + \left(1 - y_i\right)\log\left(1 - f\left(\mathbf{x};\theta\right)\right)$$

Logistic Regression

- Logistic regression gives better classification than least squares regression
- Given input training data with binary labels:

$$\mathcal{X} = \left\{ \left(x_1, y_1\right), \left(x_2, y_2\right), \ldots, \left(x_N, y_N\right) \right\} \quad x \in \mathbb{R}^D \quad y \in \left\{0,1\right\}$$

- Find a theta that minimizes this risk using gradient descent:

$$R\left(\theta\right) = \tfrac{1}{N} \sum_{i=1}^{N} y_i \log\left(f\left(\mathbf{x};\theta\right)\right) + \left(1 - y_i\right) \log\left(1 - f\left(\mathbf{x};\theta\right)\right)$$

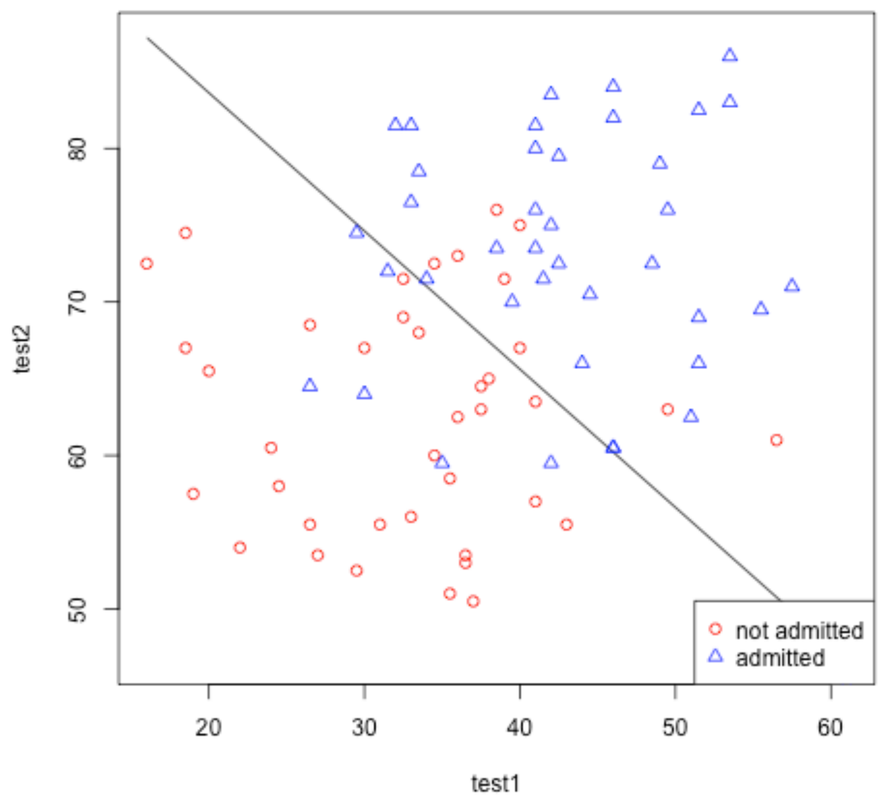
- Make predictions using this function

$$f\left(\mathbf{x};\theta\right) = \left(1 + \exp\left(-\theta^T \mathbf{x}\right)\right)^{-1}$$

- Output 1 if f > 0.5 and output 0 otherwise

Logistic Regression

- Logistic regression gives better classification than least squares regression



- Let next try even more classification improvements…

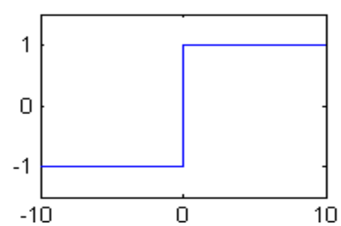
Perceptron (another Neuron)

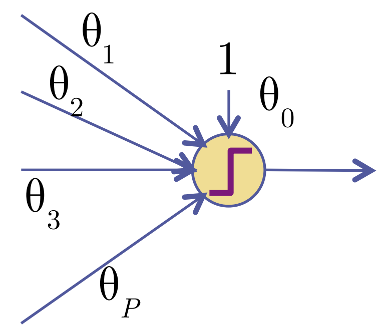
- Classification scenario once again but consider +1, -1 labels

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

- 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

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

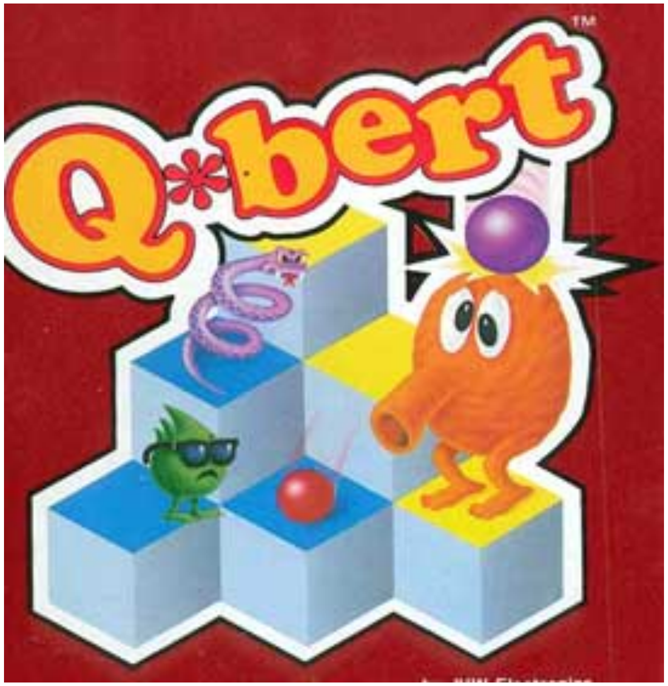
- What does this R(θ) function look like?

Perceptron & Classification Loss

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

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

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



Perceptron & Perceptron Loss

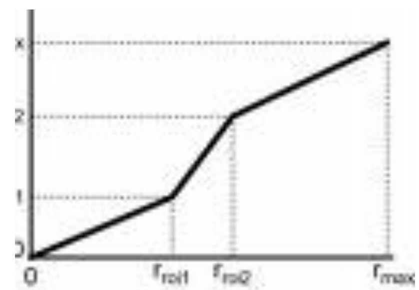
- Instead of Classification Loss

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

- Consider Perceptron Loss:

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

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



- Get reasonable gradients for gradient descent

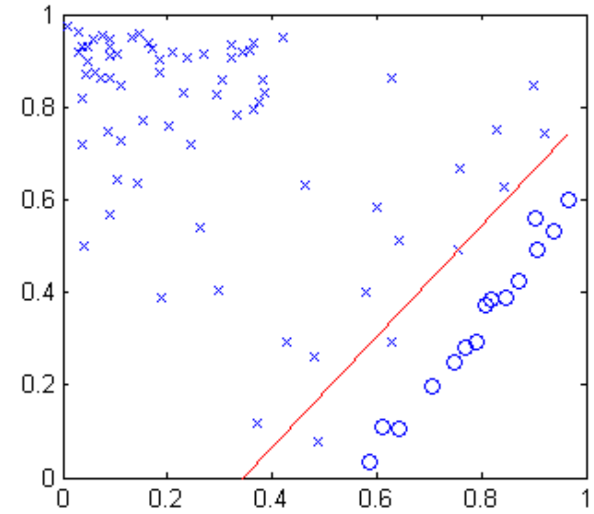
$$\nabla_\theta R^{per}(\theta) = -\frac{1}{N}\sum_{i \in misclassified} y_i \mathbf{x}_i$$

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

Perceptron vs. Linear Regression

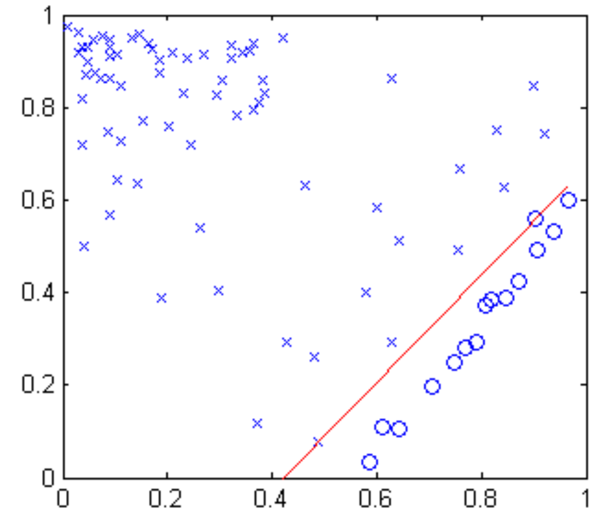
- Linear regression gets close but doesn't do perfectly

  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

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

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

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

- Also, set η to 1 without loss of generality

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

Online Perceptron

- Iterate cycling through examples i=1…N one at a time.
  If i'th example is properly classified: $\theta^{t+1} = \theta^{t}$
  Else: $\theta^{t+1} = \theta^{t} + y_i \mathbf{x}_i$
- Therorem: converge to zero error θ^* in finite total steps t.

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

- 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

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

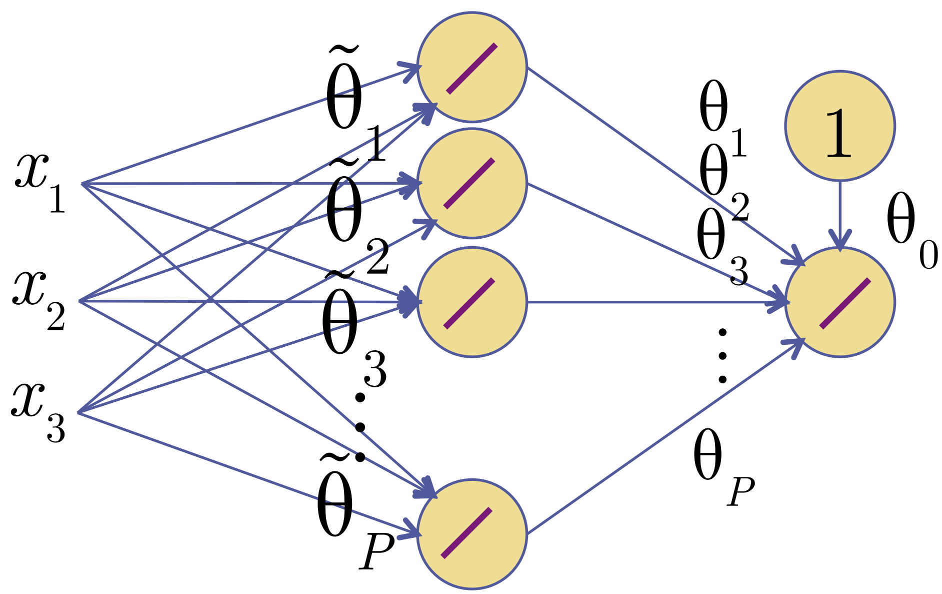
apply part 1 then part 2

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

…so t is finite!

Multi-Layer Neural Networks

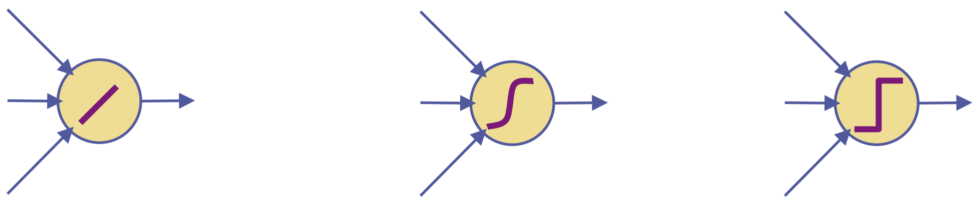
- What if we consider cascading multiple layers of network?
- Each output layer is input to the next layer
- Each layer has its own weights parameters
- Eg: each layer has linear nodes (not perceptron/logistic)



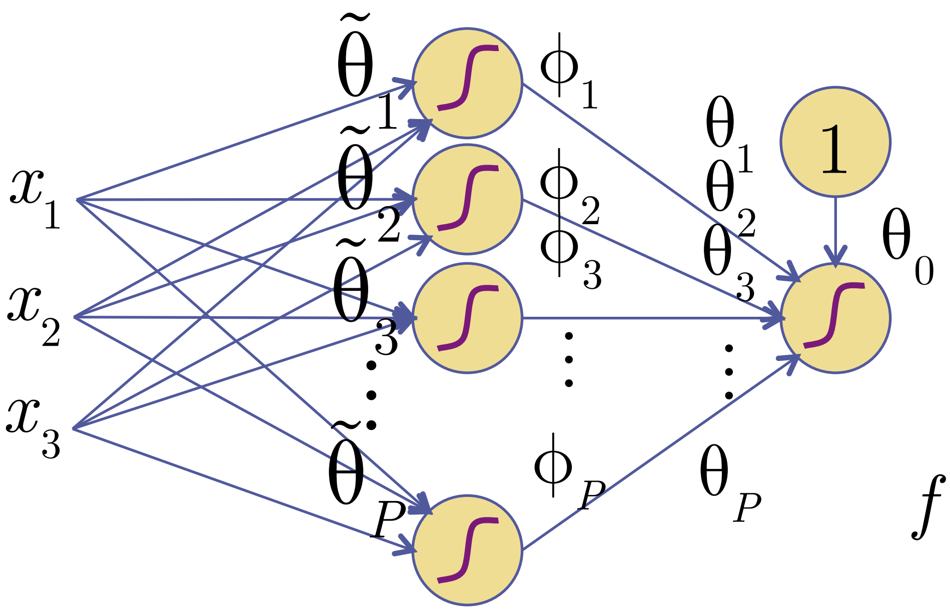
- Above Neural Net has 2 layers. What does this give?

Multi-Layer Neural Networks

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



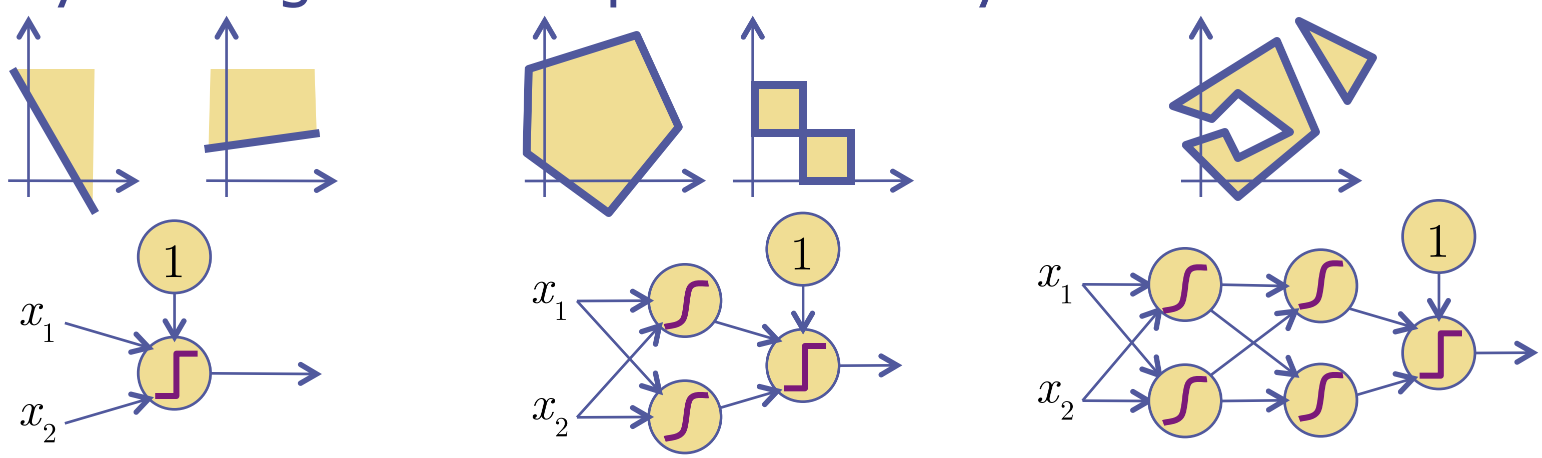
- Neural network can adjust the basis functions themselves…



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

Multi-Layer Neural Networks

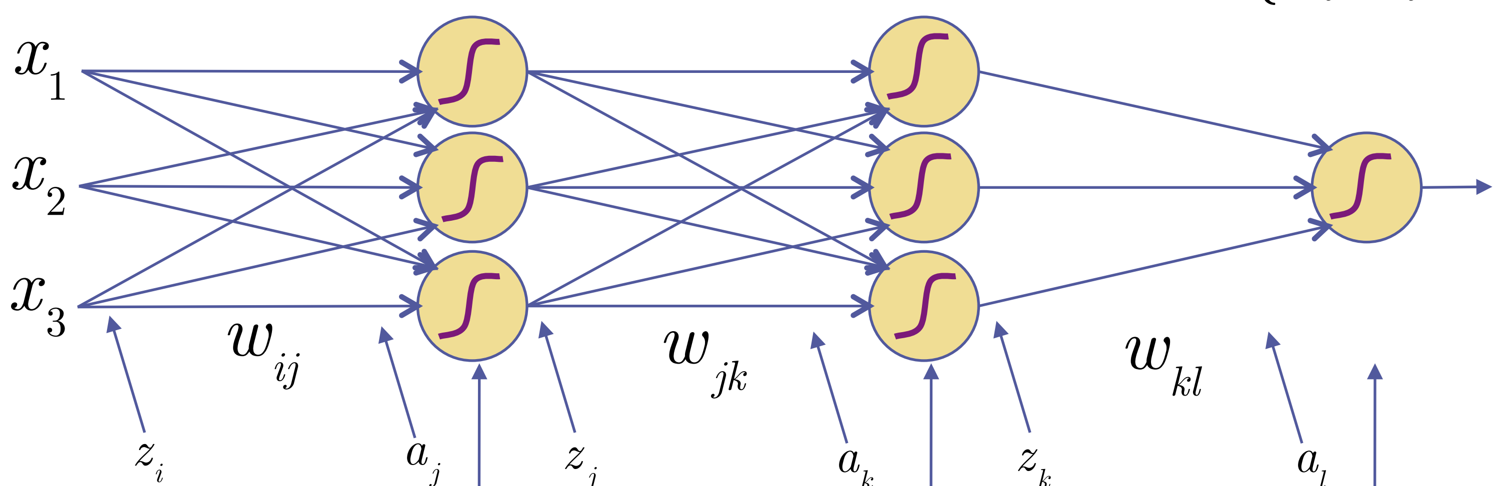
- Multi-Layer Network can handle more complex decisions
- 1-layer: is linear, can't handle XOR
- Each layer adds more flexibility (but more parameters!)
- Each node splits its input space with linear hyperplane
- 2-layer: if last layer is AND operation, get convex hull
- 2-layer: can do almost anything 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: $\theta = \left\{ w_{ij}, w_{jk}, w_{kl} \right\}$



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

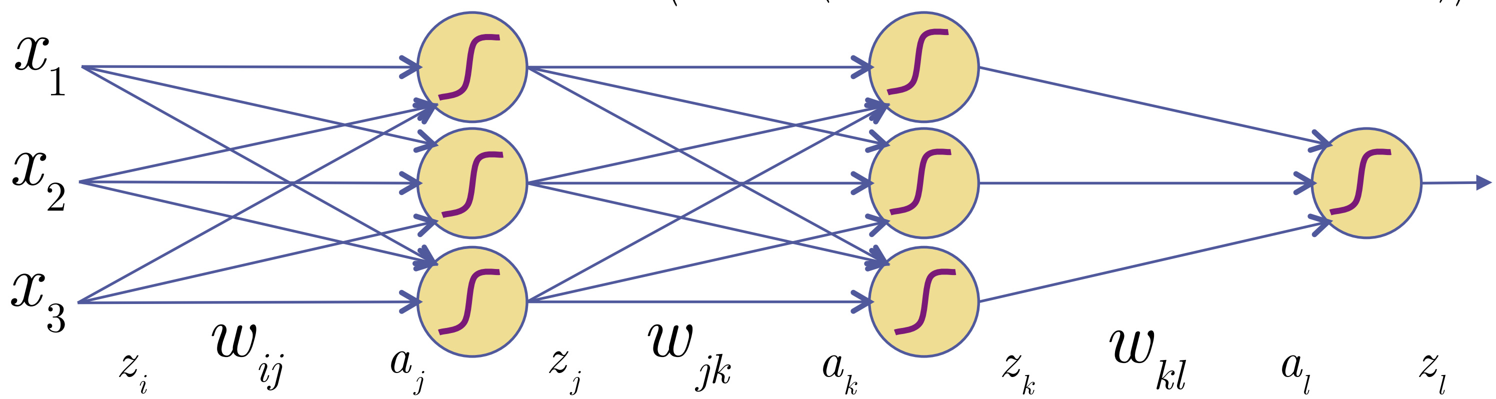
$$z_j = g\left(a_j\right) \qquad z_k = g\left(a_k\right) \qquad z_l = g\left(a_l\right)$$

- 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:

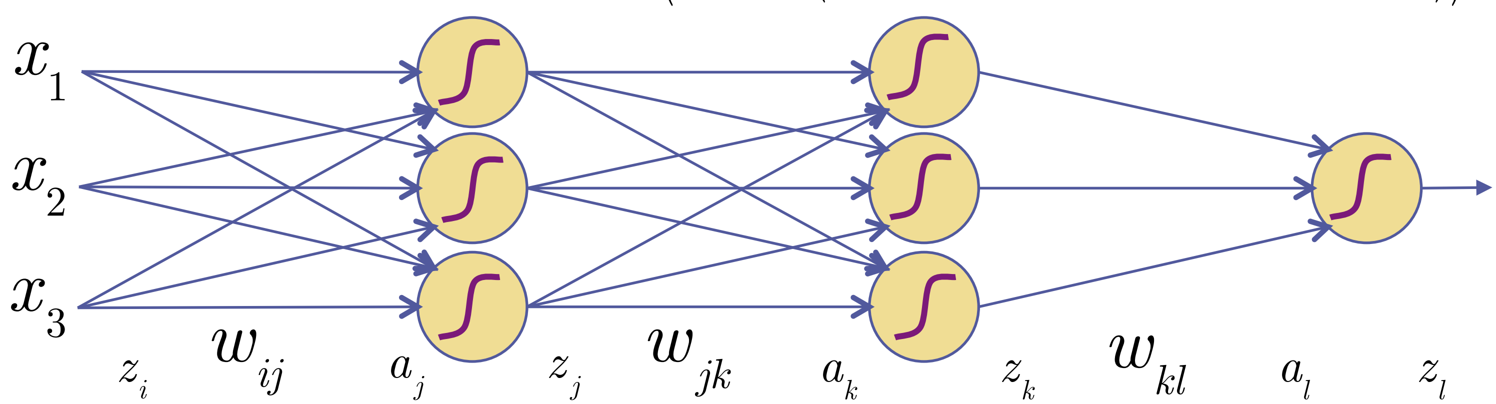
$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right)$$ **Chain Rule**

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

Back-Propagation

- 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:

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

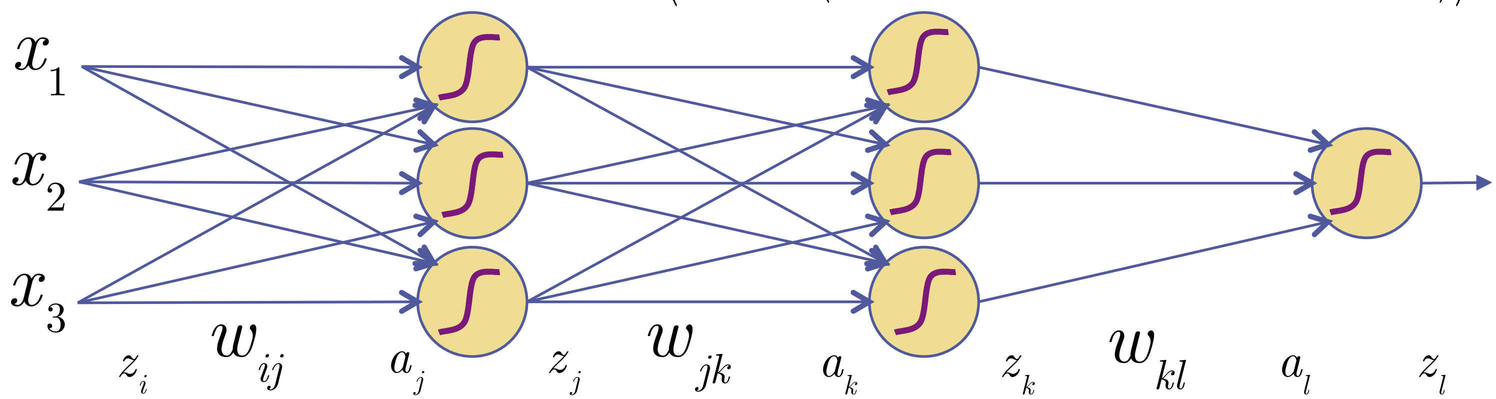
$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right) \quad \boxed{\textbf{Chain Rule}}$$

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

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:

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

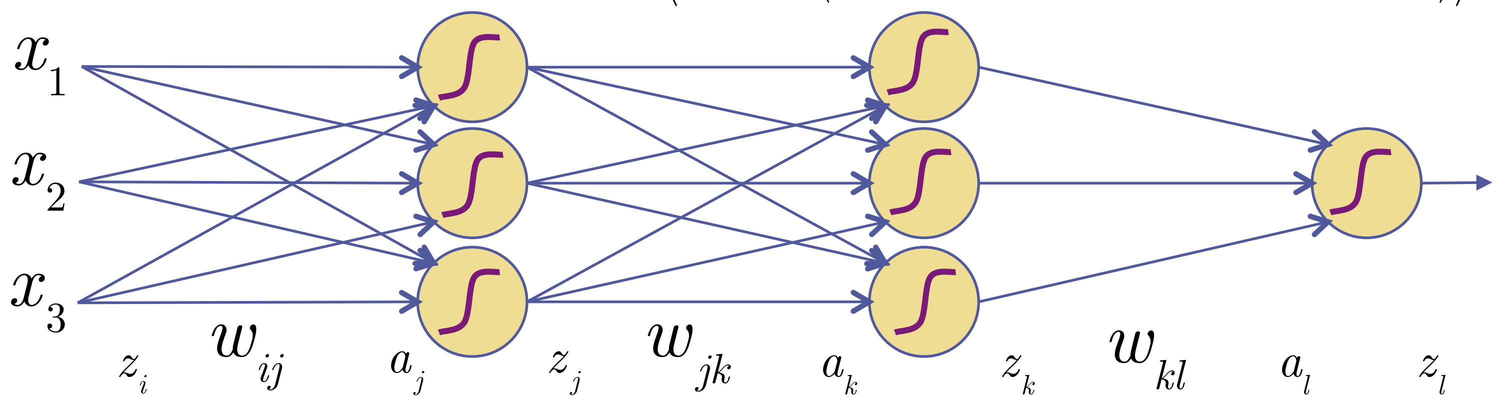
$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N}\sum_n \left[\frac{\partial L^n}{\partial a_l^n}\right]\left(\frac{\partial a_l^n}{\partial w_{kl}}\right) \quad \boxed{\textbf{Chain Rule}}$$

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

Back-Propagation

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

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



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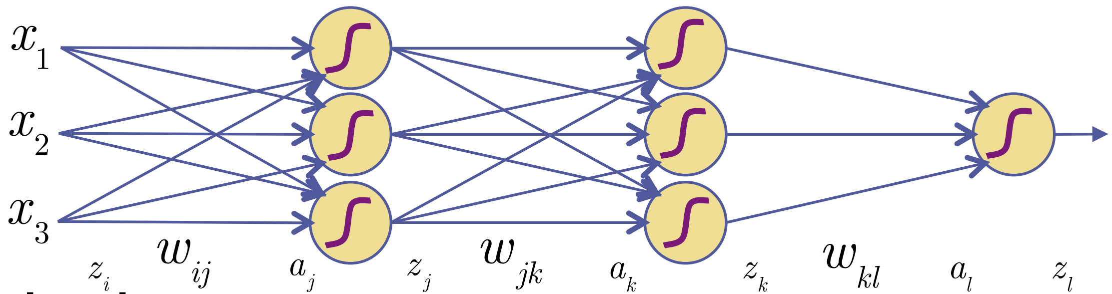
Chain Rule

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

Define as δ

Back-Propagation

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



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

- Next, hidden layer derivative:

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

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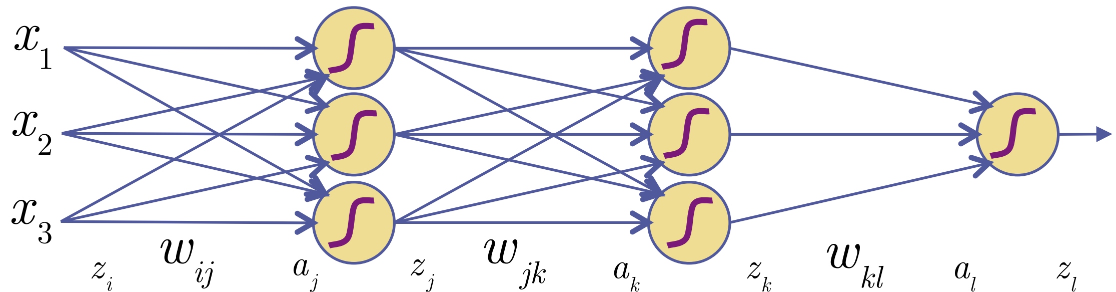

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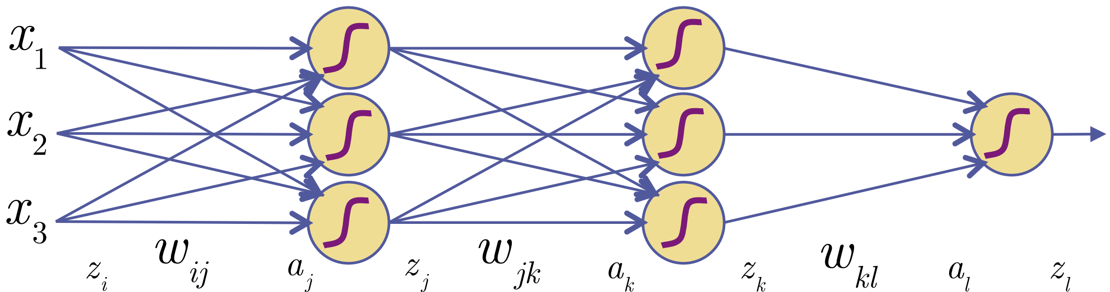
Multivariate Chain Rule

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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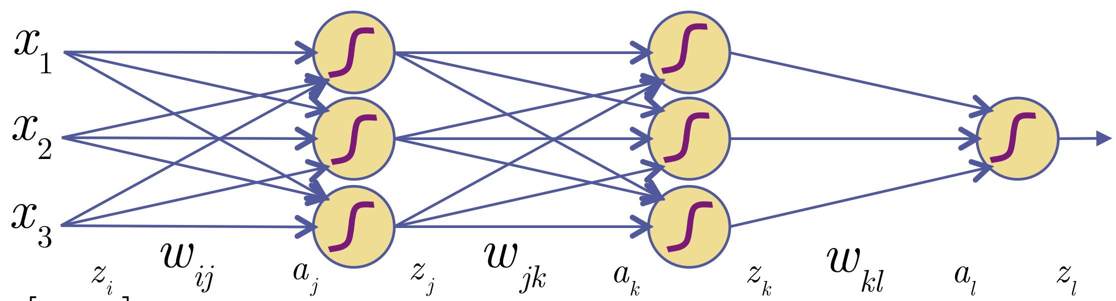
Multivariate Chain Rule

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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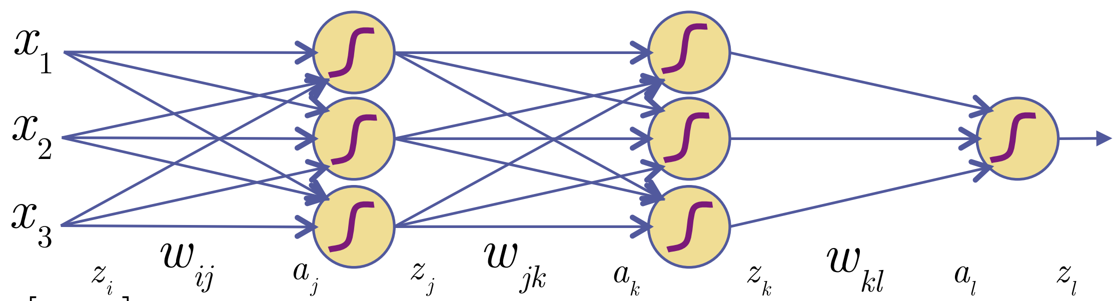
Multivariate Chain Rule

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

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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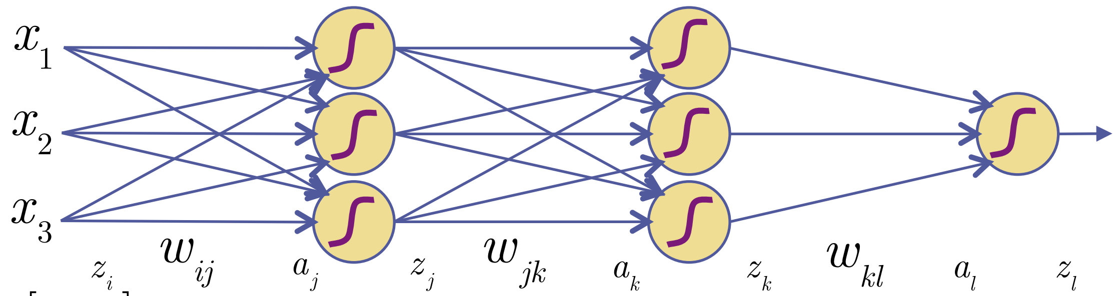

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Multivariate Chain Rule

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

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Define as δ

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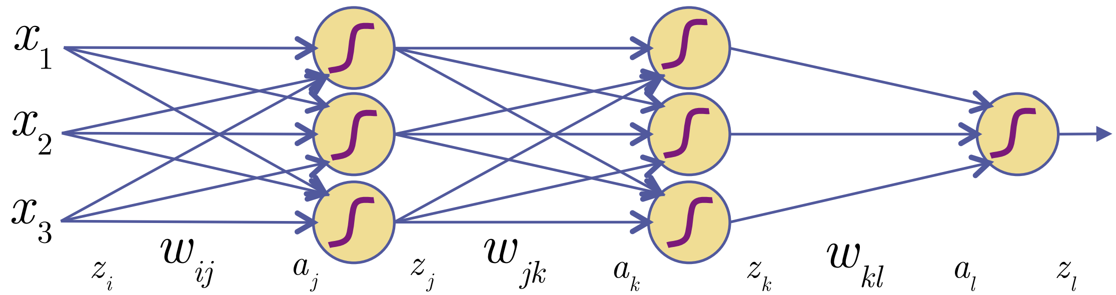
- Cost function: $R(\theta) = \frac{1}{N}\sum_n \frac{1}{2}\left(y^n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_i^n\right)\right)\right)\right)^2$



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

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

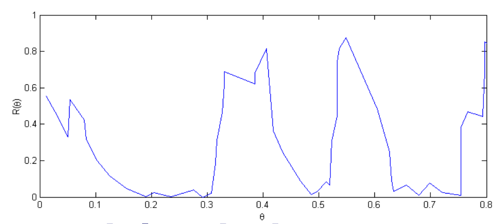
- What is this last z?

Back-Propagation

- Again, take small step in direction opposite to gradient

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

- Digits Demo: LeNet… http://yann.lecun.com
- Problems with back-prop
  is that MLP over-fits…



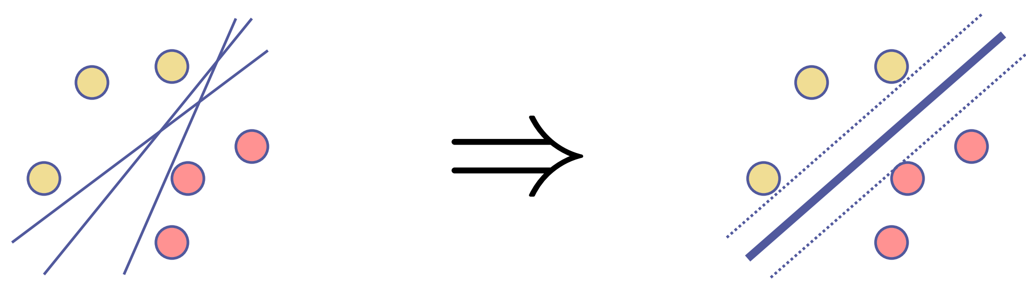
- Other problems: hard to interpret, black-box
- What are the hidden inner layers doing?
- Other main problem: minimum training error
  not minimum testing error…

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 better solution → SVMs