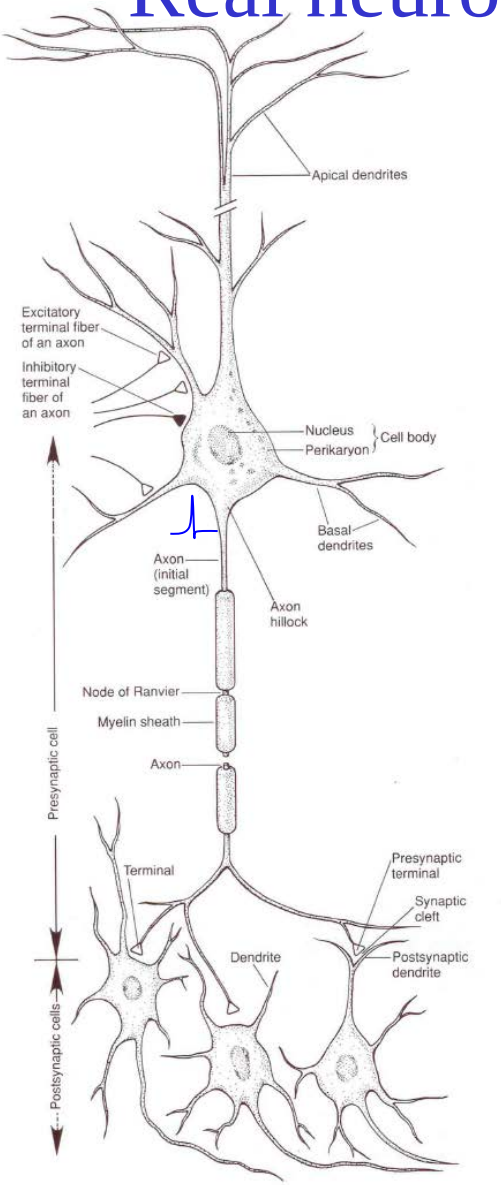
CSE 5526: Introduction to Neural Networks

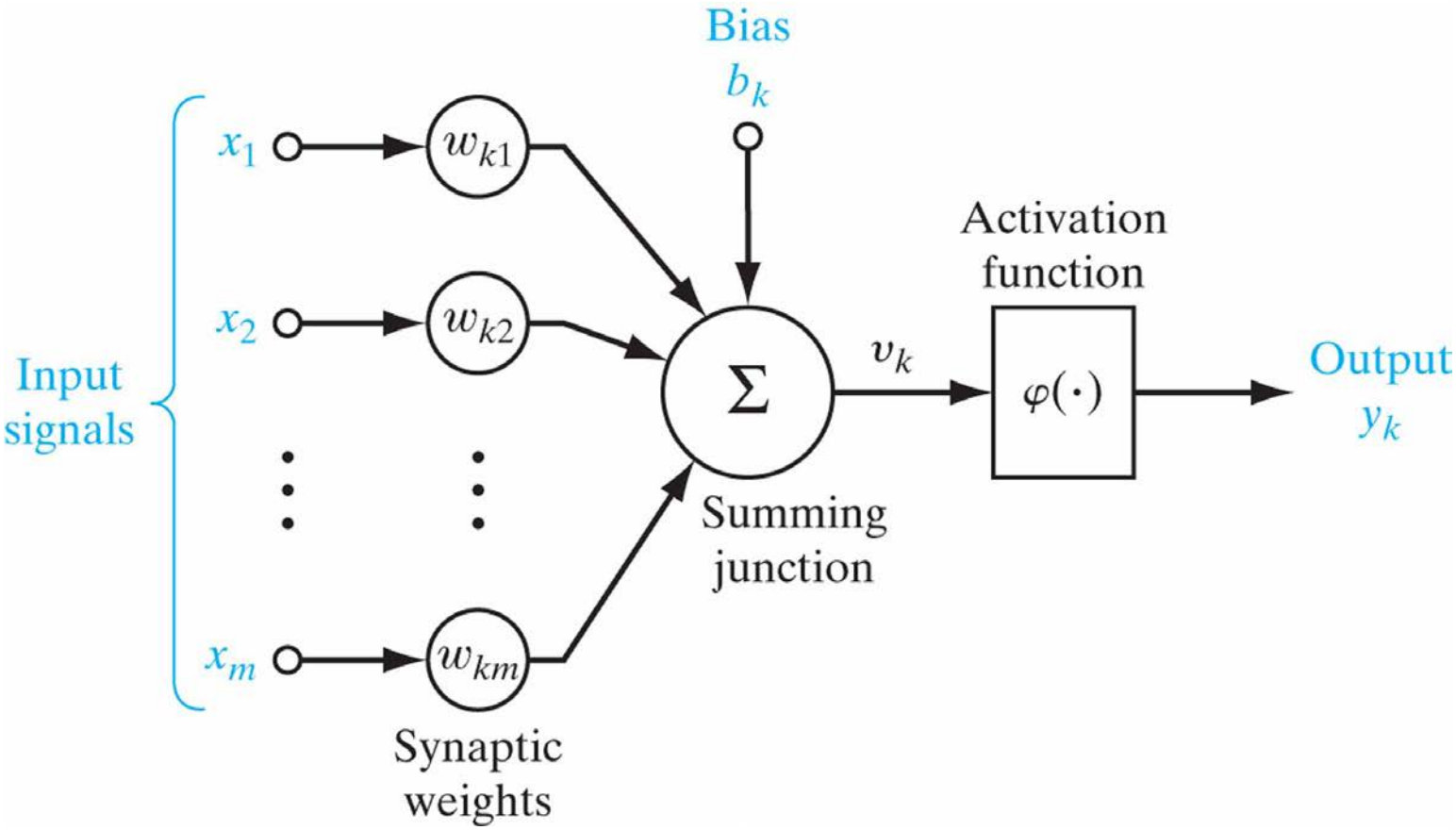
Review to date

Real neurons have three main parts



- Cell body (~50μm)
  - Initiates action potential
- Axon (0.2-20μm)
  - Transmits signal to up to 1000 other neurons
  - Insulated by myelin sheath
  - Up to 1m long
- Dendrites: receive signals
  - Synapse: junction to another neuron's axon

This model approximates the neural firing rate



McCulloch-Pitts neuron model

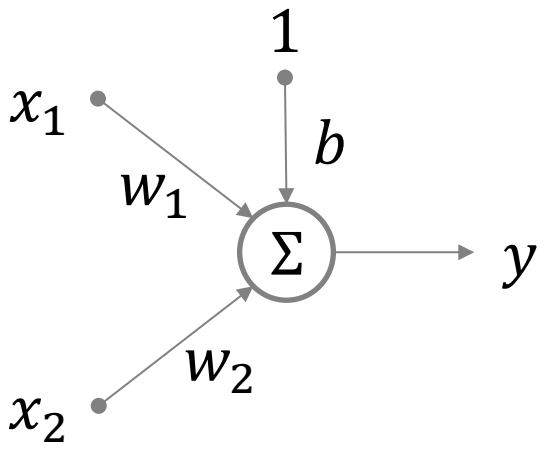
$x_i \in \{-1, 1\}$ Bipolar input

$$\varphi(v) = \begin{cases} 1 & \text{if } v \geq 0 \\ -1 & \text{if } v < 0 \end{cases}$$

A form of signum (sign) function

$$y = \varphi\left(\sum_{i=1}^{m} w_i x_i + b\right)$$

M-P neurons can implement any logic function



$$y = w_1 x_1 + w_2 x_2 + b$$

x_1	x_2	x_1 AND x_2	x_1 OR x_2	NOT x_1
-1	-1	-1	-1	1
-1	1	-1	1	1
1	-1	-1	1	-1
1	-1	1	1	-1

	x_1 AND x_2	x_1 OR x_2	NOT x_1
w_1	1	1	-1
w_2	1	1	0
b	-0.5	0.5	0

M-P neurons have a linear decision boundary

- Can we visualize the decision the perceptron would make in classifying every potential point?
- Yes, it is called the discriminant function

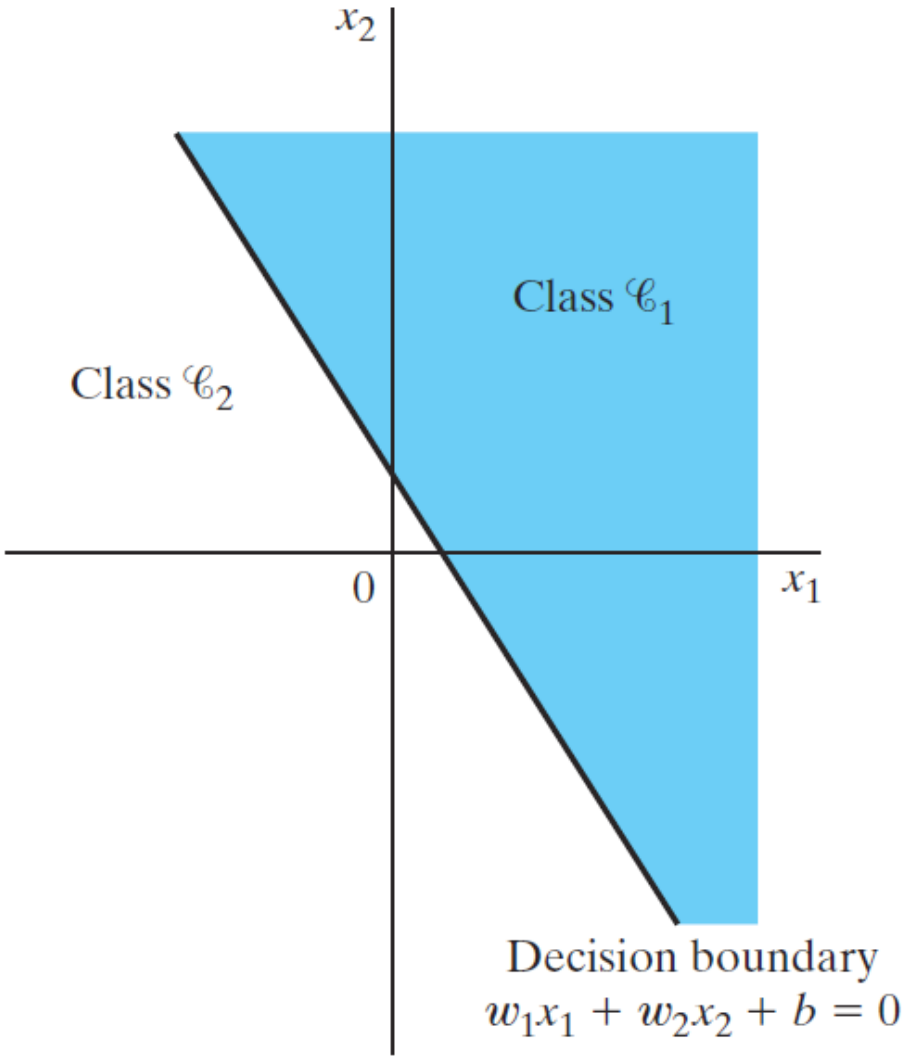
$$g(x) = x^T w = \sum_{i=0}^{m} w_i x_i$$

- What is the boundary between the two classes like?

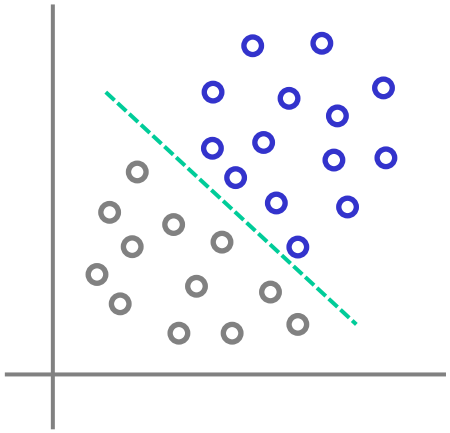
$$g(x) = x^T w = 0$$

- This is a linear function of x

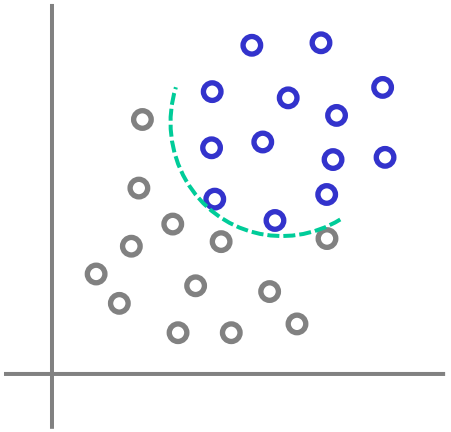
M-P neurons have a linear decision boundary



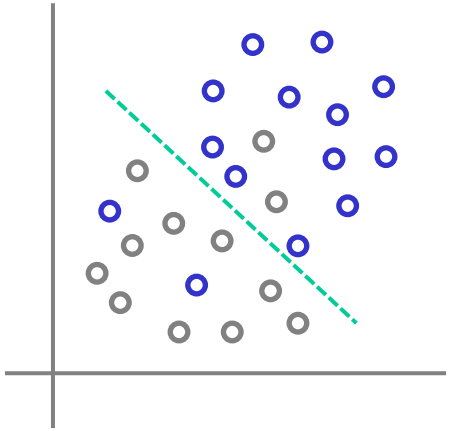
Linear decision functions can't solve all classification problems



Linearly separable



Non-linearly separable



Not separable

Distinction depends on "scale" of classifier

Perceptron algorithm learns weights from data

- Learn parameters *w* from examples (x_p, d_p)
- In an online fashion, i.e., one point at a time
- Adjust weights as necessary, i.e. when incorrect
- Adjust weights to be more like d=1 points and more like negative d=-1 points

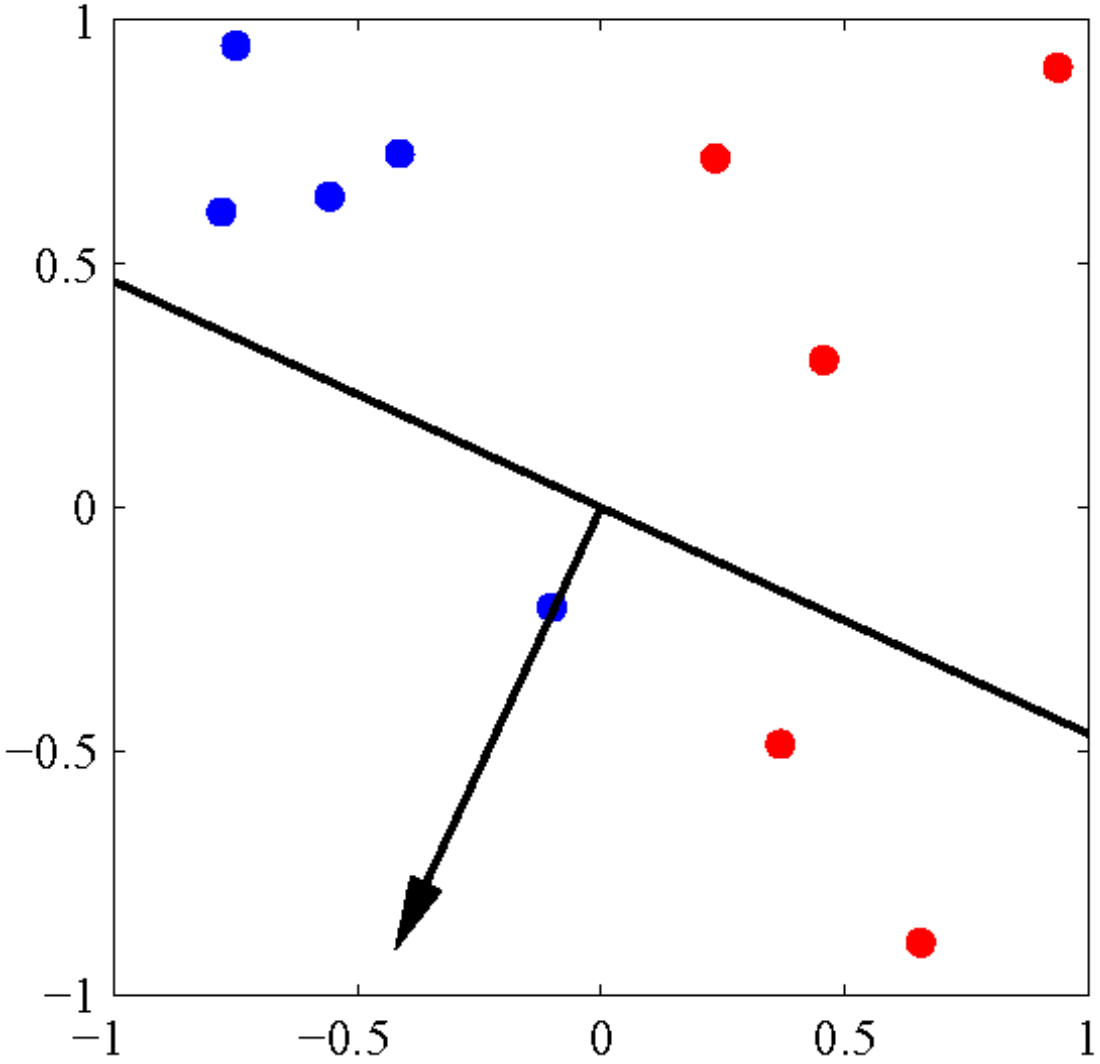
Perceptron algorithm learns weights from data

$$w(n+1) = w(n) + \Delta w(n)$$

$$= w(n) + \eta[d(n) - y(n)]x(n)$$

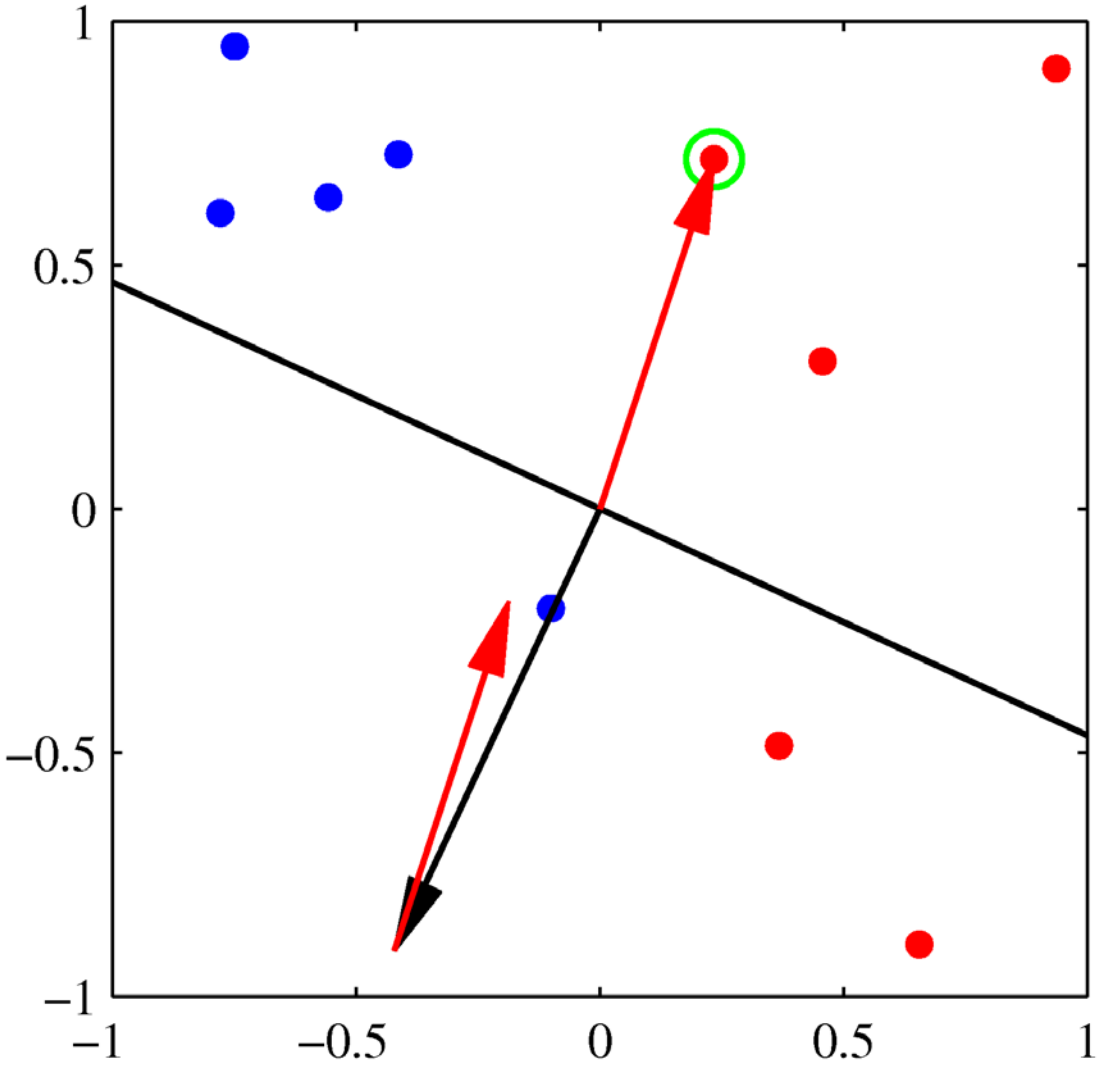
- n: iteration number, iterating over points in turn
- η: step size or learning rate, = 1 WLOG
- Only updates w when y(n) is incorrect

Visualization of perceptron learning



From Bishop (2006)

Visualization of perceptron learning



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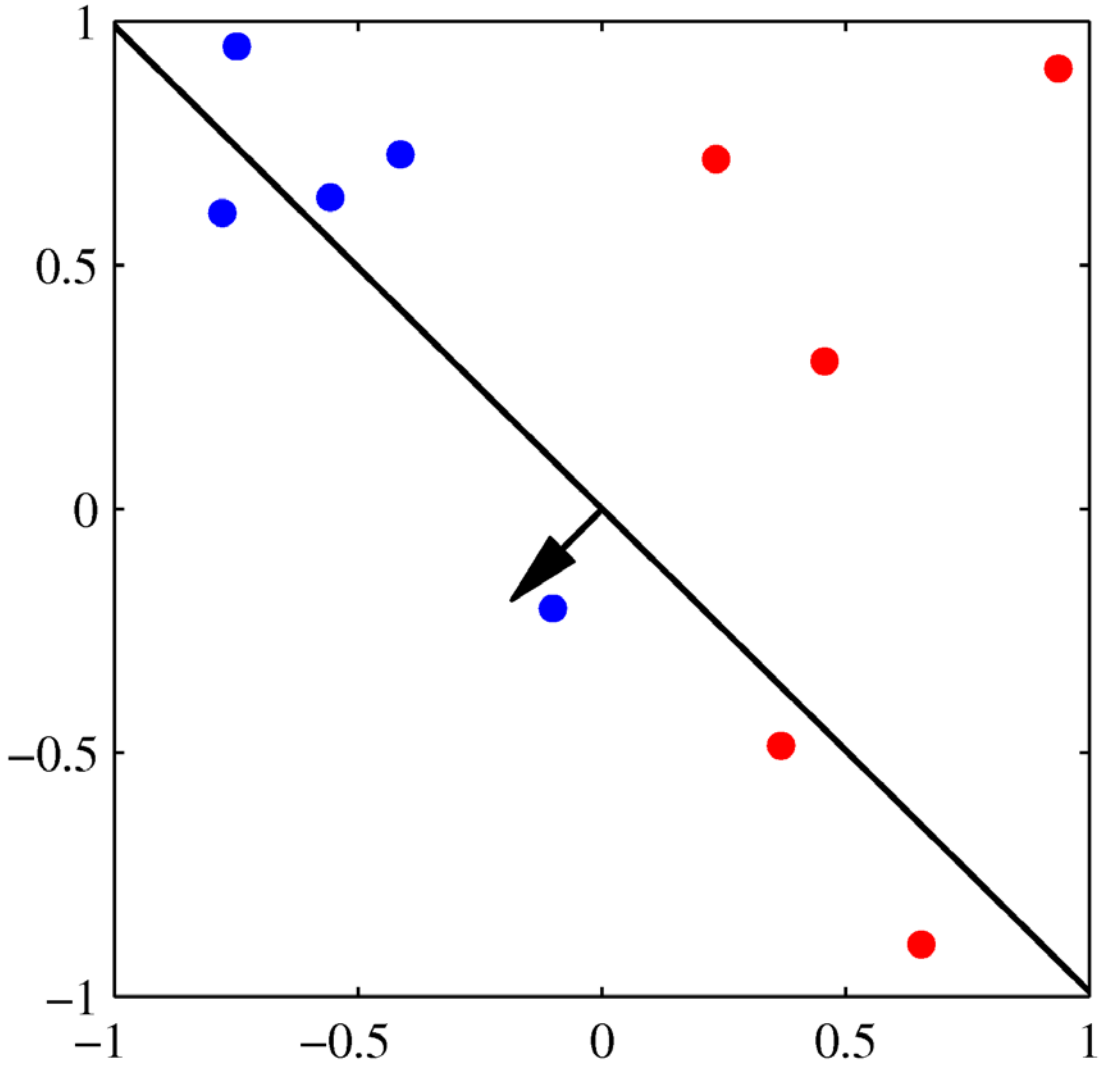
Visualization of perceptron learning



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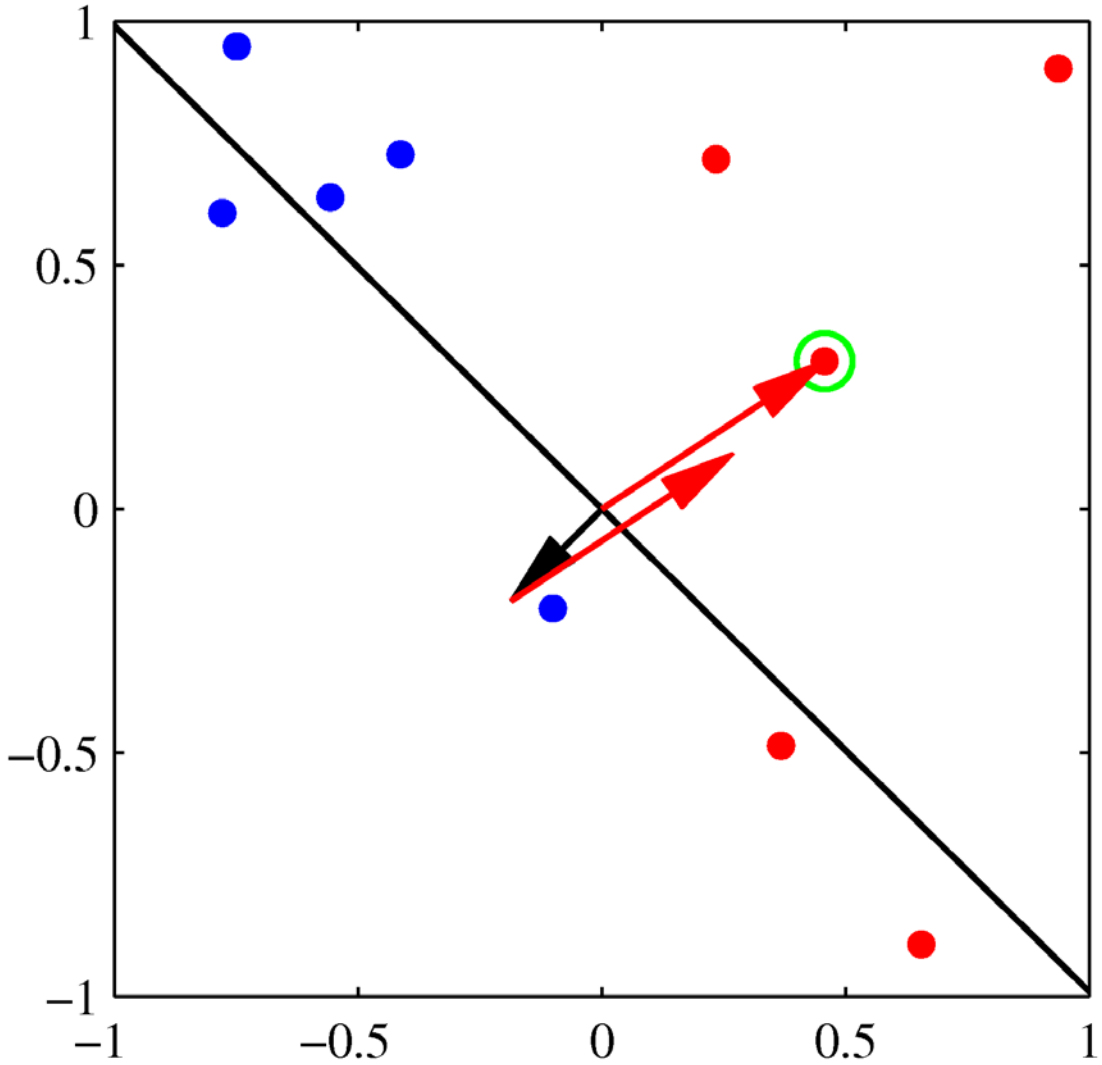
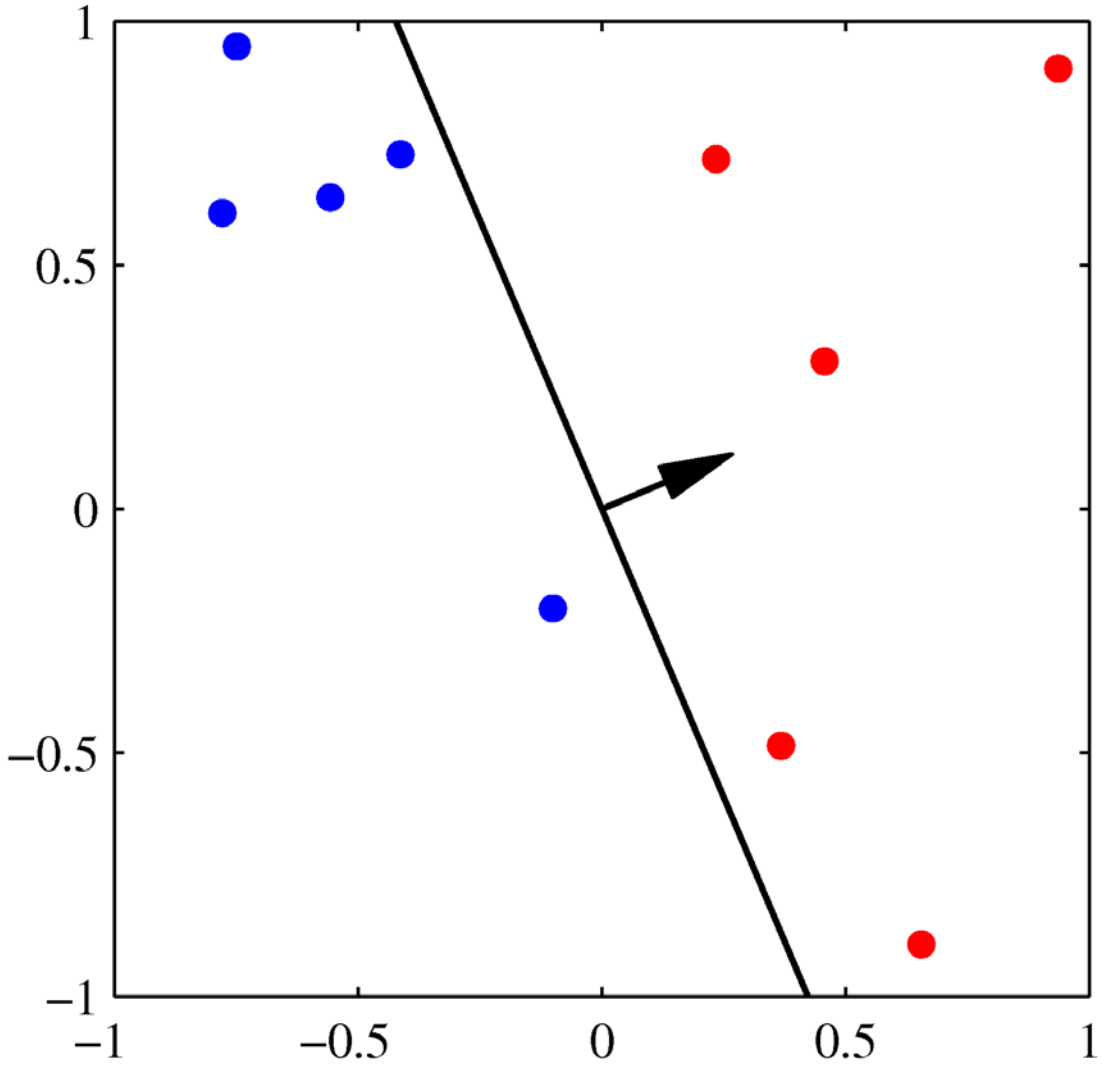
Visualization of perceptron learning



From Bishop (2006)

Visualization of perceptron learning



From Bishop (2006)

Summary of perceptron learning algorithm

- Definition
  - $w(n)$: (m+1)-by-1 weight vector (including bias) at step n
- Inputs
  - $x(n)$: n^{th} (m+1)-by-1 input vector with first element = 1
  - $d(n)$: n^{th} desired response
- Initialization: set w(0) = 0
- Repeat until no points are mis-classified
  - Compute response: $y(n) = \text{signum}\{w(n)^T x(n)\}$
  - Update: $w(n+1) = w(n) + [d(n) - y(n)]x(n)$

Perceptron learning can be interpreted as gradient descent

- Consider the total amount by which a neuron mis-classifies all of the points

$$E(w) = -\sum_p \left(d_p - y_p\right) w^T x_p$$

- Then the gradient of this WRT w is

$$\nabla_w E(w) = -\sum_p \left(d_p - y_p\right) x_p$$

- So the gradient descent update is

$$w(n+1) = w(n) - \eta \nabla_w E = w(n) + \left(d_p - y_p\right) x_p$$

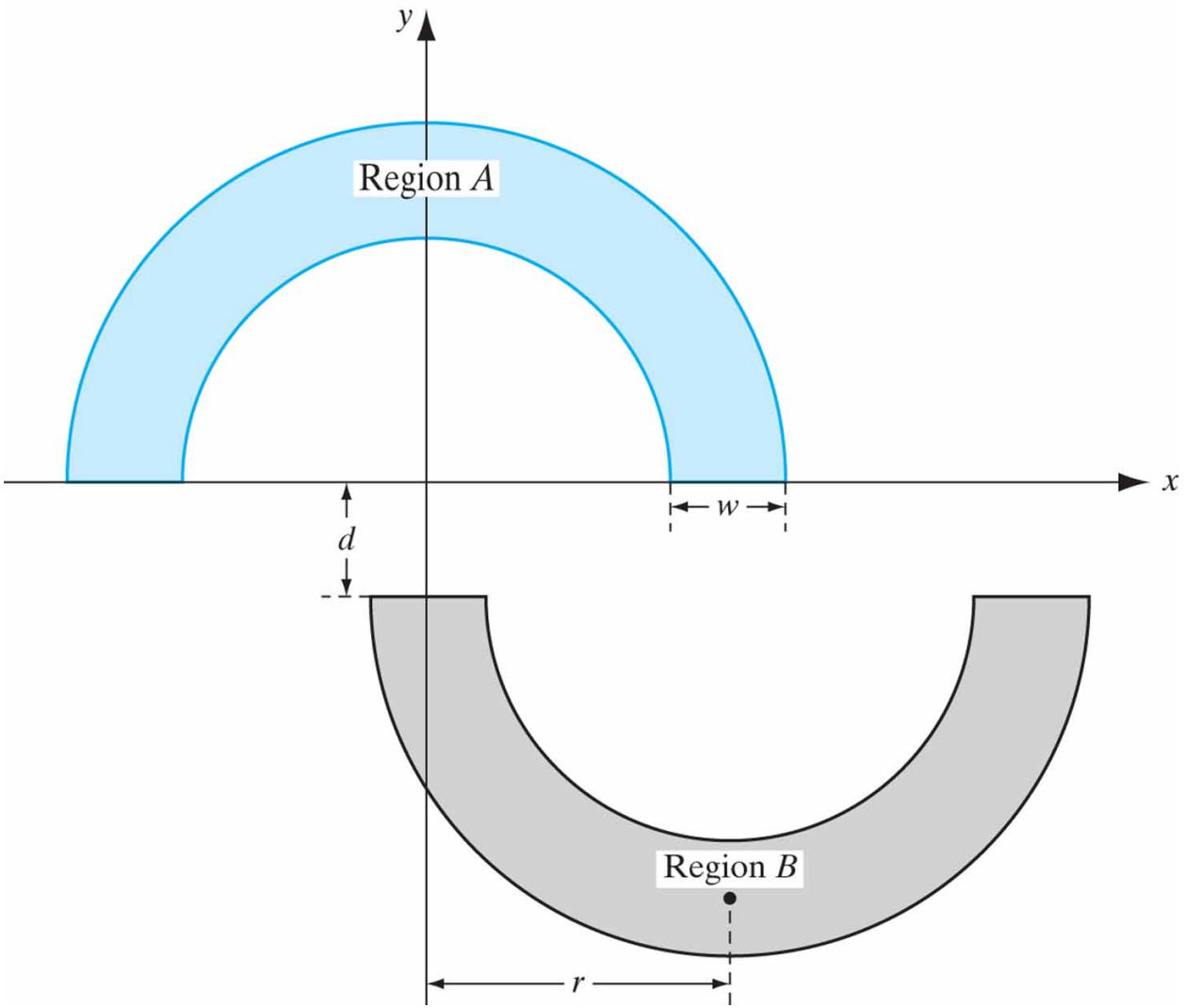
Perceptron convergence theorem

- Theorem:
  - Assume that there exists some unit vector w_0 and some α such that $d(n)w_0^T x(n) \geq \alpha$
    - i.e., the data are linearly separable
  - Assume also that there exists some R such that $\|x(n)\| = \sqrt{x(n)^T x(n)} \leq R \quad \forall n$
    - i.e., the data lie within a sphere of radius R
  - Then the perceptron algorithm makes at most $\frac{R^2}{\alpha^2}$ errors
    - i.e., it converges in at most $\frac{R^2}{\alpha^2}$ iterations

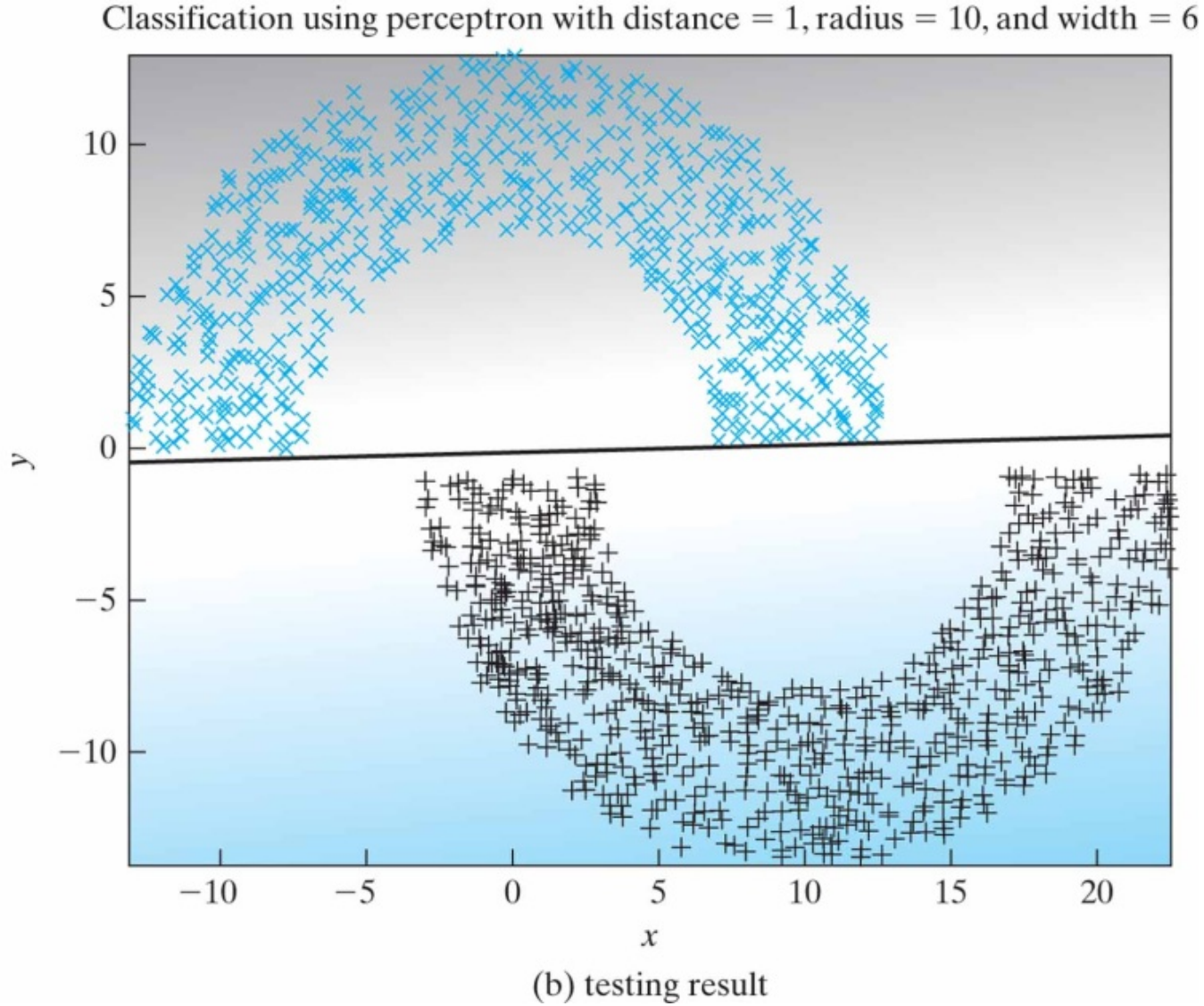
Perceptron convergence proof sketch

- Define w_k as the parameter vector when the algorithm makes its k^{th} error (note $w_1 = 0$)
- First show $k\alpha \leq \|w_{k+1}\|$ by induction
  - The weight vector grows in length proportionally with k
  - because of the separability of the data
- Second show $\|w_{k+1}\|^2 \leq kR^2$ by induction
  - But it can grow no faster than $\sqrt{k}$
  - because of the radius of the data
- Then it follows that $k \leq R^2/\alpha^2$
  - The perceptron makes a finite number of errors

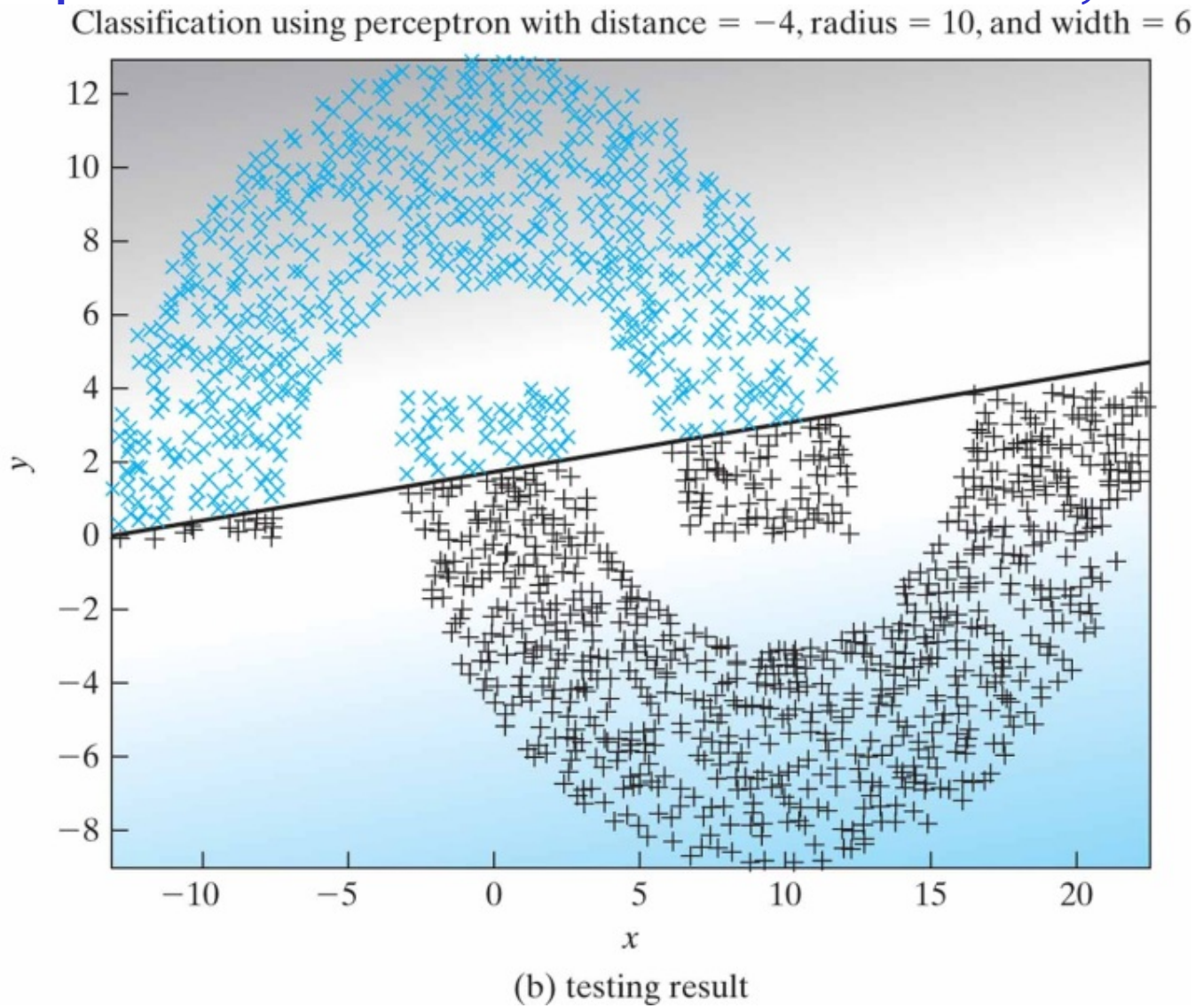
The double-moon classification problem



Perceptron learns double-moon, $d = 1$



Perceptron does not learn double-moon, d = -4



Linear regression has a closed-form solution

- Predict desired output d_p
- As a linear function of observations, $\boldsymbol{x}_p$

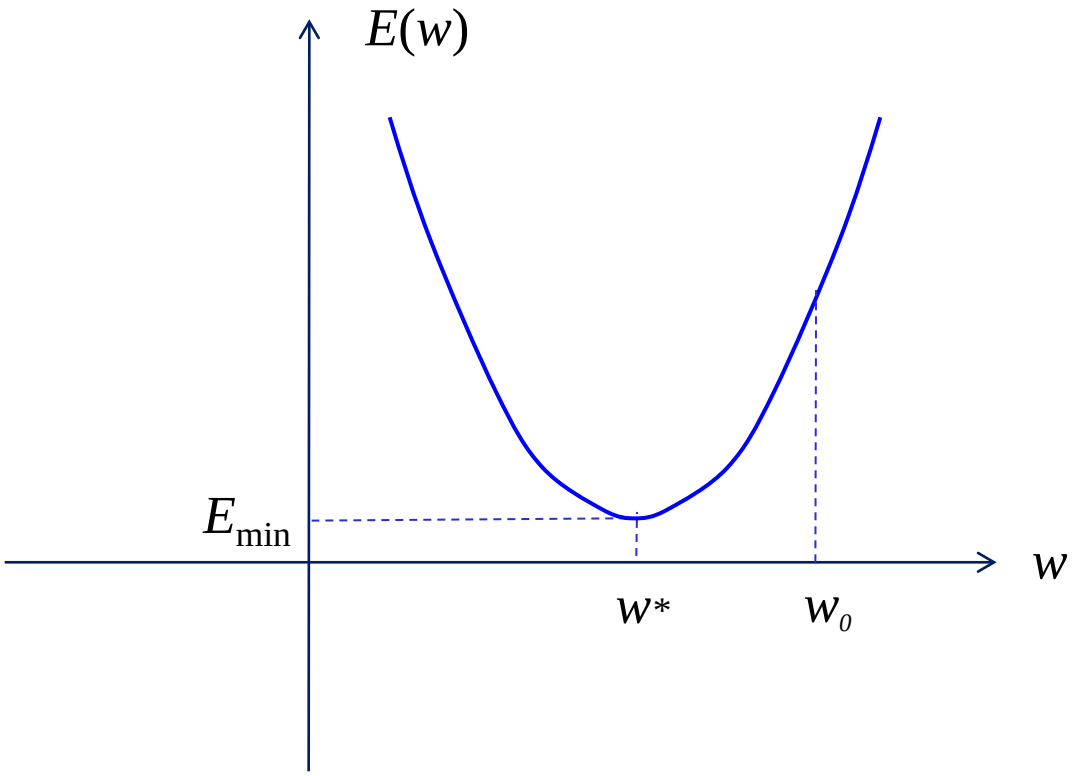
$$y_p = \boldsymbol{w}^T \boldsymbol{x}_p$$

- Find parameters $\boldsymbol{w}$ that minimize the mean square error of the predictions

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_p \left(d_p - y_p\right)^2$$

- Set gradient of error WRT $\boldsymbol{w}$ to 0
  - Solve for $\boldsymbol{w}$ analytically

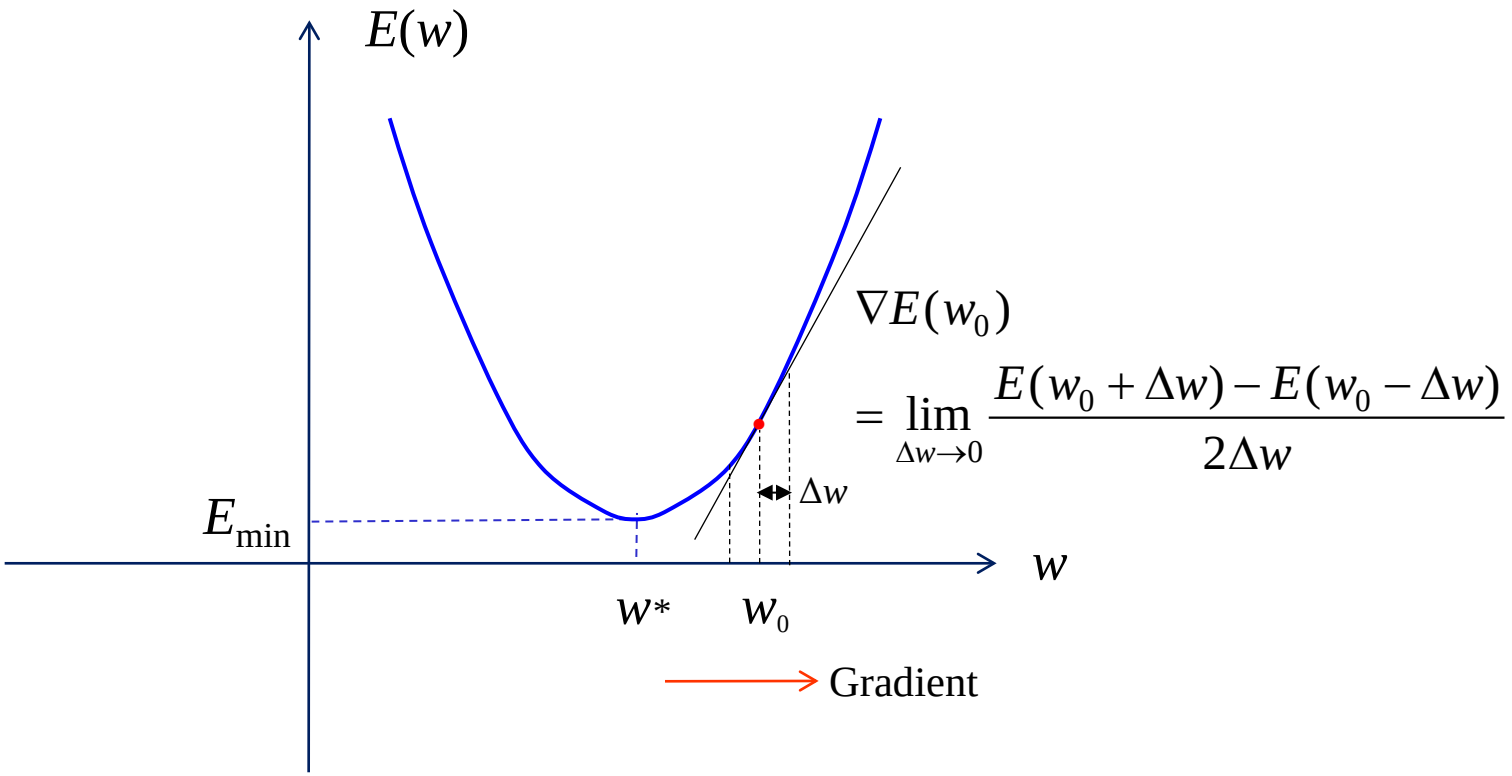
The mean square error defines a parabolic cost function



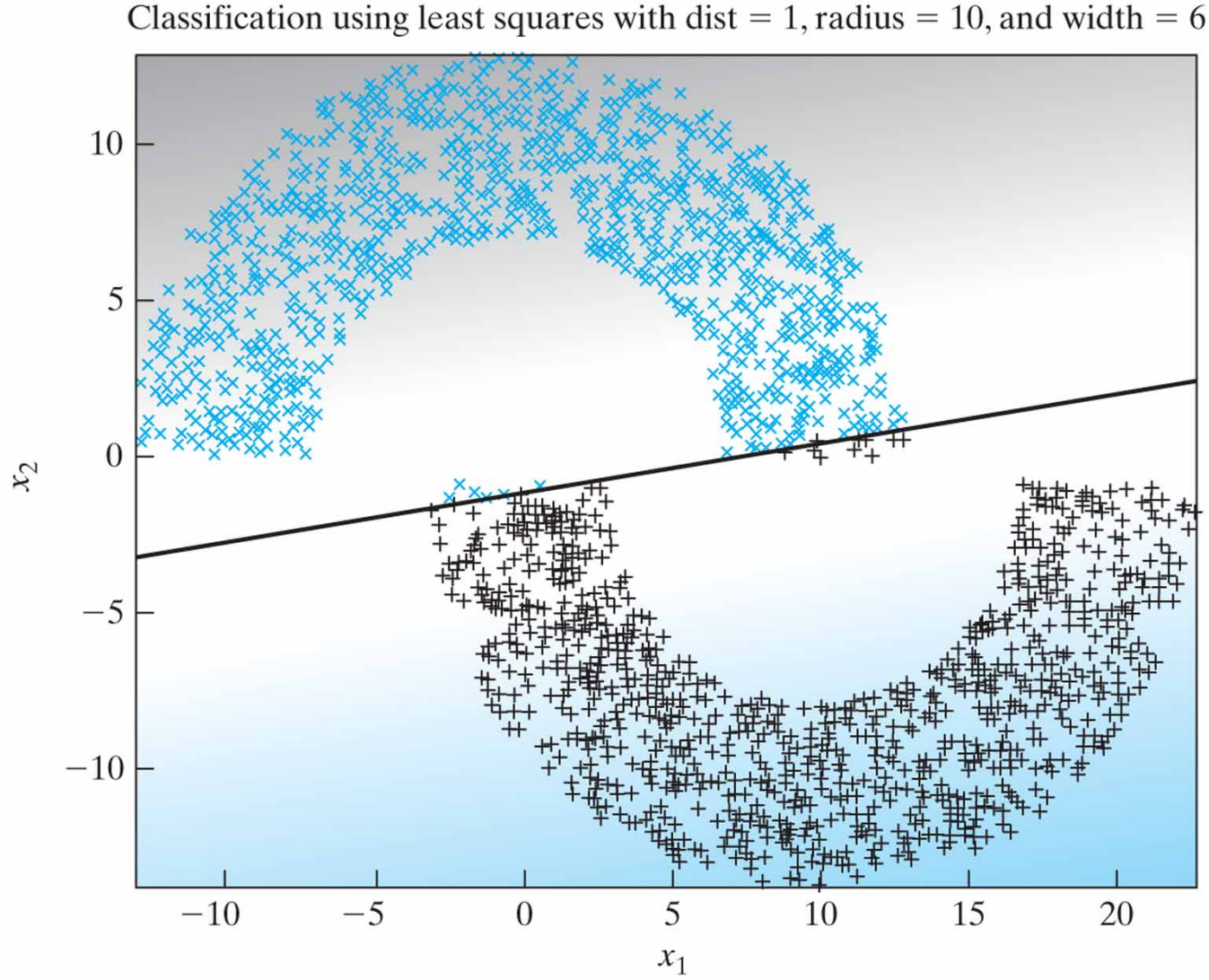
Optimal parameters can be found via search

- Often there is no closed form solution for
$$\nabla_{\boldsymbol{w}} E(\boldsymbol{w}) = 0$$
- We can still use the gradient in a numerical solution
- This is called gradient descent
$$\boldsymbol{w}(n+1) = \boldsymbol{w}(n) - \eta \nabla_{\boldsymbol{w}} E(\boldsymbol{w})$$
- At the minimum of $E(\boldsymbol{w})$, the gradient is 0
  - And $\boldsymbol{w}$ stays constant because $\boldsymbol{w}(n+1) = \boldsymbol{w}(n) - 0$

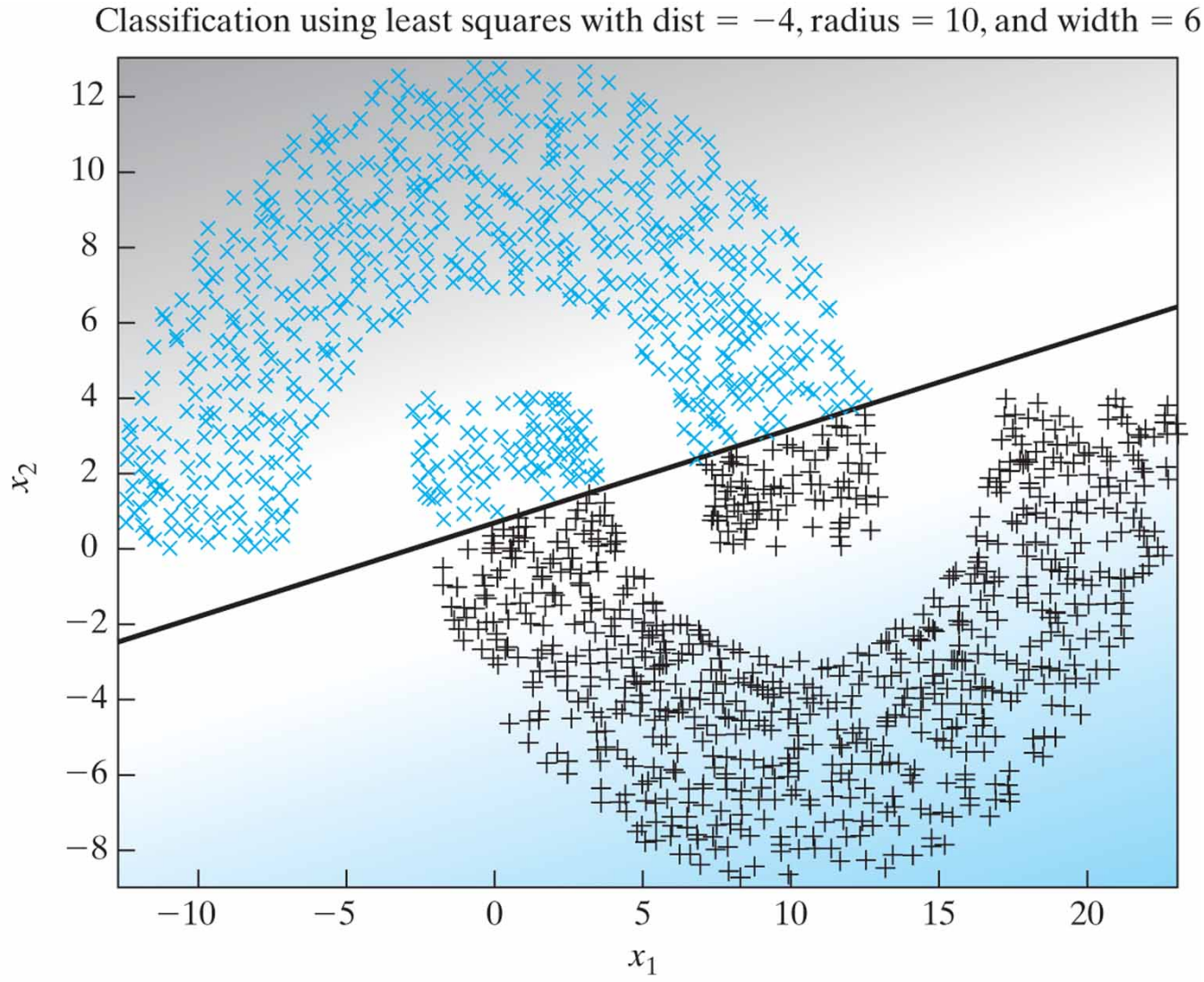
The gradient is the slope and direction of steepest ascent of the error function



Least squares classification works pretty well for double-moon, d = 1



Least squares classification works less well for double-moon, d = -4



LMS algorithm solves least squares on-line

- Stochastic gradient descent solution to linear regression is called the LMS algorithm
- Minimizes the error on one data point at a time

$$2E_p(w) = e_p^2(\boldsymbol{w}) = \left(d_p - y_p\right)^2 = \left(d_p - \boldsymbol{w}^T\boldsymbol{x}_p\right)^2$$

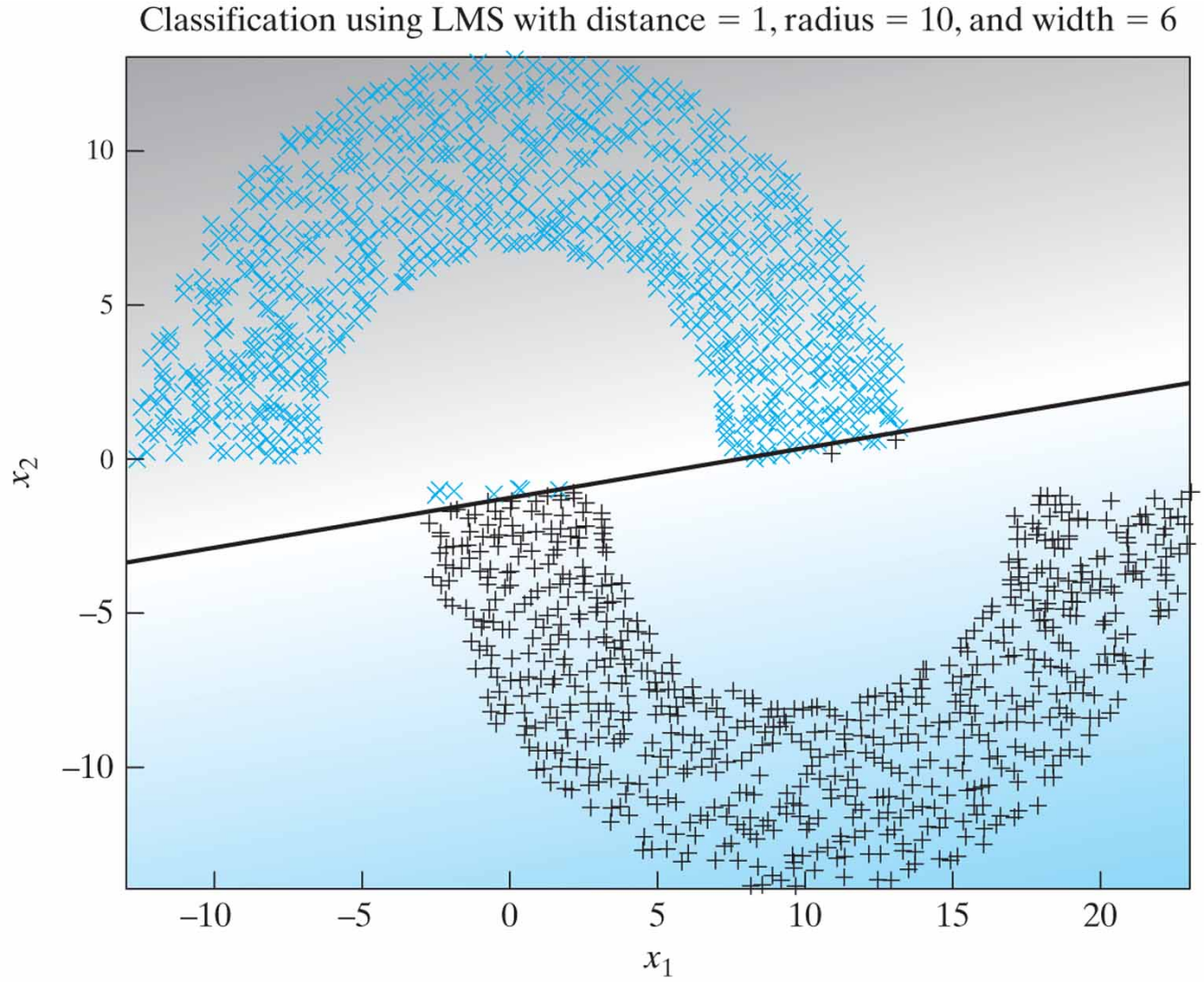
- The gradient is

$$\nabla_{\boldsymbol{w}} E_p(\boldsymbol{w}) = -\left(d_p - \boldsymbol{w}^T\boldsymbol{x}_p\right)\boldsymbol{x}_p = -e_p(\boldsymbol{w})\boldsymbol{x}_p$$

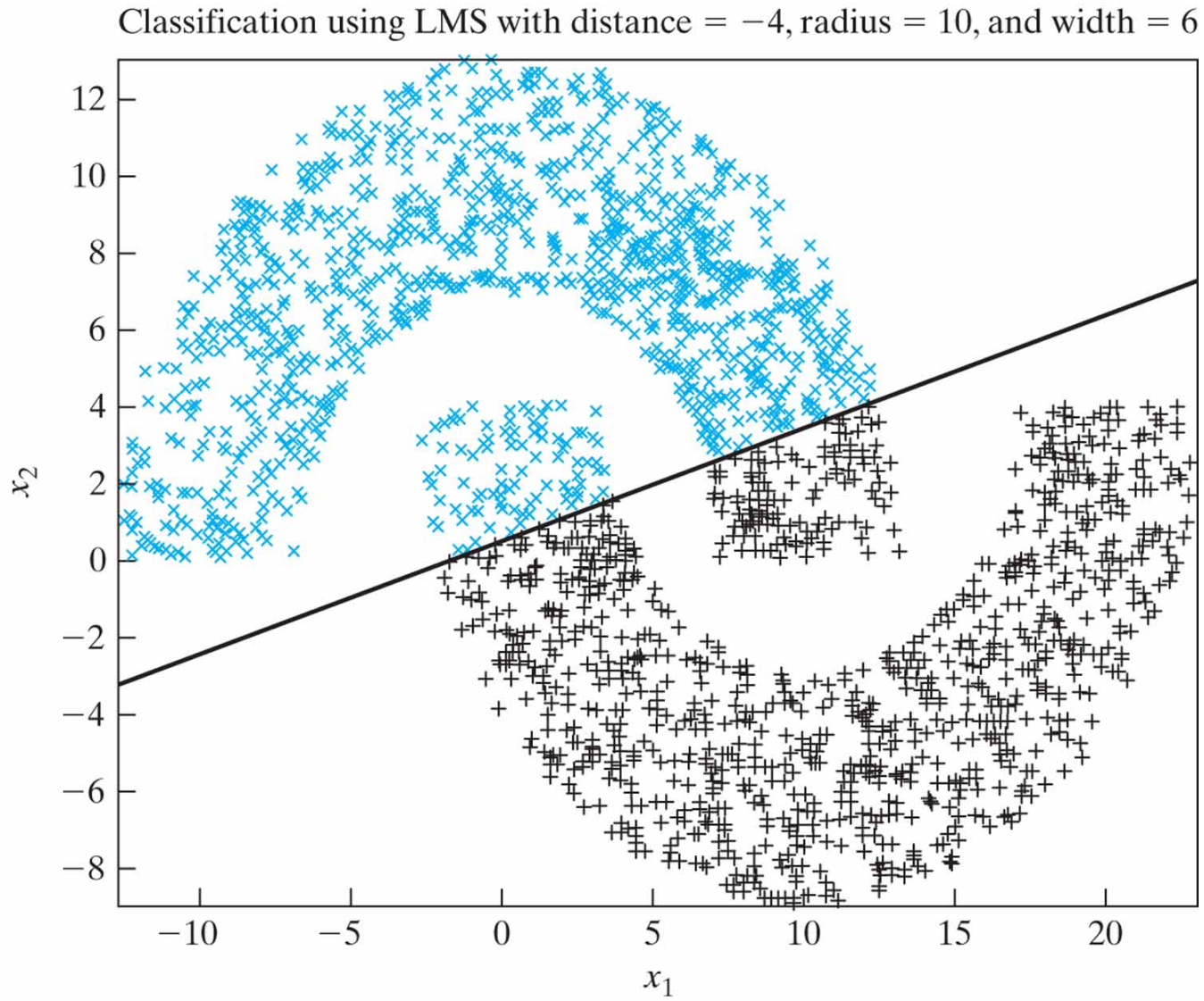
- So the LMS update is

$$\begin{aligned}\boldsymbol{w}(n+1) &= \boldsymbol{w}(n) - \eta\nabla_{\boldsymbol{w}} E_p(\boldsymbol{w}) \\ &= \boldsymbol{w}(n) + \eta e_p\,(\boldsymbol{w})\boldsymbol{x}_p\end{aligned}$$

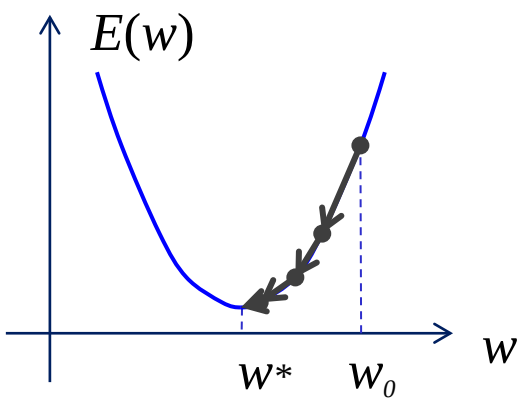
LMS achieves the least squares solution for double-moon, d = 1



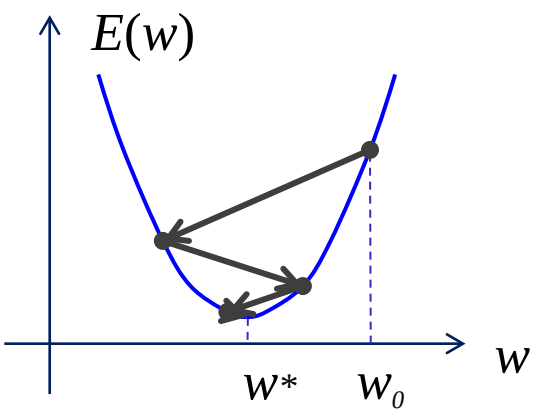
LMS achieves the least squares solution for double-moon, d=-4



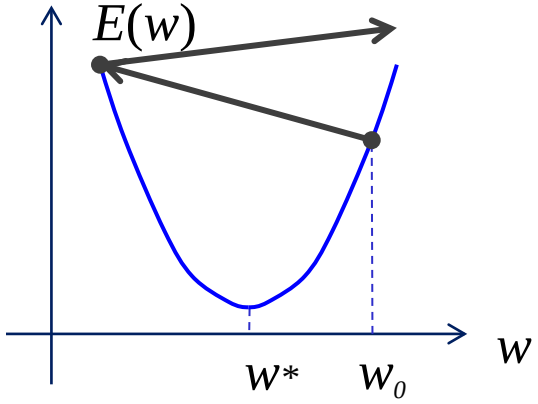
The optimal learning rate for a parabola is the reciprocal of the second derivative



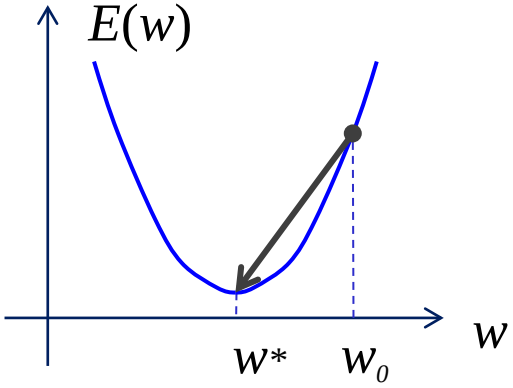
$\eta < (E''(w))^{-1}$



$\eta > (E''(w))^{-1}$

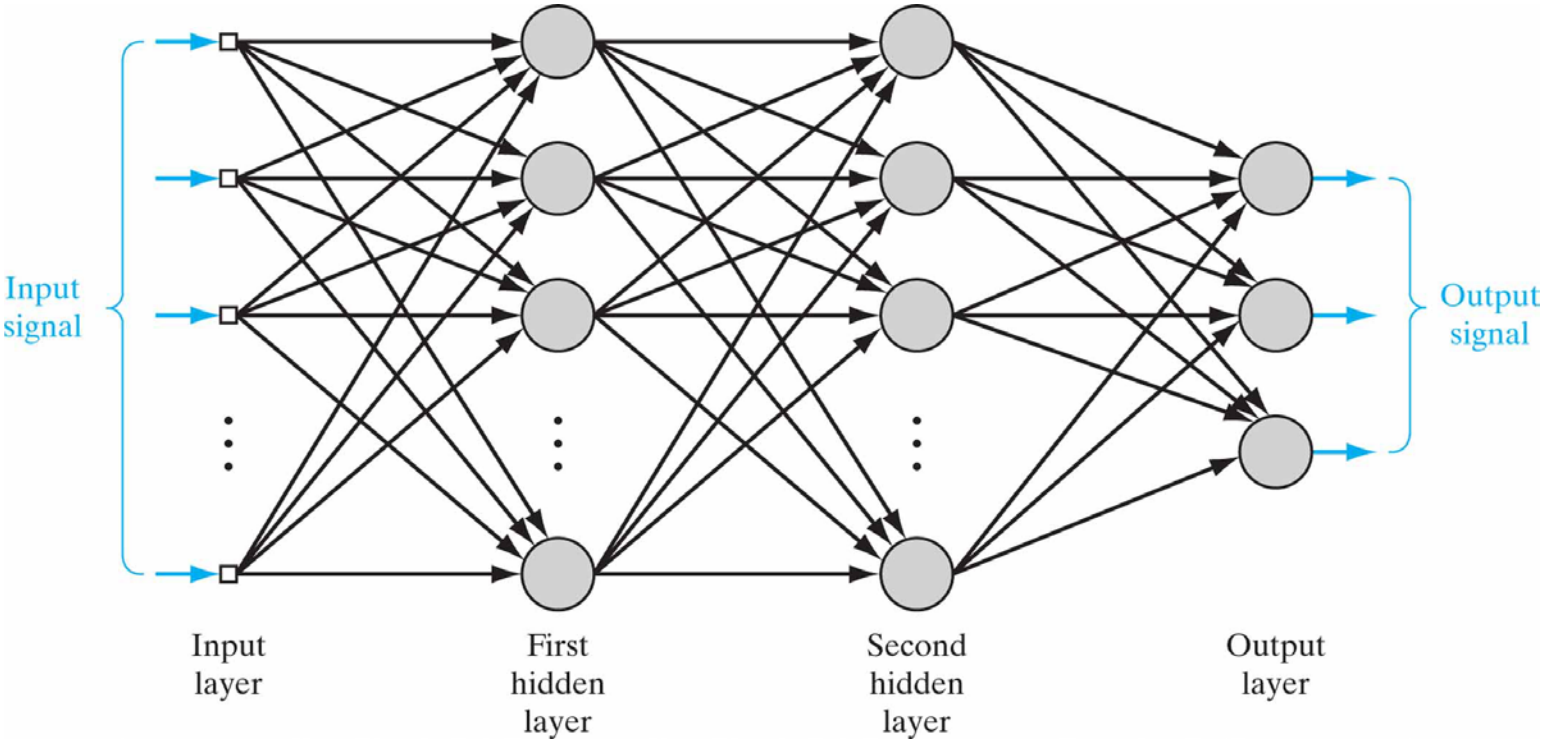


$\eta > 2(E''(w))^{-1}$



$\eta = (E''(w))^{-1}$

Multilayer perceptrons aren't really perceptrons



MLPs can be trained to minimize the MSE

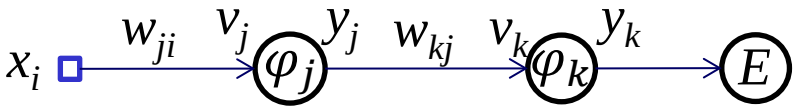
- Think of an MLP as a complicated, non-linear function of its input parametrized by $\boldsymbol{w}$:

$$\mathbf{y} = F(\boldsymbol{x}; \boldsymbol{w})$$

- Given a set of training data $\{\boldsymbol{x}_p, \boldsymbol{d}_p\}$, adjust $\boldsymbol{w}$ to minimize the mean square error of its predictions

$$\bar{E}(\boldsymbol{w}) = \sum_p E_p(\boldsymbol{w}) = \sum_p \frac{1}{2} \left\| \boldsymbol{d}_p - F(\boldsymbol{x}_p; \boldsymbol{w}) \right\|^2$$

Gradient descent in MLPs is called backprop



- Error assigned to each neuron

$$e_k = (d_k - y_k)$$

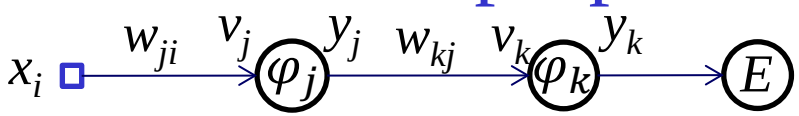
$$e_j = \sum_k e_k \varphi'(v_k) w_{kj}$$

- Gradients computed for each weight

$$\frac{\partial}{\partial w_{kj}} E(\boldsymbol{w}) = -e_k \varphi'(v_k) y_j$$

$$\frac{\partial}{\partial w_{ji}} E(\boldsymbol{w}) = -e_j \varphi'(v_j) x_i$$

Gradient descent in MLPs is called backprop



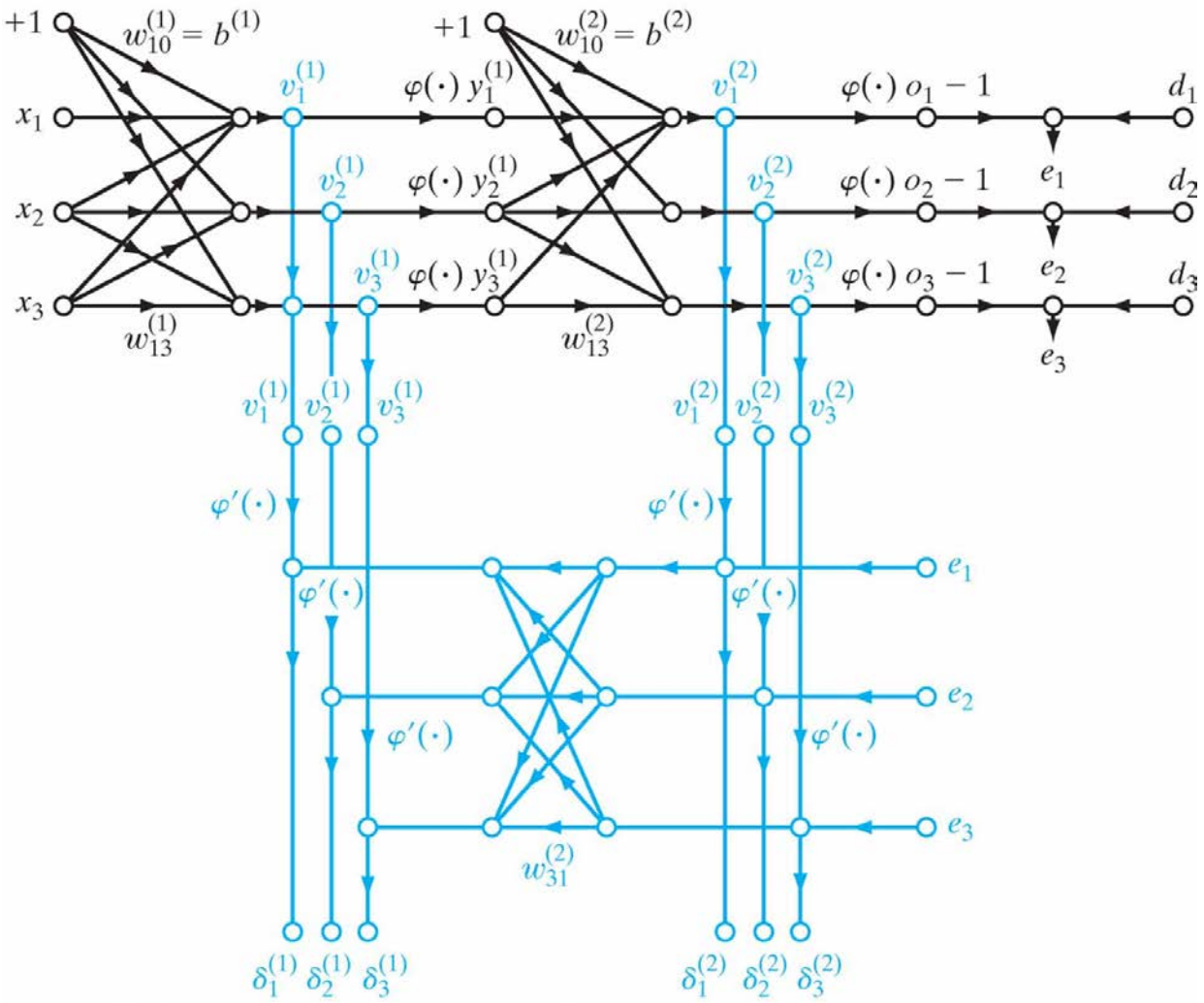
- So the weights are updated as

$$w_{kj}(n+1) = w_{kj}(n) + \eta e_k \varphi'(v_k) y_j$$

$$w_{ji}(n+1) = w_{ji}(n) + \eta e_j \varphi'\left(v_j\right) x_i$$

- Easy to extend to more layers
  - Although the gradient itself is less well behaved
  - So second-order methods are more necessary

Backprop can be visualized as a flow chart



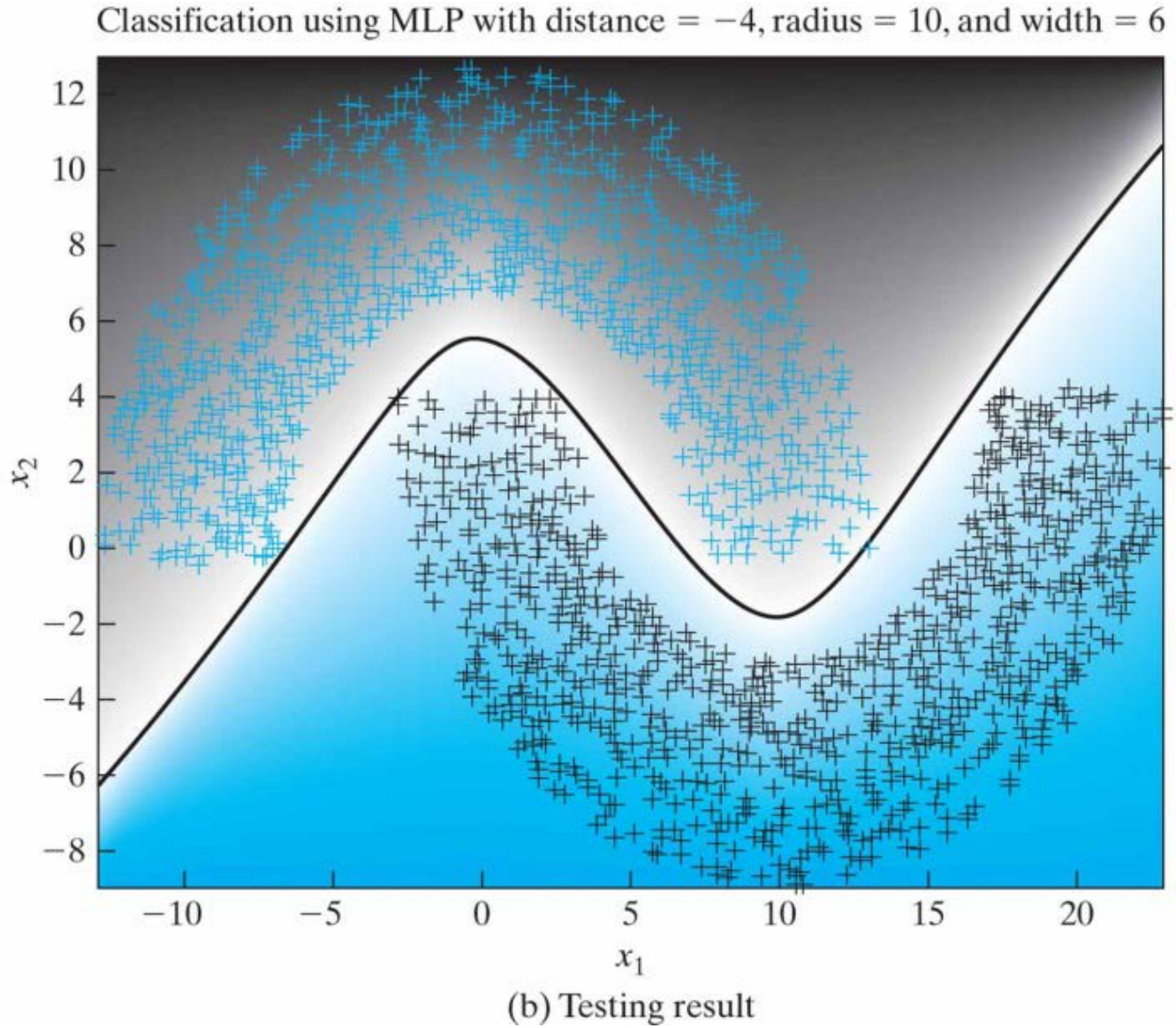
Must set several parameters to build an MLP

- Model parameters
  - Number of hidden layers
  - Number of units in each hidden layer
  - Activation function
  - Error function
- It is best to compare different settings empirically

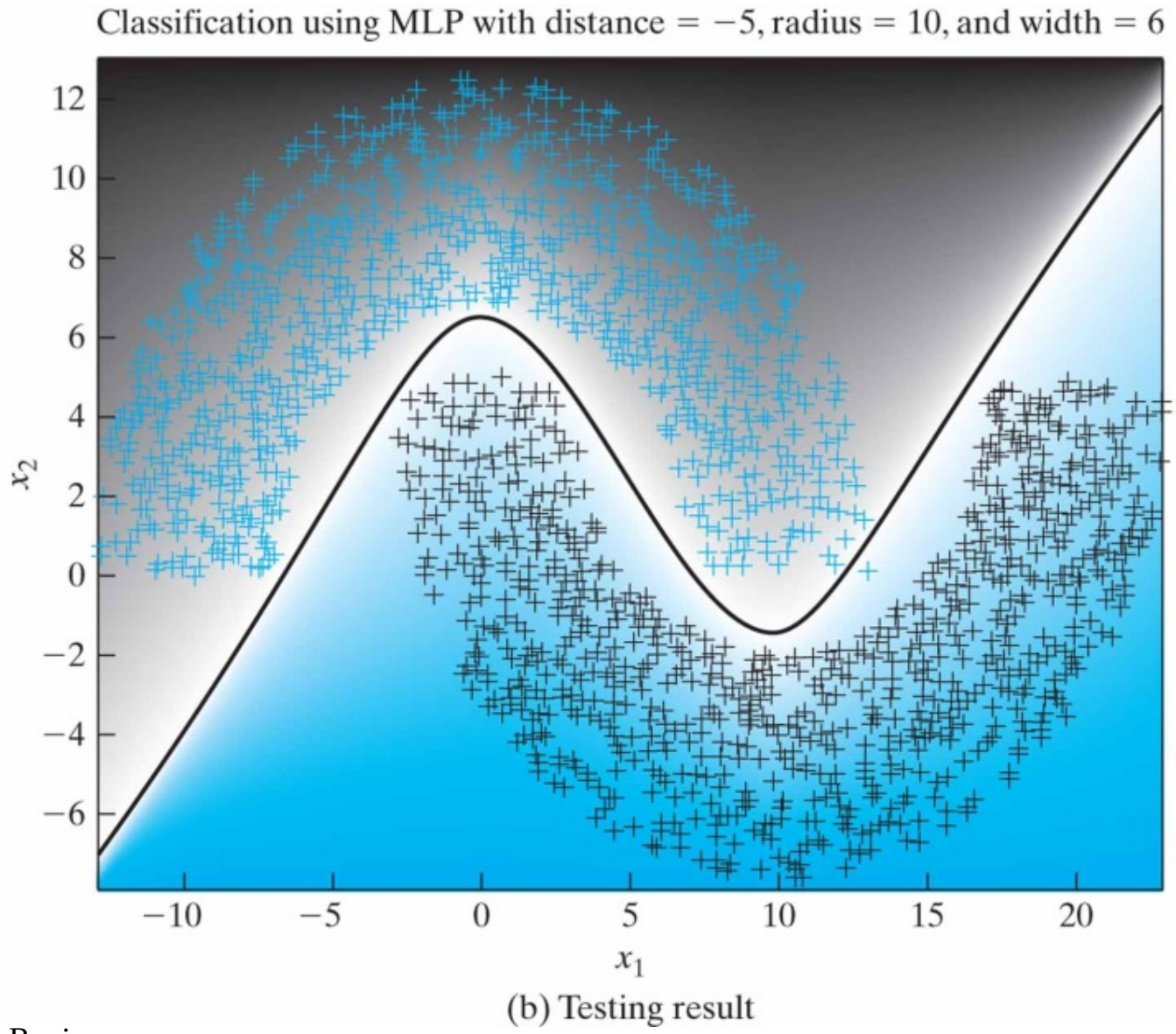
There are many optimization tricks for finding better local minima in backprop

- Momentum: mix in gradient from step $n - 1$
- Weight initialization: small random values
- Stopping criterion: early stopping
- Learning rate annealing: start large, slowly shrink
- Second order methods: use a separate η for each pair of parameters based on local curvature
- Randomize training example order
- Regularization: terms in $E(\boldsymbol{w})$ that only depend on $\boldsymbol{w}$

MLP learns double-moon, d = -4



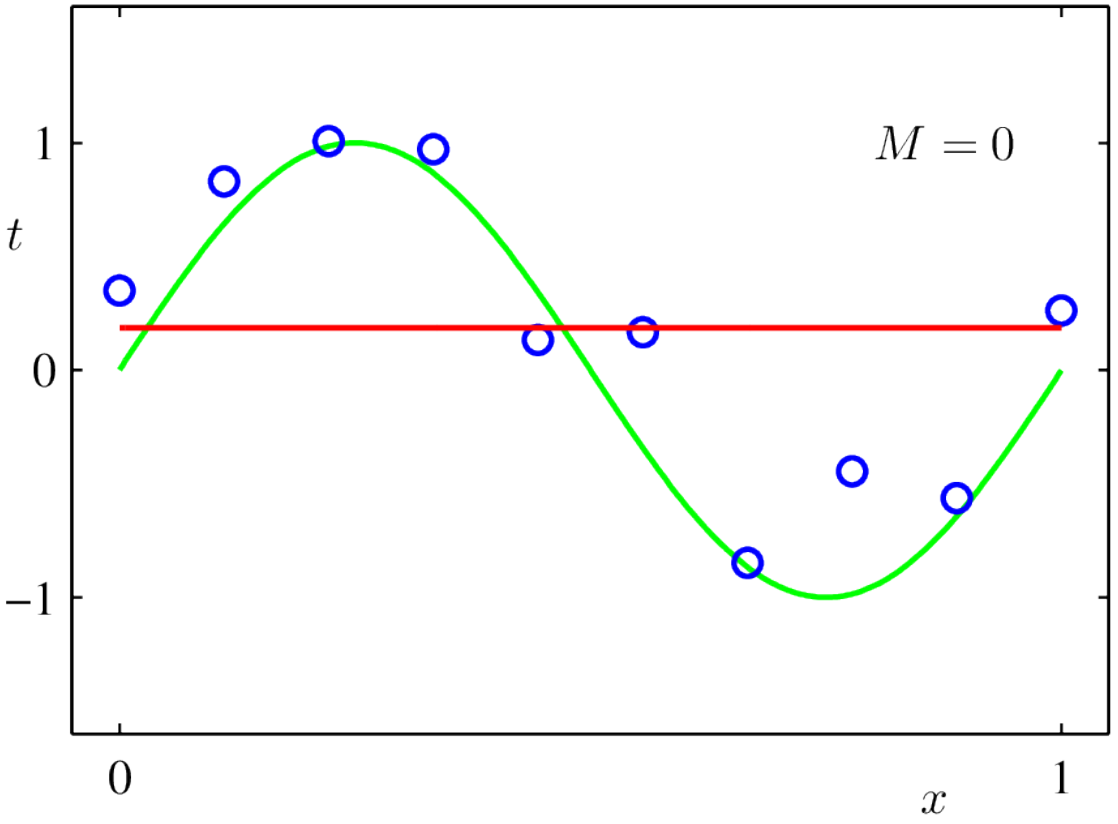
MLP learns double-moon, d = -5



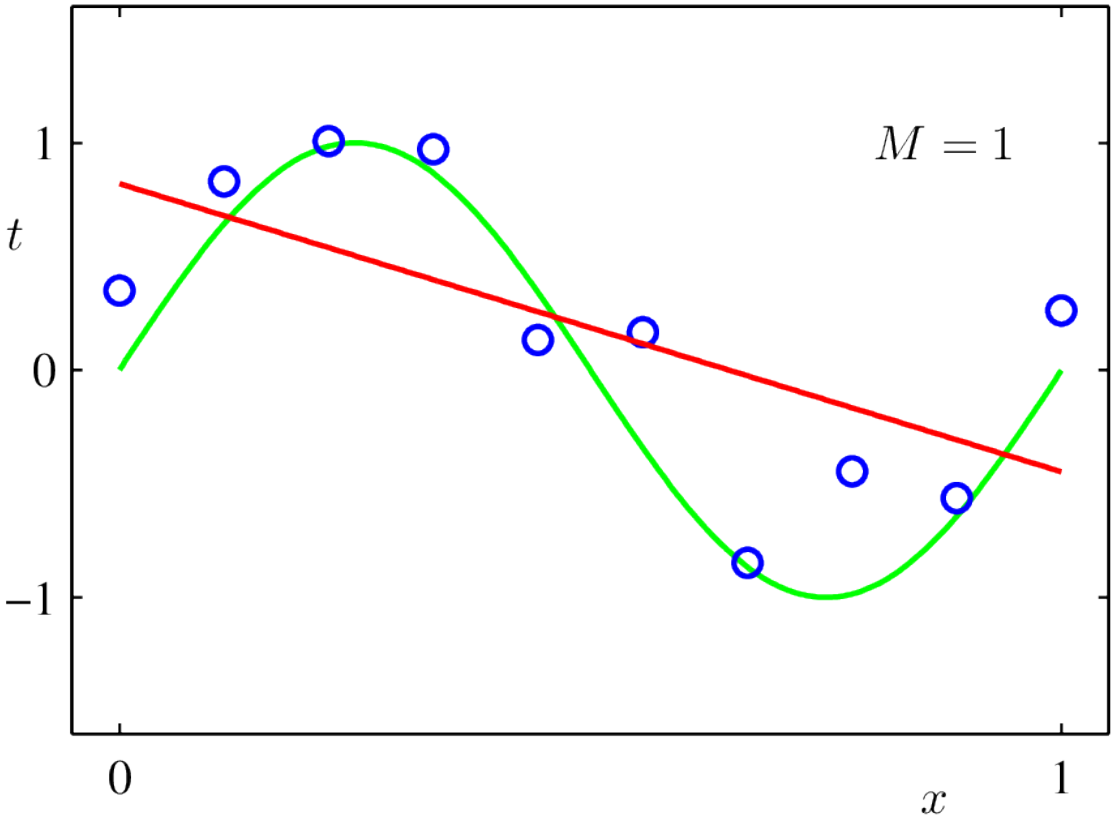
Our goal is to train models that generalize

- Models must be complex enough to capture important variations in the training data
- But not so complex that they capture the random variations in the training data
- We evaluate generalization by measuring performance on a held-out test or validation set

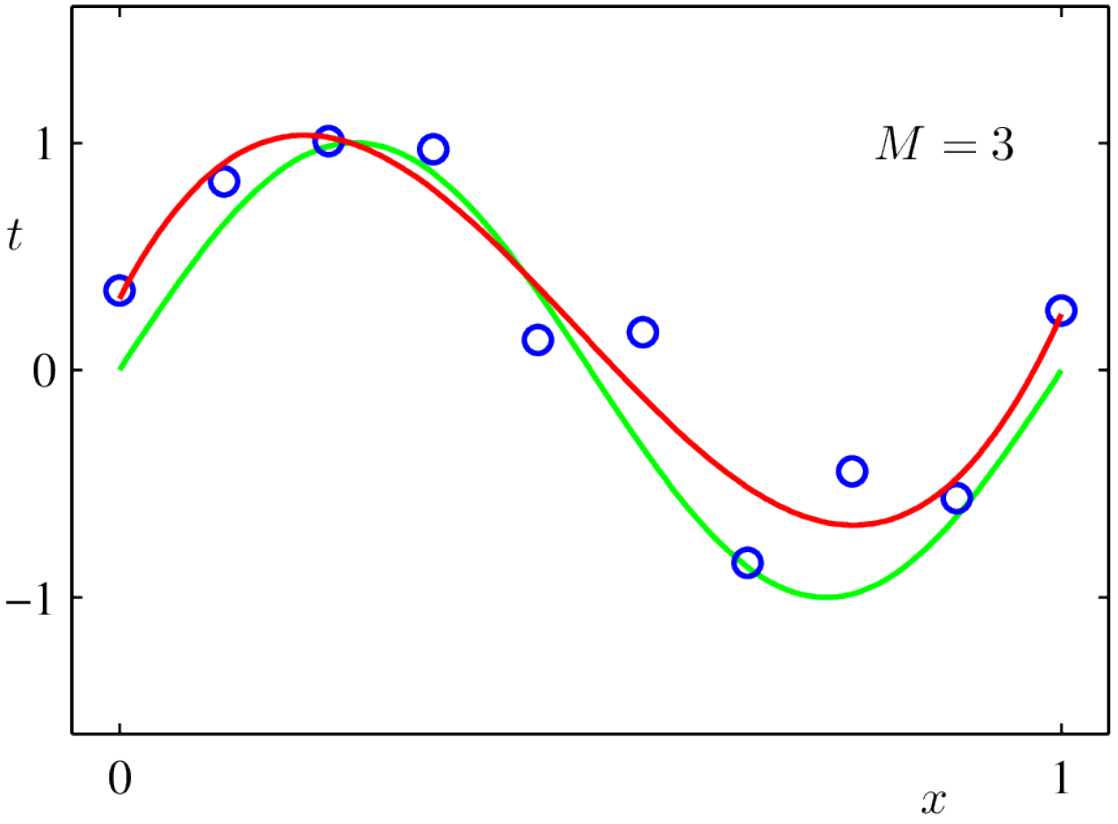
Polynomial of order 0
cannot capture important variations



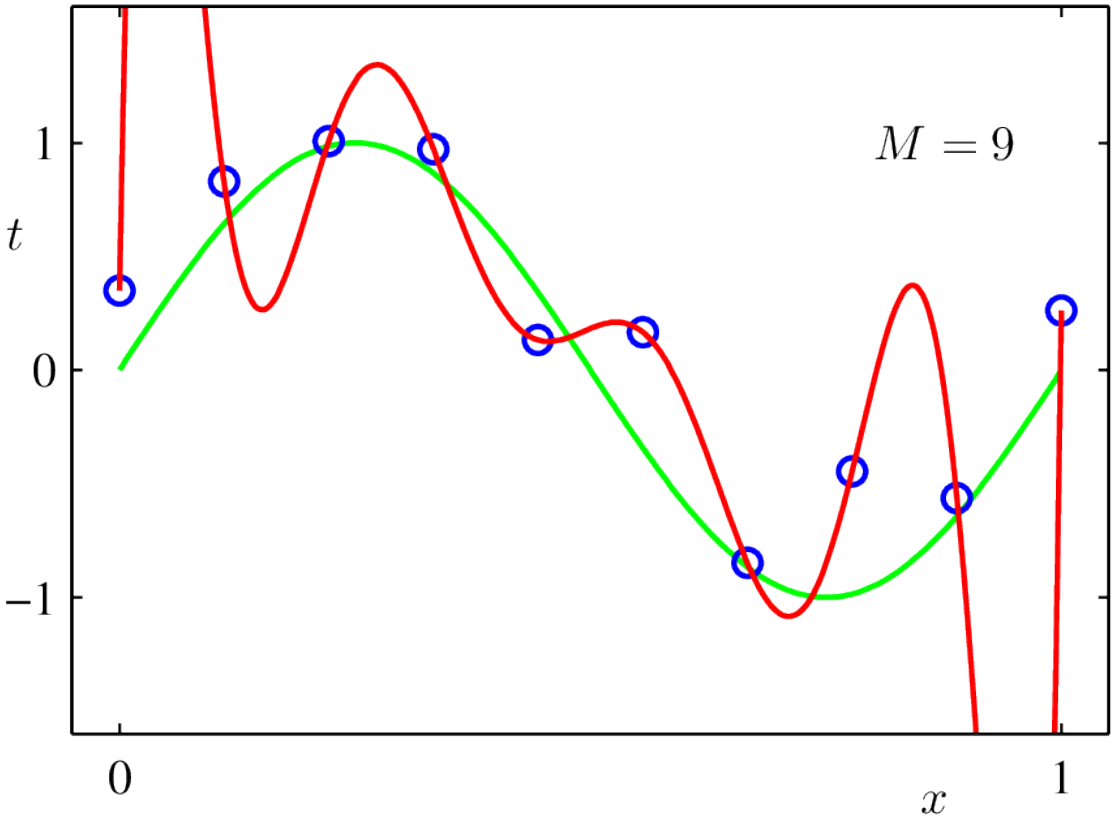
Polynomial of order 1
cannot capture important variations



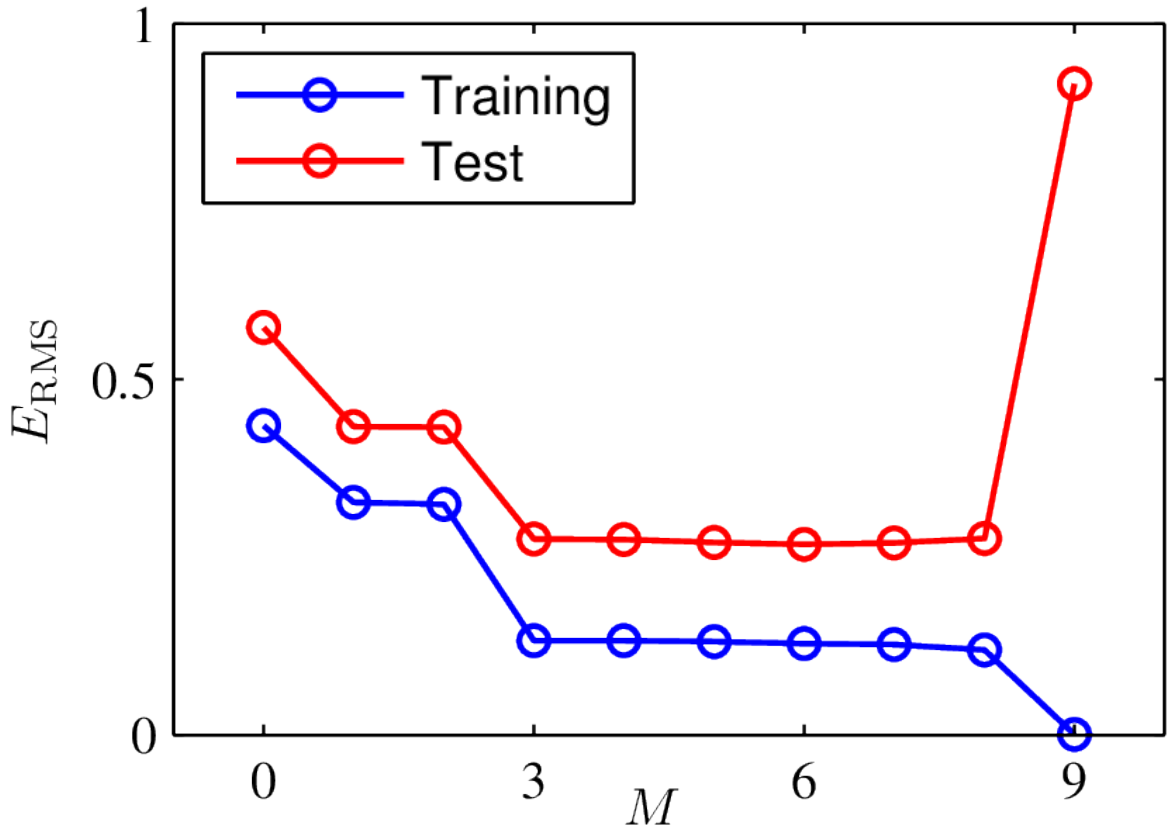
Polynomial of order 3 can capture important variations



Polynomial of order 9 captures unimportant variations

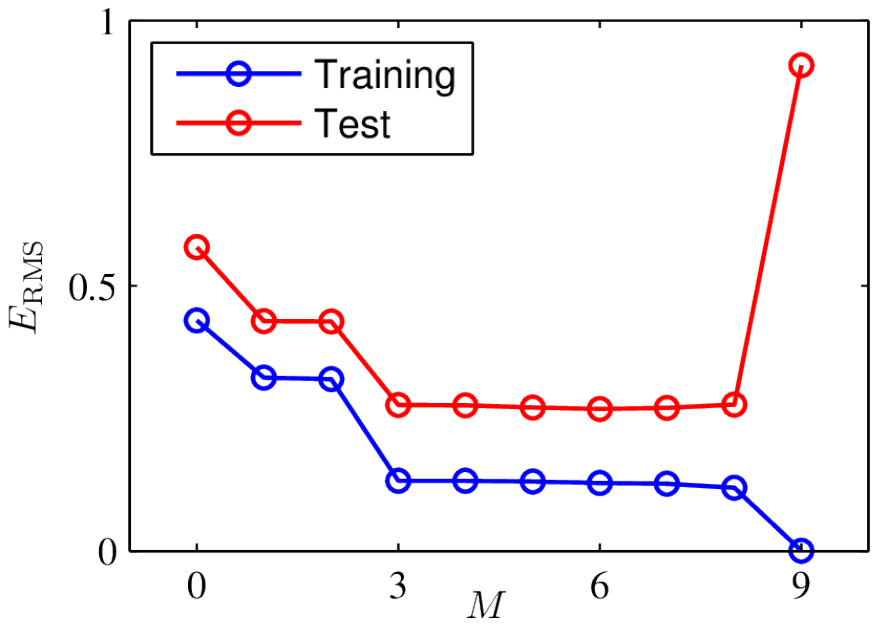


Learning curves can tell you whether a model is too complex or too simple



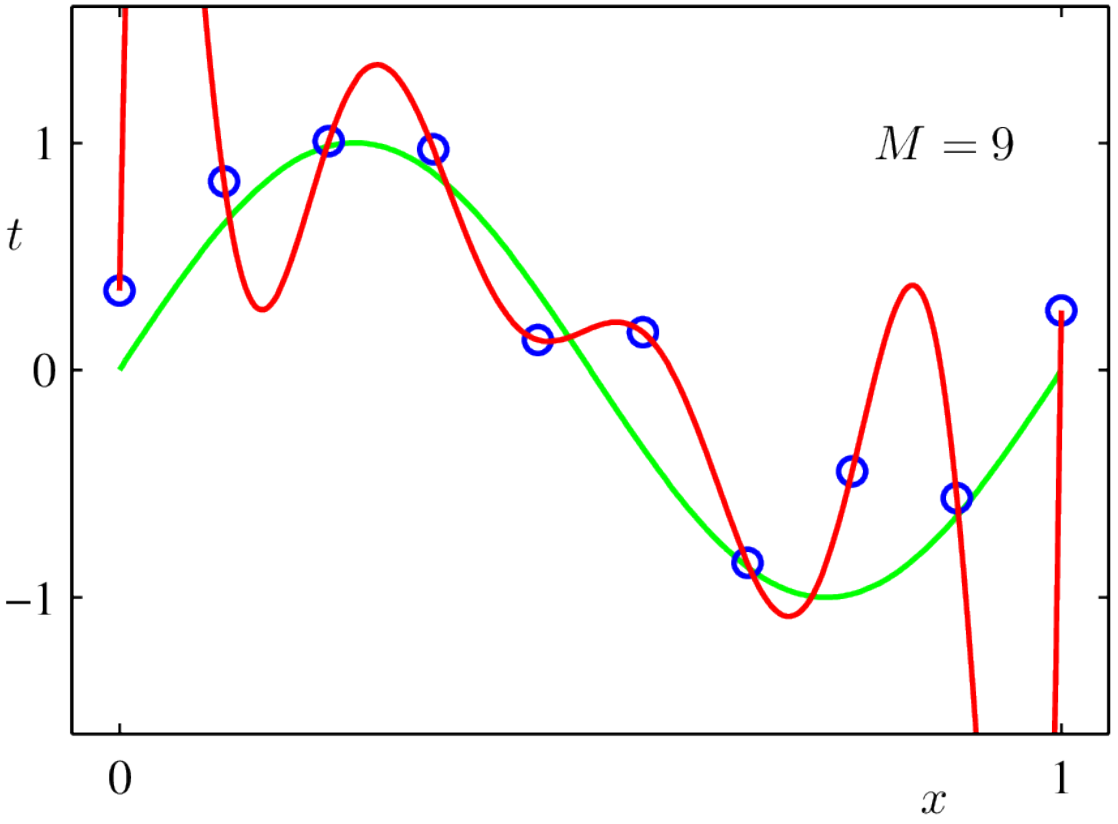
Simple models under-fit
complex models over-fit

	Under-fit	Good fit	Over-fit
Training error	High	Low	Low
Testing error	High	Low	High



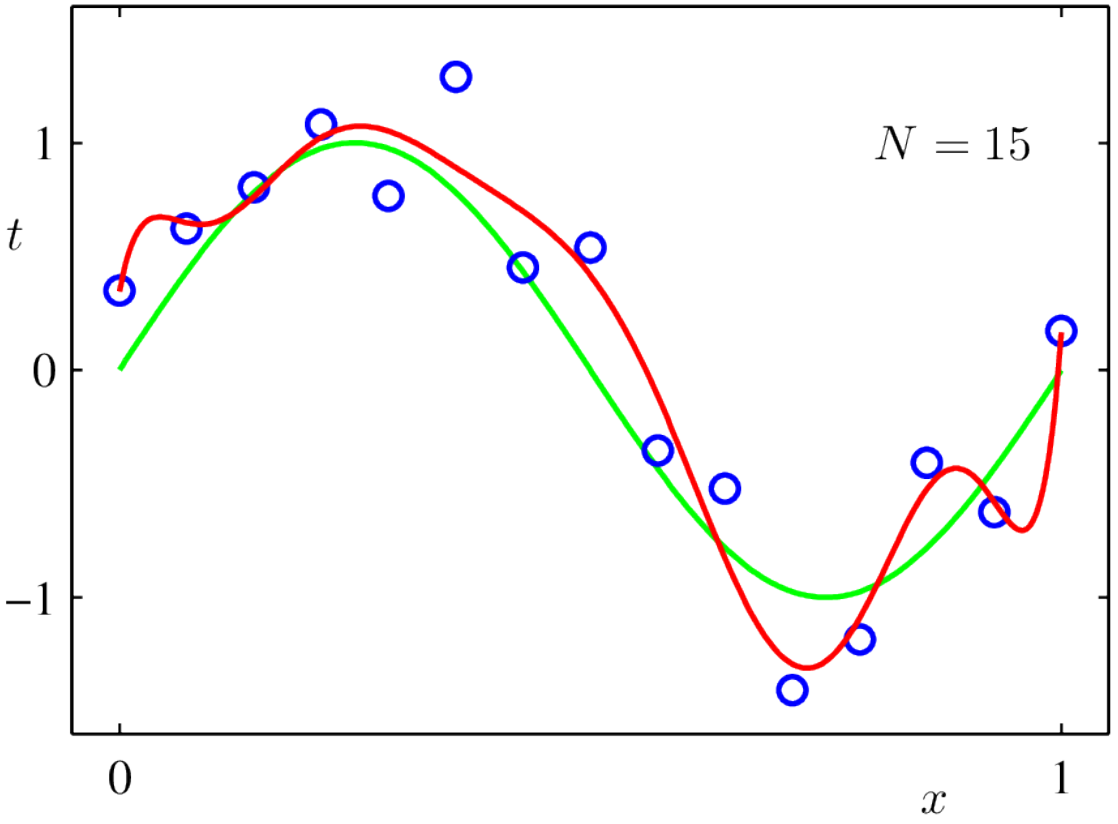
Fit is relative to the amount of training data

- Polynomial of order 9 fit to 10 points



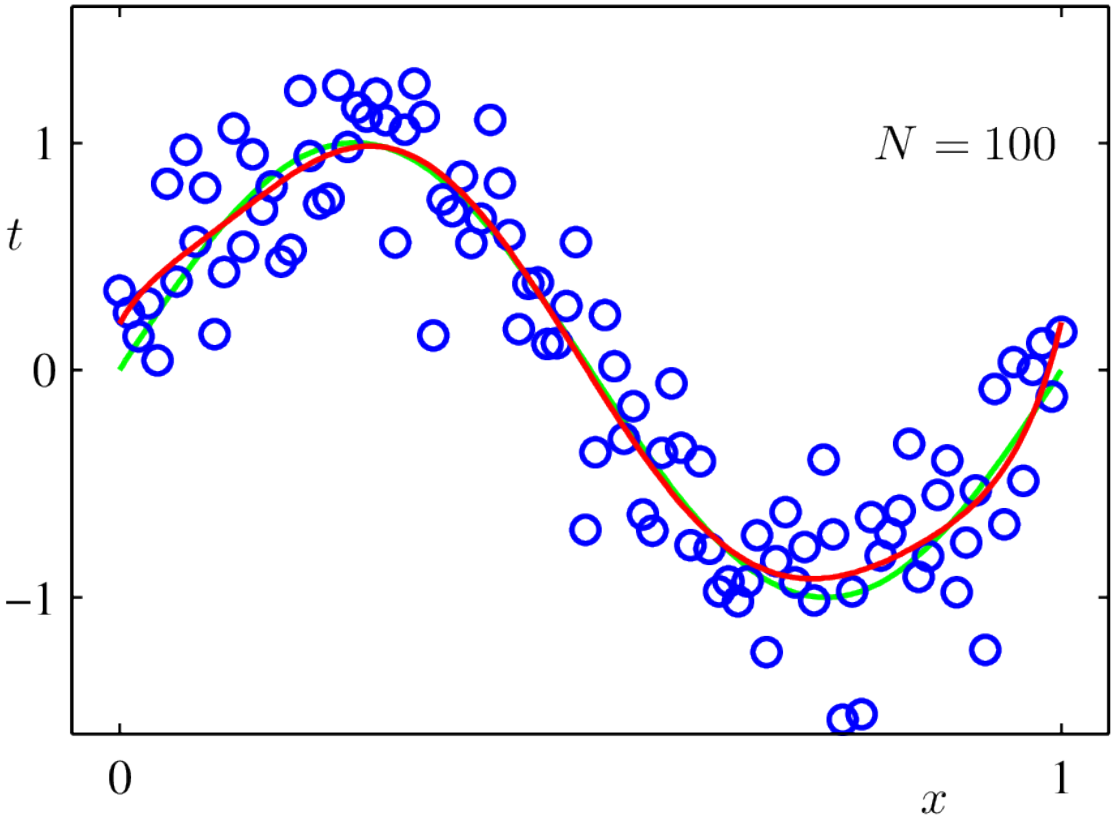
Fit is relative to the amount of training data

- Polynomial of order 9 fit to 15 points

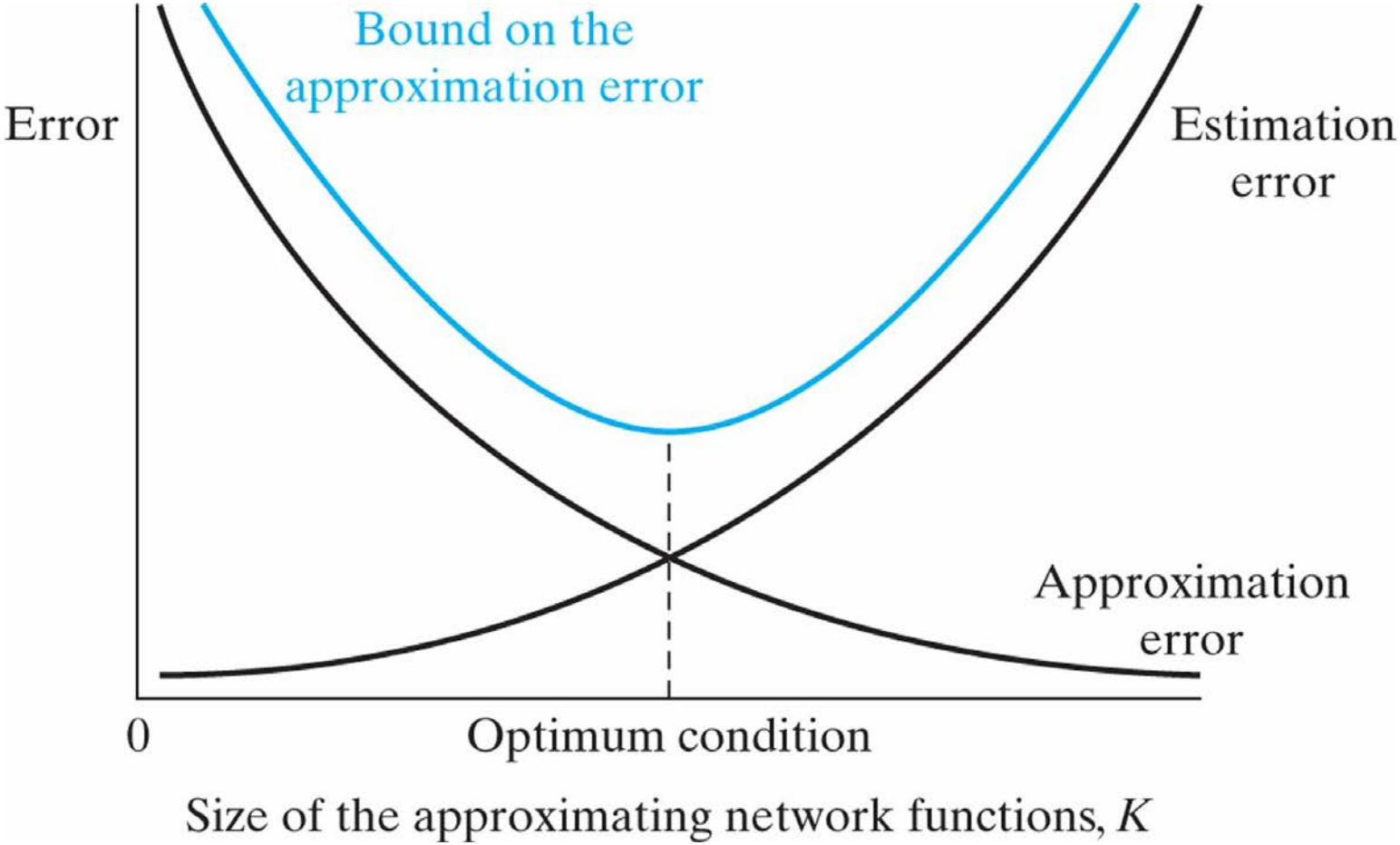


Fit is relative to the amount of training data

- Polynomial of order 9 fit to 100 points



Simple networks are dominated by bias complex networks are dominated by variance



Function approximation

- Think of the MSE as a measure of goodness of fit for function approximation
- We have discussed several function approximators

Model	$\boldsymbol{y_p = f(x_p)}$
M-P Neuron	$y = \text{signum}(\boldsymbol{w}^T \boldsymbol{x})$
Linear regression	$y = \boldsymbol{w}^T \boldsymbol{x}$
MLP	$y_k = \varphi\left(\sum_j w_{kj}\, \varphi\left(\sum_i w_{ji} x_i\right)_j\right)_k$
RBF network	$y = \sum_k w_k \varphi\left(\|\boldsymbol{x} - \boldsymbol{\mu}_k\|\right)$

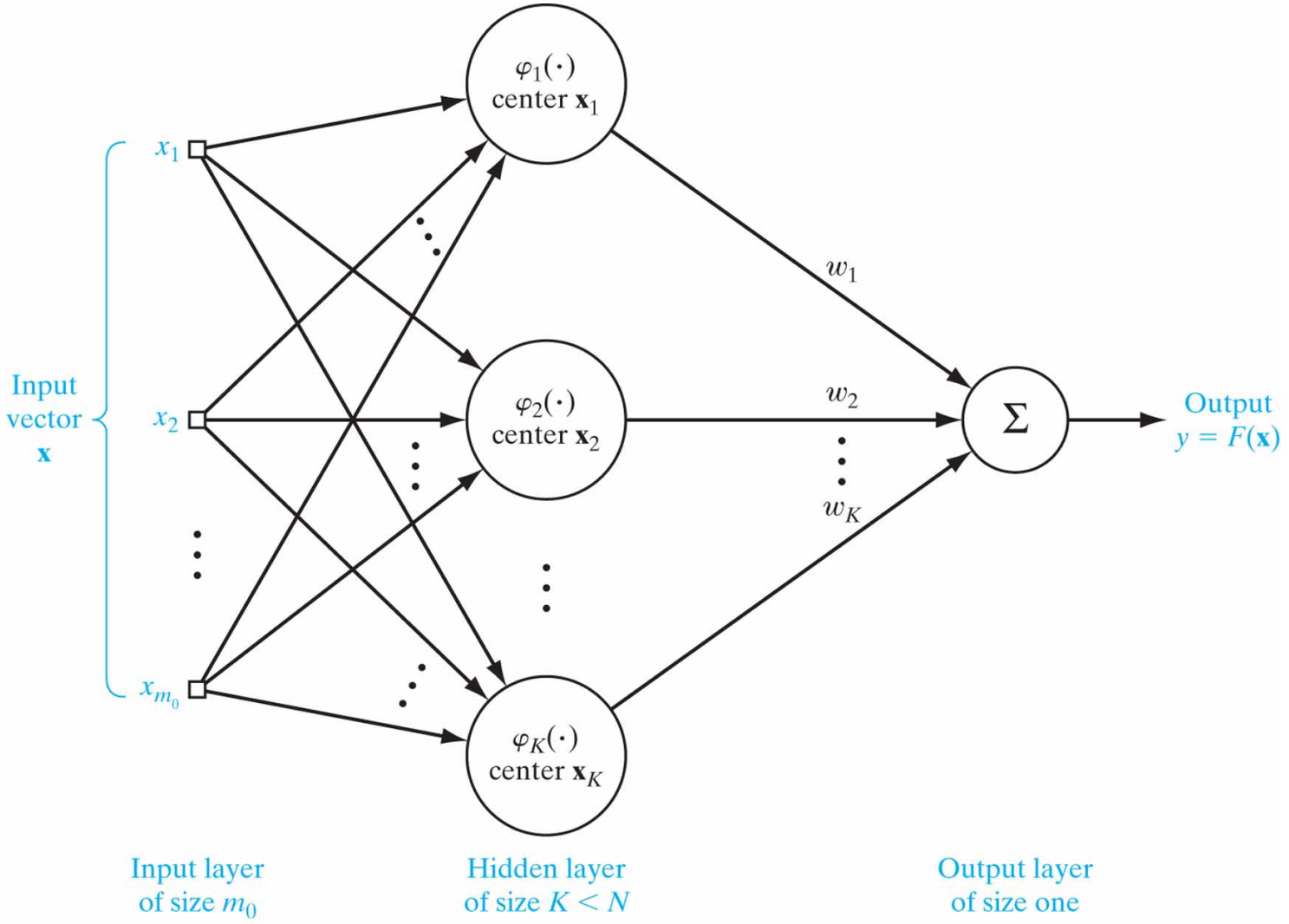
Linear projection computes weights for bases

- It is possible to approximate a function $f(\boldsymbol{x})$ by a linear combination of simpler functions

$$F(\boldsymbol{x}) = \sum_j w_j \varphi_j(\boldsymbol{x})$$

- If w_j's can be chosen so that approximation error is arbitrarily small for any function $f(\boldsymbol{x})$ over the domain of interest, then $\{\varphi_j\}$ has the property of universal approximation, or $\{\varphi_j\}$ is complete

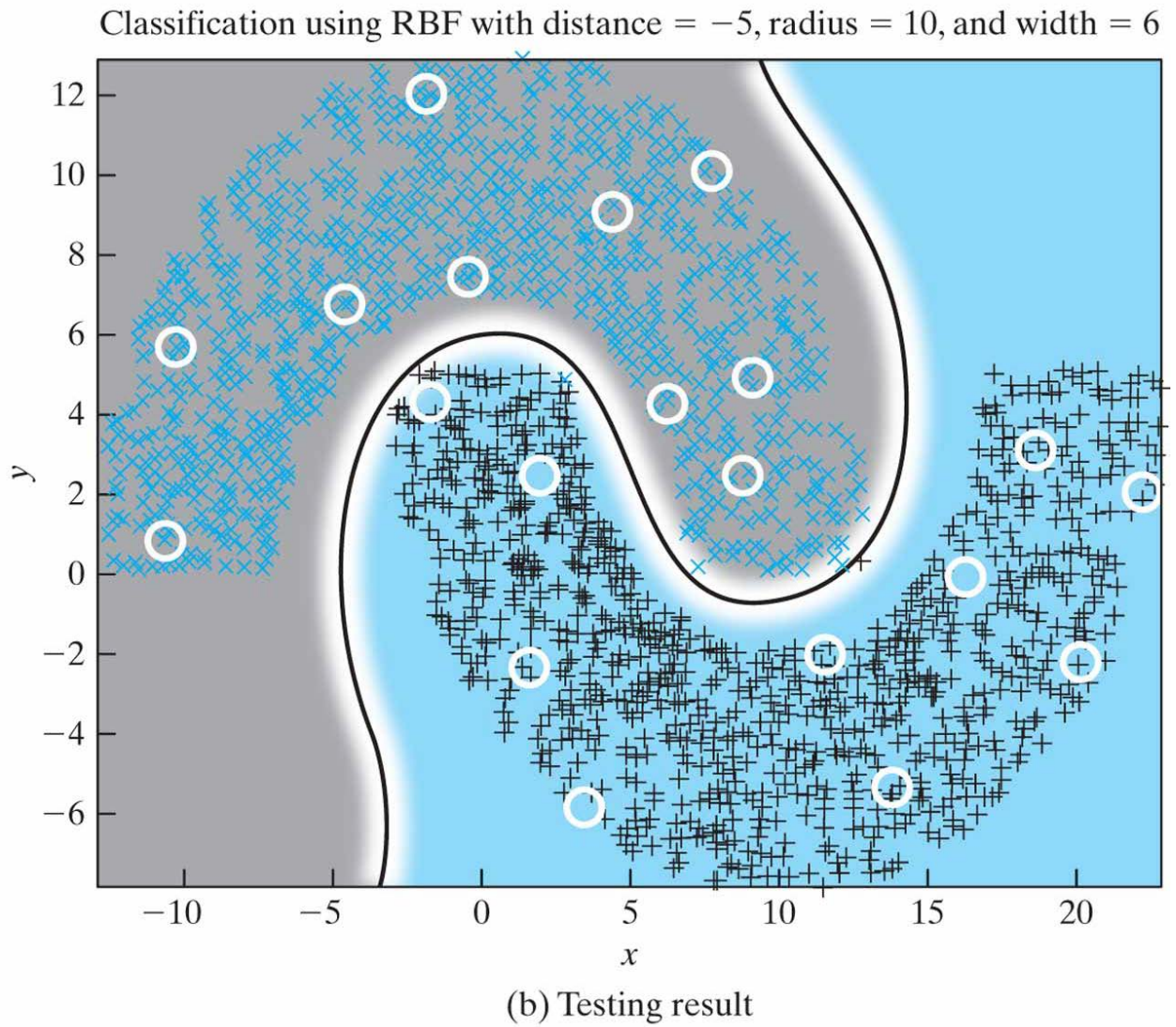
Radial basis function networks are similar to MLPs in structure



RBF nets are trained in three steps

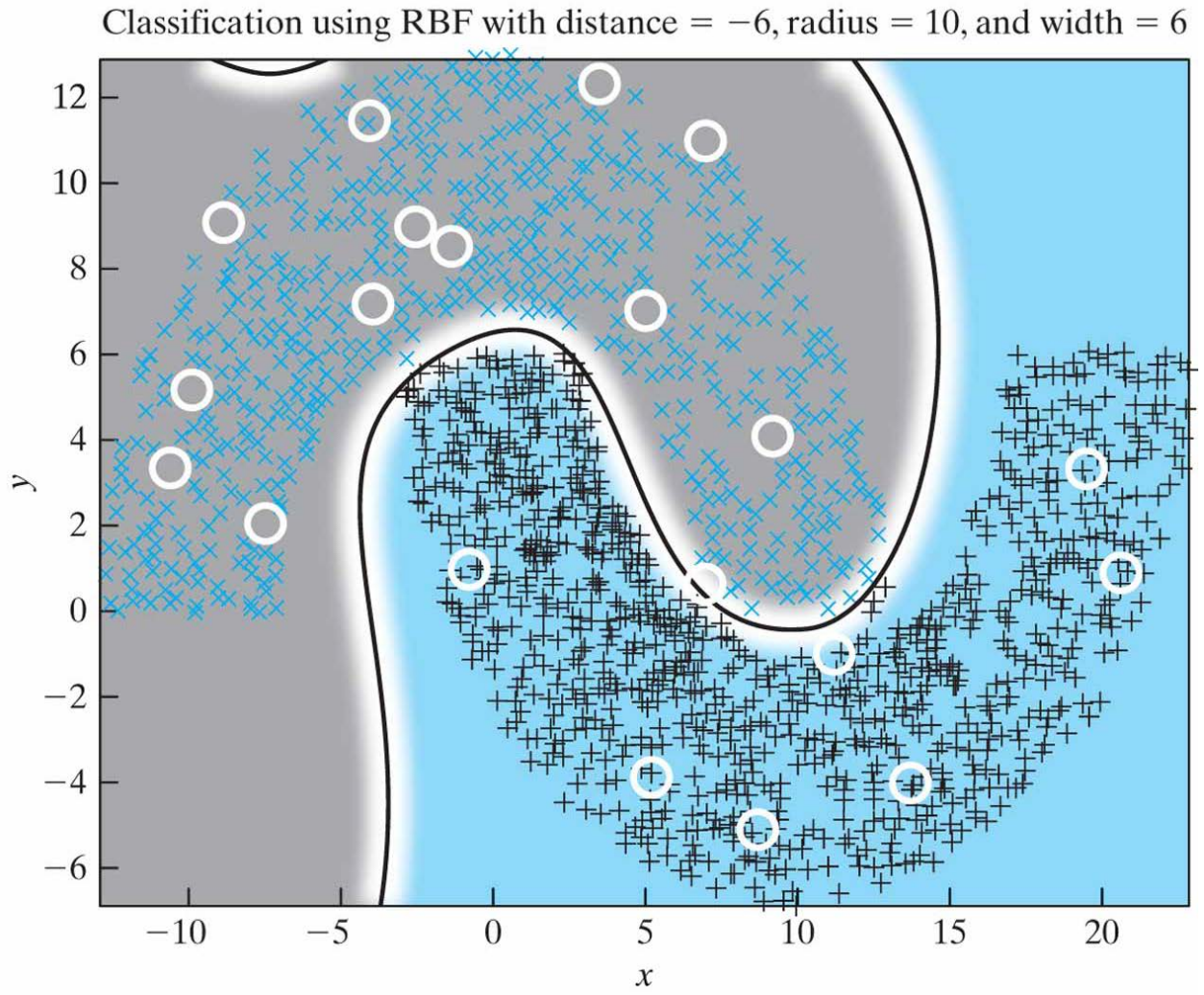
- To train
  1. Choose the Gaussian centers using *K*-means, etc.
  2. Determine the Gaussian widths as the variance of each cluster, or using $d_{\max}$
  3. Determine the weights w_j using linear regression
- Select the number of bases using (cross-)validation

RBF learns double-moon, d = -5



(b) Testing result

RBF net learns double-moon, d = -6



(b) Testing result