Artificial Intelligence: Representation and Problem Solving

15-381

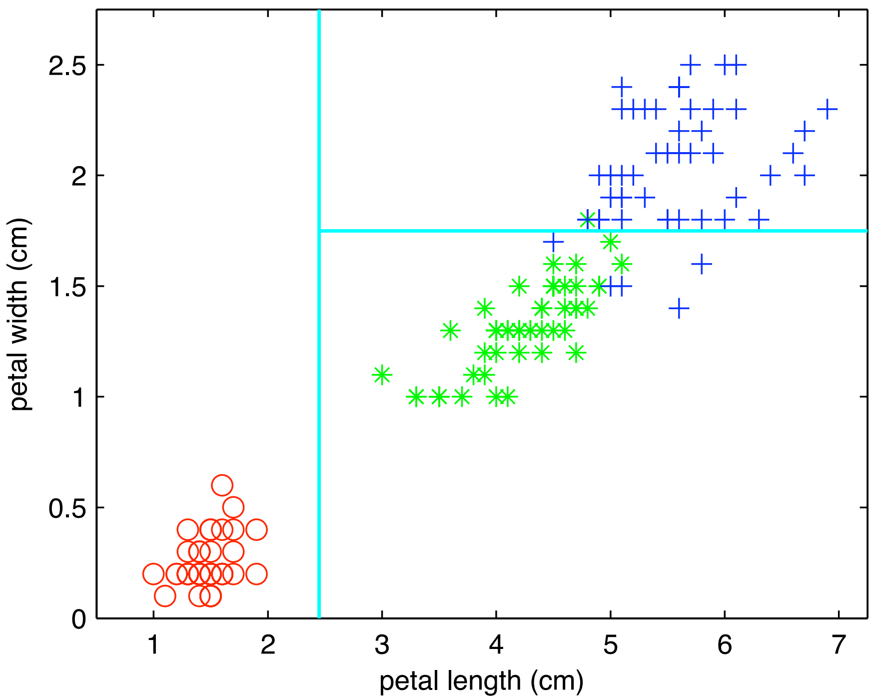
January 16, 2007

Neural Networks

Topics

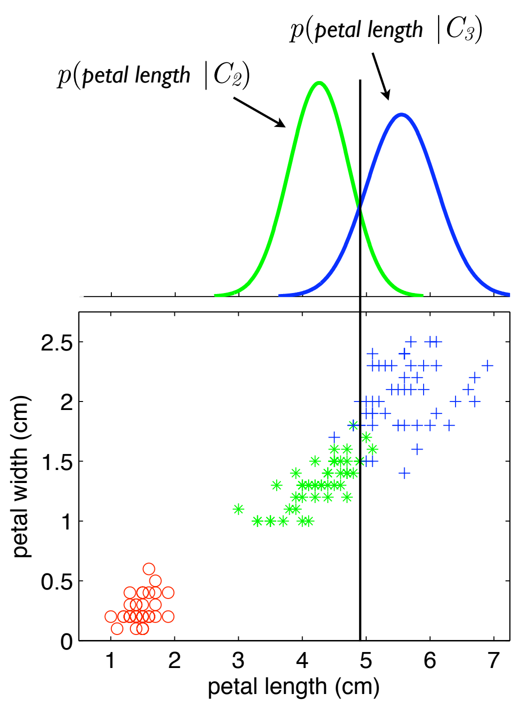
- decision boundaries
- linear discriminants
- perceptron
- gradient learning
- neural networks

The Iris dataset with decision tree boundaries

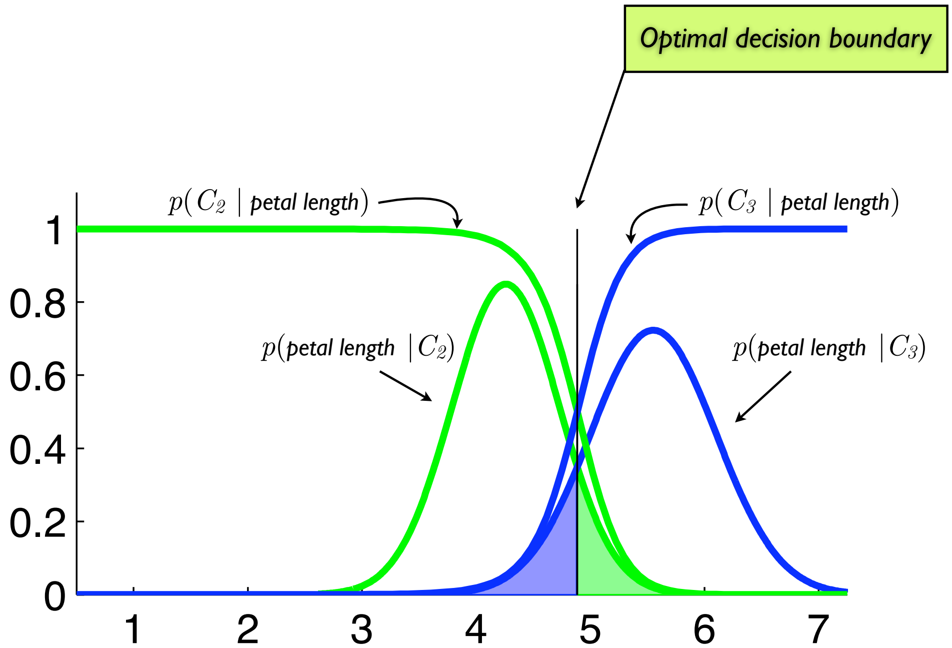


The optimal decision boundary for C_2 vs C_3

- optimal decision boundary is determined from the statistical *distribution* of the classes
- optimal only if model is correct
- assigns precise degree of uncertainty to classification

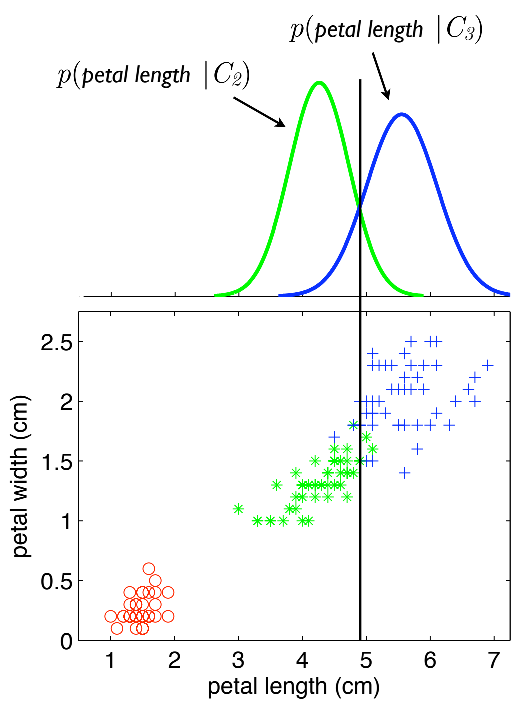


Optimal decision boundary

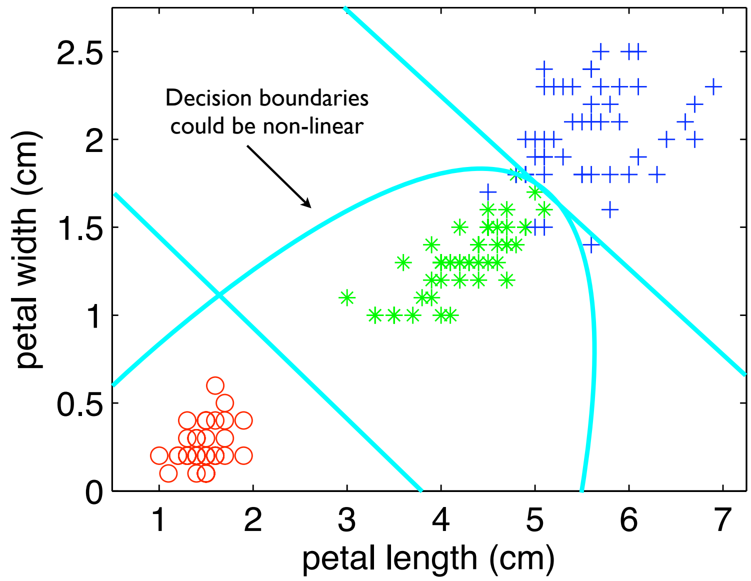


Can we do better?

- only way is to use more information
- DTs use both petal width and petal length



Arbitrary decision boundaries would be more powerful



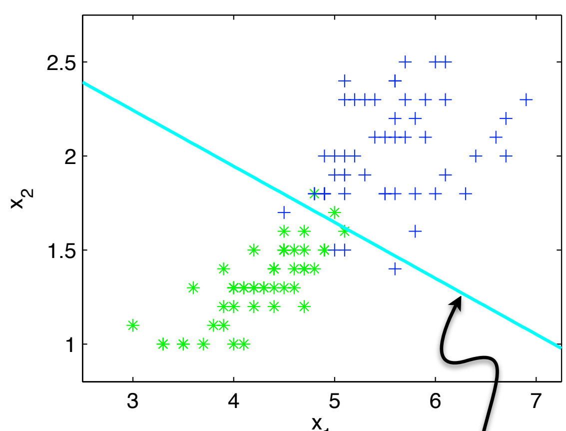
Defining a decision boundary

- consider just two classes
- want points on one side of line in class 1, otherwise class 2.
- 2D *linear discriminant function:*

$$\begin{aligned} y &= \mathbf{m}^T \mathbf{x} + b \\ &= m_1 x_1 + m_2 x_2 + b \\ &= \sum_i m_i x_i + b \end{aligned}$$

- This defines a 2D plane which leads to the decision:

$$\mathbf{x} \in \begin{cases} \text{class 1} & \text{if } y \geq 0, \\ \text{class 2} & \text{if } y < 0. \end{cases}$$



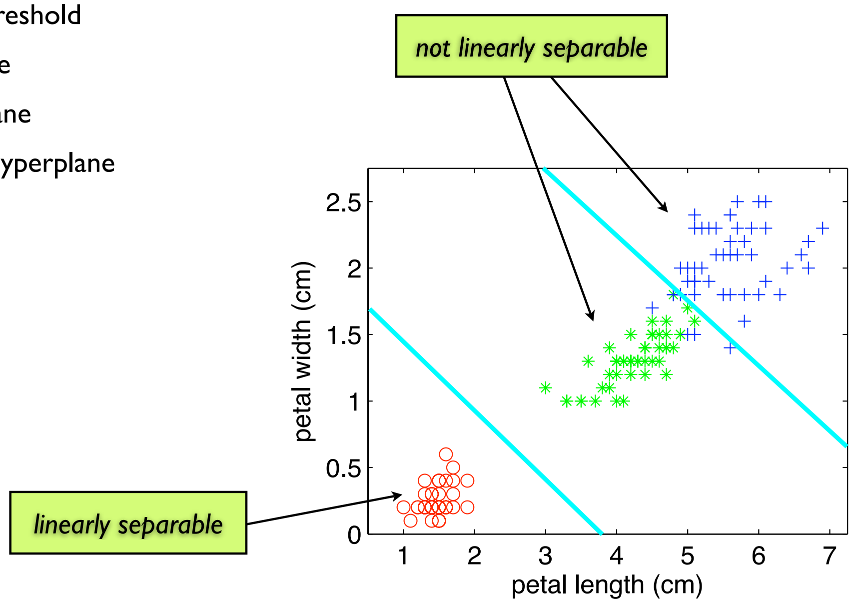
The decision *boundary*:
$y = \mathbf{m}^T \mathbf{x} + b = 0$

Or in terms of scalars:

$$\begin{aligned} m_1 x_1 + m_2 x_2 &= -b \\ \Rightarrow x_2 &= -\frac{m_1 x_1 + b}{m_2} \end{aligned}$$

Linear separability

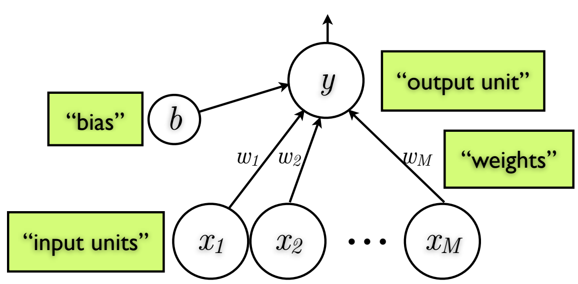
- Two classes are linearly separable if they can be separated by a linear combination of attributes
  - 1D: threshold
  - 2D: line
  - 3D: plane
  - M-D: hyperplane



Diagraming the classifier as a "neural" network

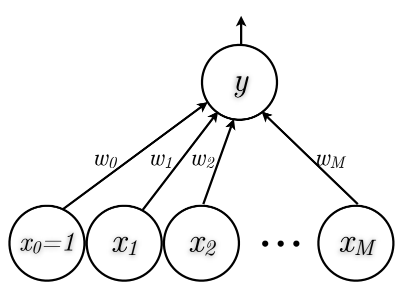
- The feedforward neural network is specified by weights w_i and bias b:

$$
\begin{aligned}
y &= \mathbf{w}^T \mathbf{x} + b \\
&= \sum_{i=1}^{M} w_i x_i + b
\end{aligned}
$$



- It can written equivalently as

$$
y = \mathbf{w}^T \mathbf{x} = \sum_{i=0}^{M} w_i x_i
$$



- where $w_0 = b$ is the bias and a "dummy" input x_0 that is always 1.

Determining, ie learning, the optimal linear discriminant

- First we must define an *objective function*, ie the goal of learning
- Simple idea: adjust weights so that output $y(\mathbf{x}_n)$ matches class c_n
- *Objective*: minimize sum-squared error over all patterns $\mathbf{x}_n$:

$$E = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{w}^T\mathbf{x}_n - c_n)^2$$

- Note the notation $\mathbf{x}_n$ defines a *pattern vector*:

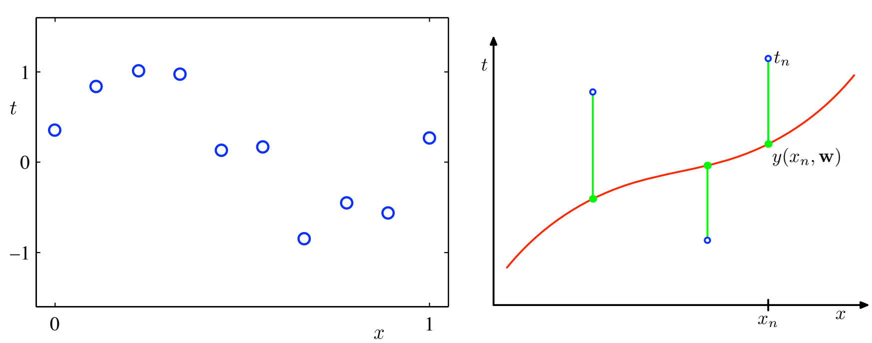
$$\mathbf{x}_n = \{x_1, \ldots, x_M\}_n$$

- We can define the desired class as:

$$c_n = \begin{cases} 0 & \mathbf{x}_n \in \text{class } 1 \\ 1 & \mathbf{x}_n \in \text{class } 2 \end{cases}$$

We've seen this before: curve fitting

$$t = \sin(2\pi x) + \text{noise}$$



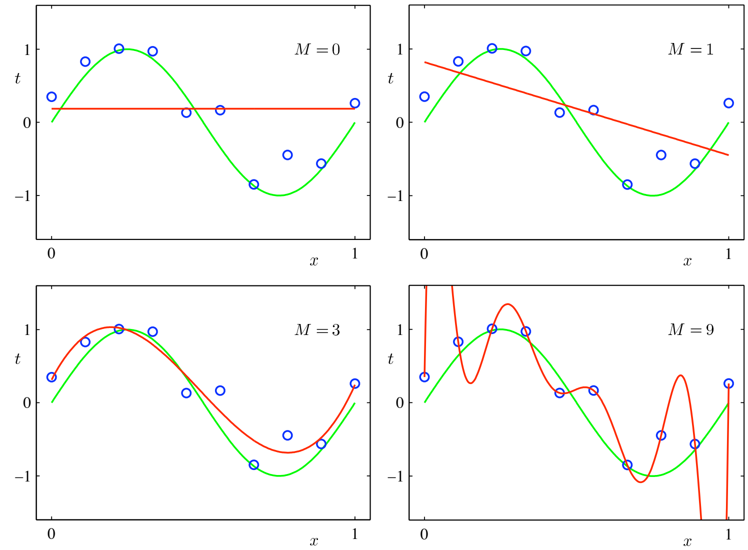
example from Bishop (2006), *Pattern Recognition and Machine Learning*

Neural networks compared to polynomial curve fitting

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} [y(x_n, \mathbf{w}) - t_n]^2$$

For the linear network, M=1 and there are multiple input dimensions



example from Bishop (2006), *Pattern Recognition and Machine Learning*

General form of a linear network

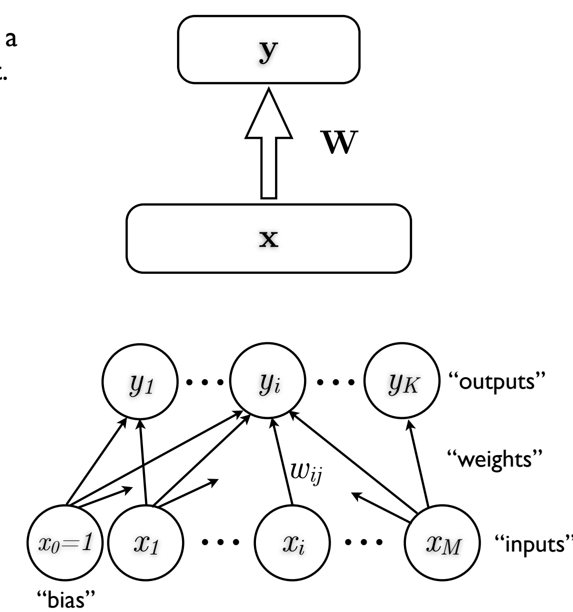
- A linear neural network is simply a linear transformation of the input.

$$y_j = \sum_{i=0}^{M} w_{i,j} x_i$$

- Or, in matrix-vector form:

$$\mathbf{y} = \mathbf{W}\mathbf{x}$$

- Multiple outputs corresponds to *multivariate regression*



Training the network: Optimization by gradient descent

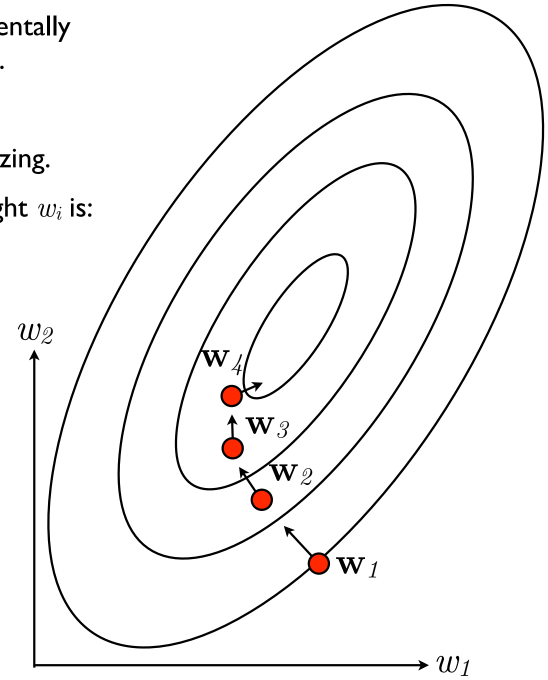
- We can adjust the weights incrementally to minimize the objective function.
- This is called *gradient descent*
- Or gradient *ascent* if we're maximizing.
- The gradient descent rule for weight w_i is:

$$w_i^{t+1} = w_i^t - \epsilon \frac{\partial E}{w_i}$$

- Or in vector form:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \epsilon \frac{\partial E}{\mathbf{w}}$$

- For gradient *ascent*, the *sign* of the gradient step changes.



Computing the gradient

- Idea: minimize error by gradient descent
- Take the derivative of the objective function wrt the weights:

$$\begin{aligned} E &= \frac{1}{2}\sum_{n=1}^{N}(\mathbf{w}^T\mathbf{x}_n - c_n)^2 \\ \frac{\partial E}{w_i} &= \frac{2}{2}\sum_{n=1}^{N}(w_0 x_{0,n} + \cdots + w_i x_{i,n} + \cdots + w_M x_{M,n} - c_n) x_{i,n} \\ &= \sum_{n=1}^{N}(\mathbf{w}^T\mathbf{x}_n - c_n) x_{i,n} \end{aligned}$$

- And in vector form:

$$\frac{\partial E}{\mathbf{w}} = \sum_{n=1}^{N}(\mathbf{w}^T\mathbf{x}_n - c_n)\mathbf{x}_n$$

Simulation: learning the decision boundary

- Each iteration updates the gradient:

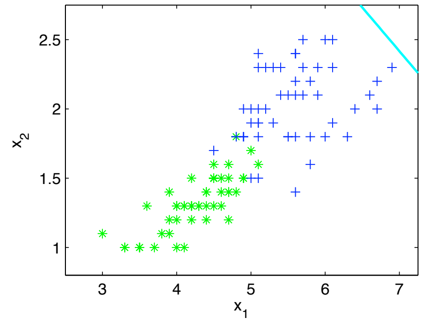
$$w_i^{t+1} = w_i^t - \epsilon \frac{\partial E}{w_i}$$

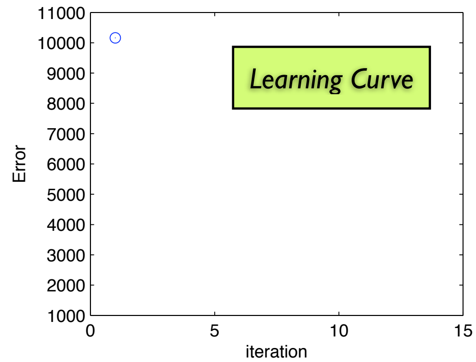
$$\frac{\partial E}{w_i} = \sum_{n=1}^{N} (\mathbf{w}^T \mathbf{x}_n - c_n) x_{i,n}$$

- Epsilon is a small value:

  ϵ = 0.1/N

- Epsilon too large:
  - learning diverges
- Epsilon too small:
  - convergence slow





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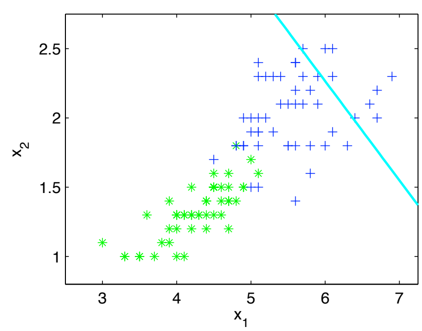

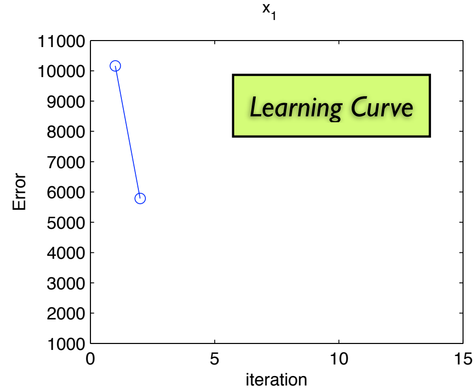

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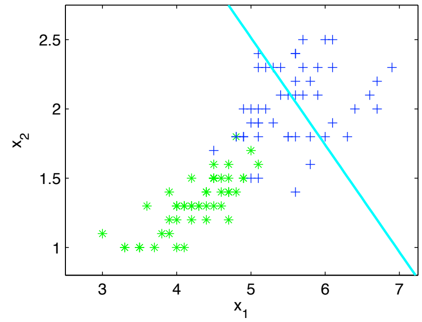

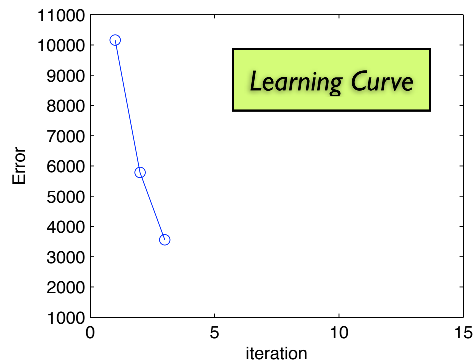

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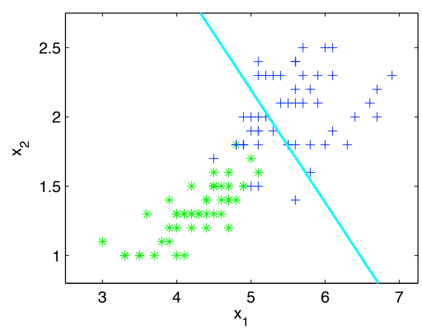

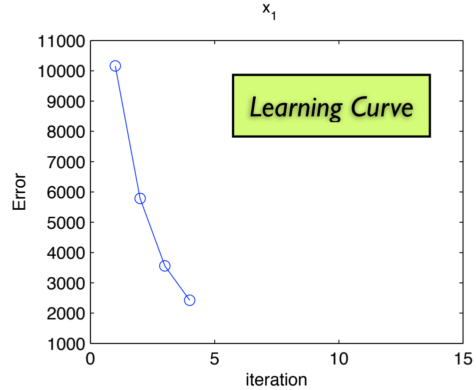

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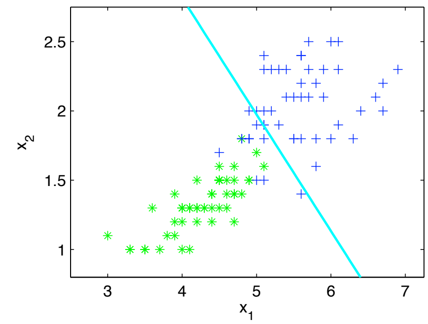

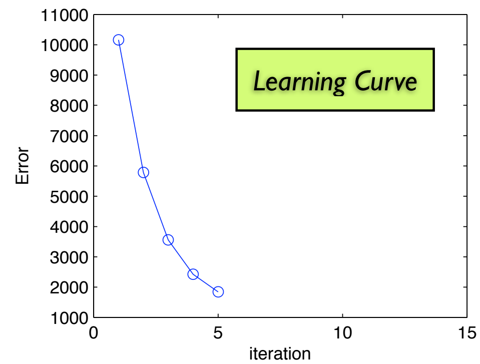

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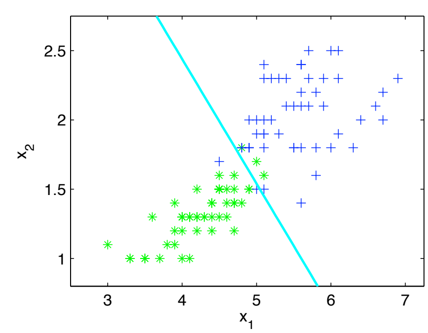

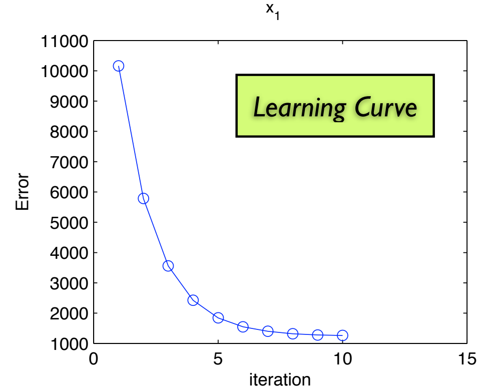

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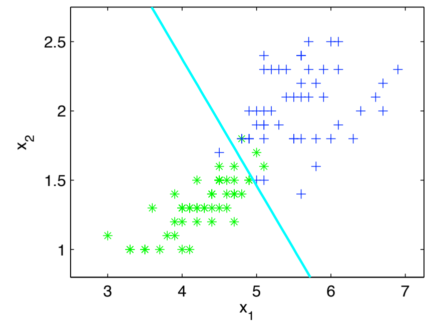
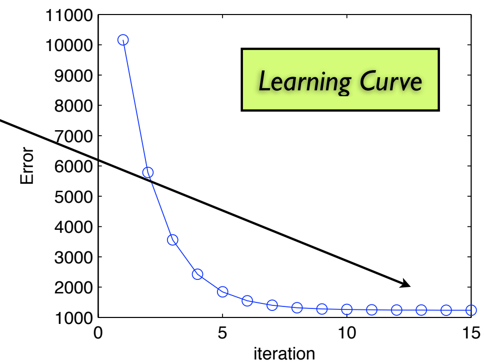
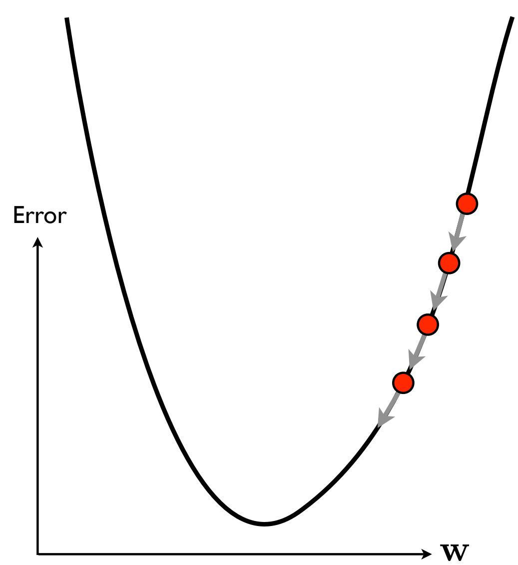


- Learning converges onto the solution that minimizes the error.
- For linear networks, this is guaranteed to converge to the minimum
- It is also possible to derive a closed-form solution (covered later)



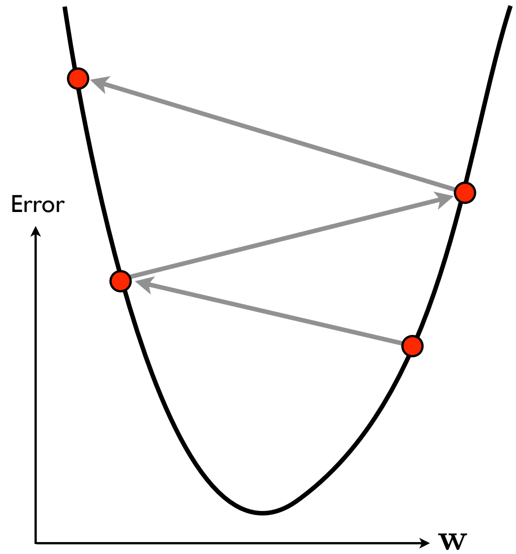
Learning is slow when epsilon is too small

- Here, larger step sizes would converge more quickly to the minimum



Divergence when epsilon is too large

- If the step size is too large, learning can oscillate between different sides of the minimum



Multi-layer networks

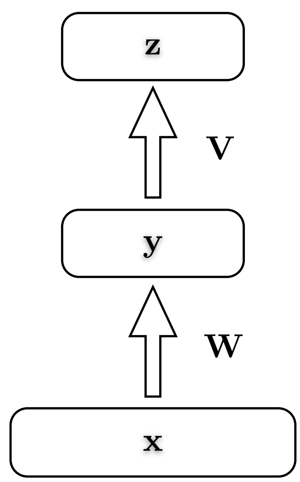
- Can we extend our network to multiple layers? We have:

$$
\begin{aligned}
y_j &= \sum_i w_{i,j} x_i \\
z_j &= \sum_k v_{j,k} y_j \\
&= \sum_k v_{j,k} \sum_i w_{i,j} x_i
\end{aligned}
$$

- Or in matrix form

$$
\begin{aligned}
\mathbf{z} &= \mathbf{V}\mathbf{y} \\
&= \mathbf{V}\mathbf{W}\mathbf{x}
\end{aligned}
$$

- Thus a two-layer linear network is equivalent to a one-layer linear network with weights $\mathbf{U}=\mathbf{V}\mathbf{W}$.
- It is *not* more powerful.



How do we address this?

Non-linear neural networks

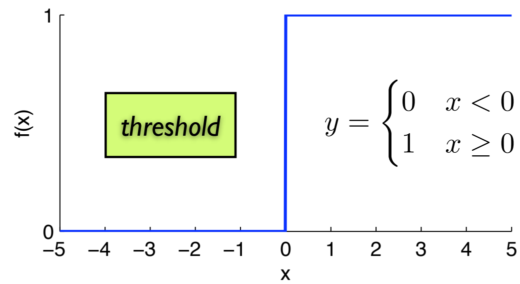
- Idea introduce a non-linearity:

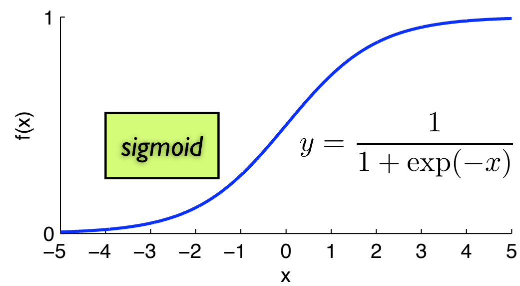
$$y_j = f(\sum_i w_{i,j} x_i)$$

- Now, multiple layers are *not* equivalent

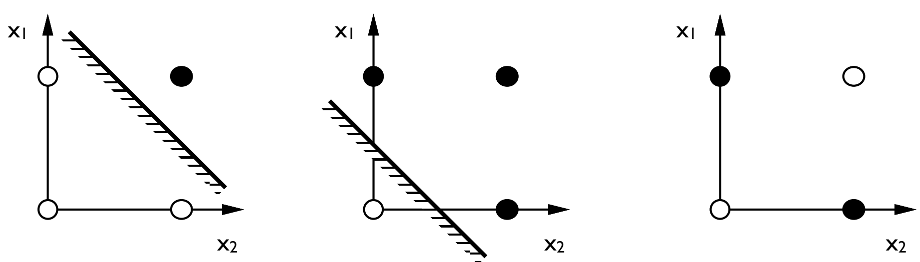
$$\begin{aligned} z_j &= f(\sum_k v_{j,k}\, y_j) \\ &= f(\sum_k v_{j,k}\, f(\sum_i w_{i,j} x_i)) \end{aligned}$$

- Common nonlinearities:
  - threshold
  - sigmoid





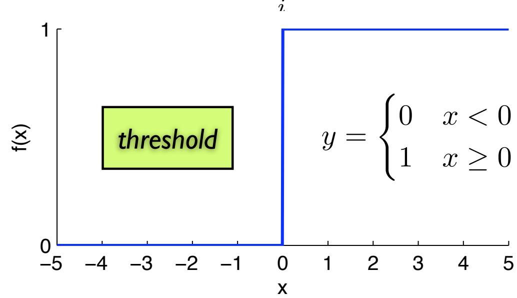
Modeling logical operators



x_1 AND x_2 x_1 OR x_2 x_1 XOR x_2

- A one-layer binary-threshold network can implement the logical operators AND and OR, but not XOR.
- Why not?

$$y_j = f(\sum_i w_{i,j} x_i)$$



Posterior odds interpretation of a sigmoid

The general classification/regression problem

desired output
$\mathbf{y} = \{y_1, \ldots, y_K\}$

for classification:

$$y_i = \begin{cases} 1 & \text{if } \mathbf{x}_i \in C_i \equiv \text{class } i, \\ 0 & \text{otherwise} \end{cases}$$

regression for arbitrary y.

model
$\boldsymbol{\theta} = \{\theta_1, \ldots, \theta_M\}$

model (e.g. a decision tree) is defined by M parameters, **e.g. a multi-layer neural network.**

Data
$\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_T\}$
$\mathbf{x}_i = \{x_1, \ldots, x_N\}_i$

input is a set of T observations, each an N-dimensional vector (binary, discrete, or continuous)

Given data, we want to learn a model that can correctly classify novel observations **or map the inputs to the outputs**

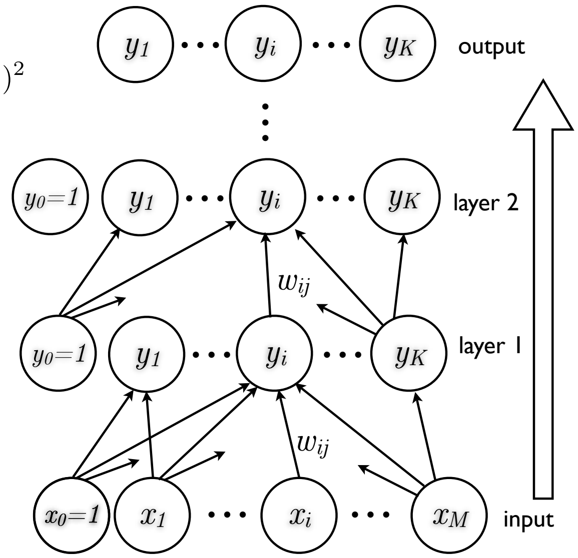
A general multi-layer neural network

- Error function is defined as before, where we use the target vector t_n to define the desired output for network output y_n.

$$E = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{y}_n(\mathbf{x_n}, \mathbf{W_{1:L}}) - \mathbf{t}_n)^2$$

- The "forward pass" computes the outputs at each layer:

$$y_j^l = f(\sum_i w_{i,j}^l \, y_j^{l-1})$$
$$l = \{1, \dots, L\}$$
$$\mathbf{x} \equiv \mathbf{y}^0$$
$$\text{output} = \mathbf{y}^L$$



Deriving the gradient for a sigmoid neural network

- Mathematical procedure for train is gradient descient: same as before, except the gradients are more complex to derive.

New problem: local minima

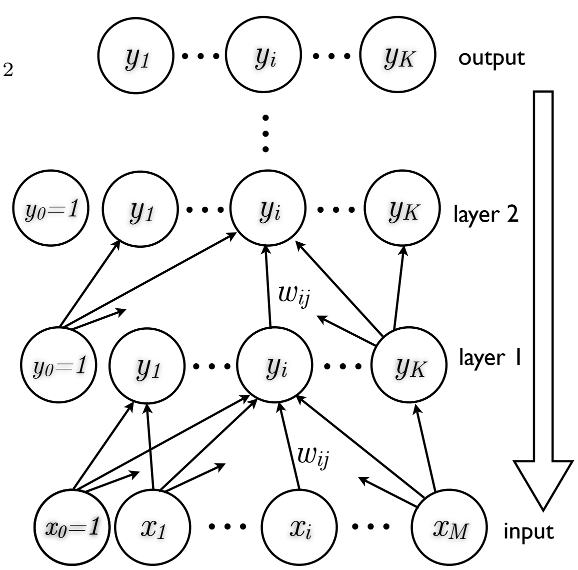
$$E = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{y}_n(\mathbf{x_n}, \mathbf{W_{1:L}}) - \mathbf{t}_n)^2$$

- Convenient fact for the sigmoid non-linearity:

$$\frac{d\sigma(x)}{dx} = \frac{d}{dx}\frac{1}{1+\exp(-x)}$$
$$= \sigma(x)(1-\sigma(x))$$

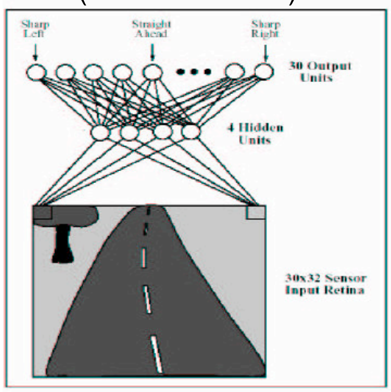
- backward pass computes the gradients: *back-propagation*

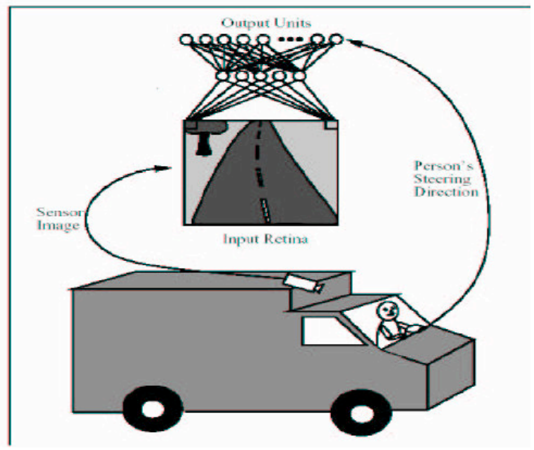
$$\mathbf{W}_{t+1} = \mathbf{W}_t + \epsilon \frac{\partial E}{\mathbf{W}}$$



Applications: Driving (output is analog: steering direction)

network with 1 layer
(4 hidden units)





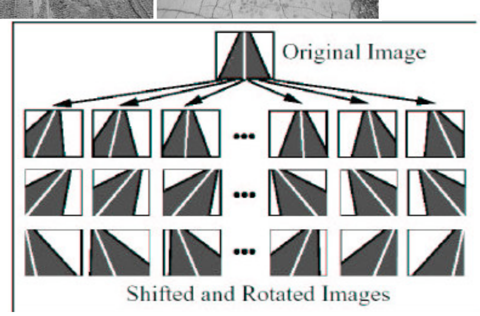
- Learns to drive on roads
- Demonstrated at highway speeds over 100s of miles

D. Pomerleau. *Neural network perception for mobile robot guidance.* Kluwer Academic Publishing, 1993.

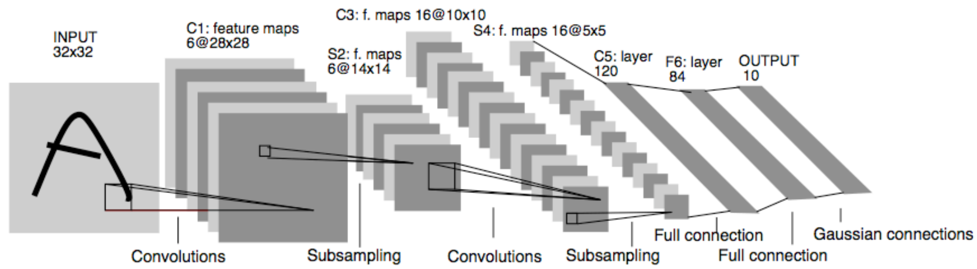
Real image input is augmented to avoid overfitting

Training data:
Images +
corresponding
steering angle

Important:
Conditioning of training data to generate new examples → avoids overfitting



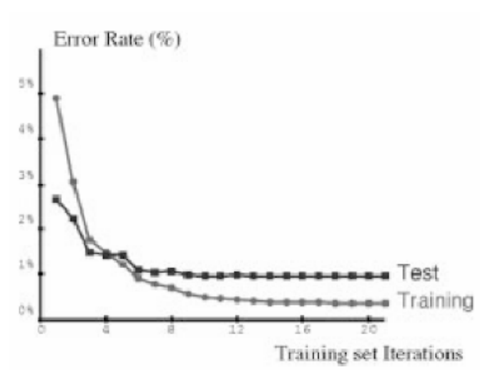
Hand-written digits: LeNet



- Takes as input image of handwritten digit
- Each pixel is an input unit
- Complex network with many layers
- Output is digit class

- Tested on large (50,000+) database of handwritten samples
- Real-time
- Used commercially

LeNet

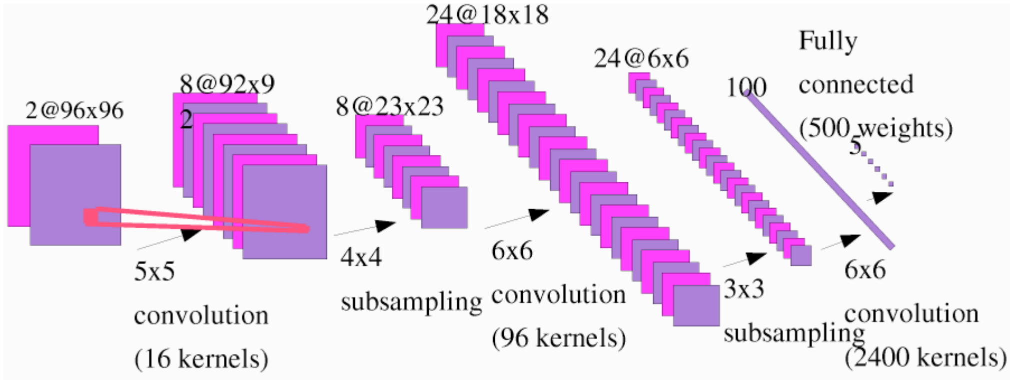


Very low error rate (<< 1%

Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, november 1998.

http://yann.lecun.com/exdb/lenet/

Object recognition



- LeCun, Huang, Bottou (2004). Learning Methods for Generic Object Recognition with Invariance to Pose and Lighting. Proceedings of CVPR 2004.
- http://www.cs.nyu.edu/~yann/research/norb/

Summary

- Decision boundaries
  - Bayes optimal
  - linear discriminant
  - linear separability
- Classification vs regression
- Optimization by gradient descent
- Degeneracy of a multi-layer linear network
- Non-linearities:: threshold, sigmoid, others?
- Issues:
  - very general architecture, can solve many problems
  - large number of parameters: need to avoid overfitting
  - usually requires a large amount of data, or special architecture
  - local minima, training can be slow, need to set stepsize