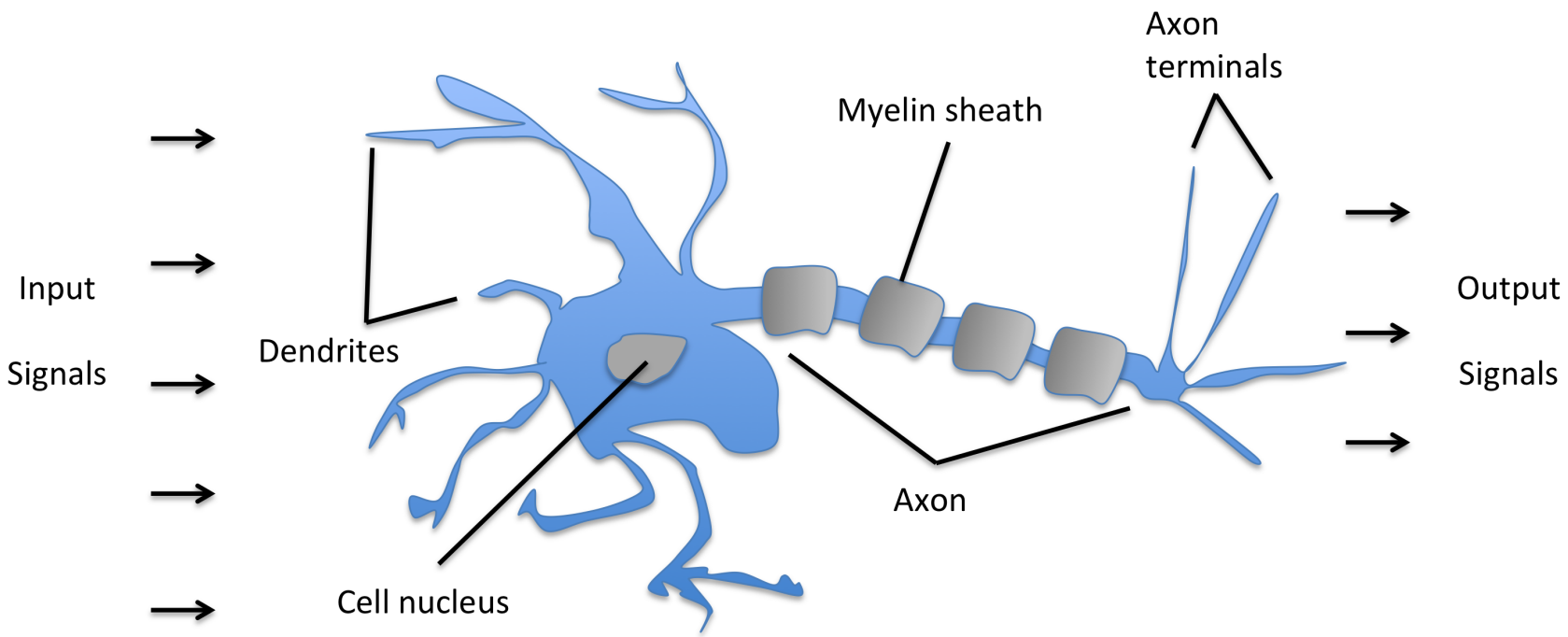
Chapter 2

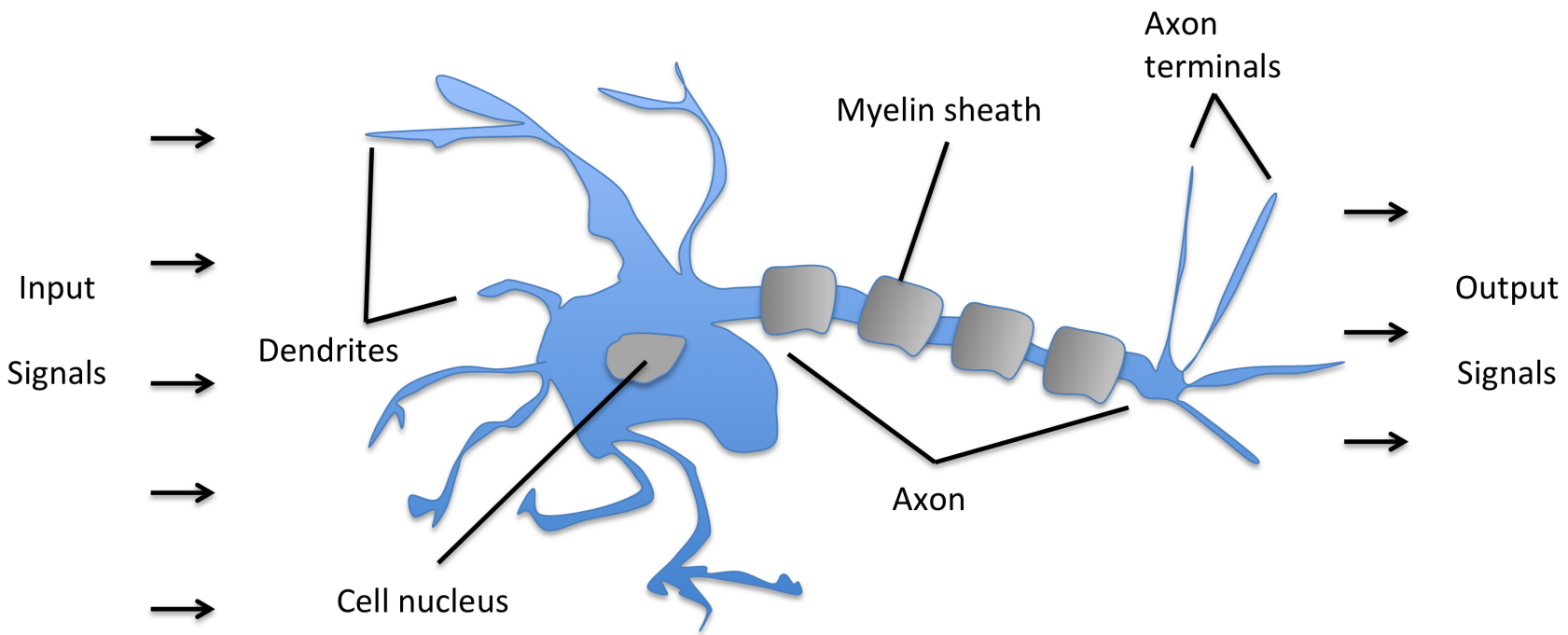
Training Machine Learning Algorithms for Classification

July 1, 2016

Biology


Axon
terminals
Myelin sheath
Input
Signals
Dendrites
Output
Signals
Axon
Cell nucleus

Logic Gate



- Simple logic gate with binary outputs
- Signals arrive at dendrites
- Integrated into cell body
- If signal exceeds threshold, generate output, and pass to axon

Rosenblatt Perceptron

- Binary classification task
- Positive class (1) vs. negative class (-1)
- Define activation function $\phi(z)$
- Takes as input a dot product of input and weights
- Net input: $z = w_1 x_1 + \cdots + w_m x_m$

$$\mathbf{w} = \begin{bmatrix} w^{(1)} \\ w^{(2)} \\ \vdots \\ w^{(m)} \end{bmatrix}, \mathbf{x} = \begin{bmatrix} x^{(1)} \\ x^{(2)} \\ \vdots \\ x^{(m)} \end{bmatrix}$$

Heaviside step function

- $\phi(z)$ known as activation
- if activation above some threshold, predict class 1
- predict class -1 otherwise

Heaviside Step Function

$$\phi(z) = \begin{cases} 1 & \text{if } z \geq \theta \\ -1 & \text{otherwise .} \end{cases}$$

Step function simplified

Bring the threshold θ to the left side of the equation and define a weight-zero as $w_0 = -\theta$ and $x_0 = 1$, so that we write $\mathbf{z}$ in a more compact form

$$z = w_0 x_0 + w_1 x_1 + \cdots + w_m x_m = \mathbf{w}^\mathbf{T} \mathbf{x}$$

and

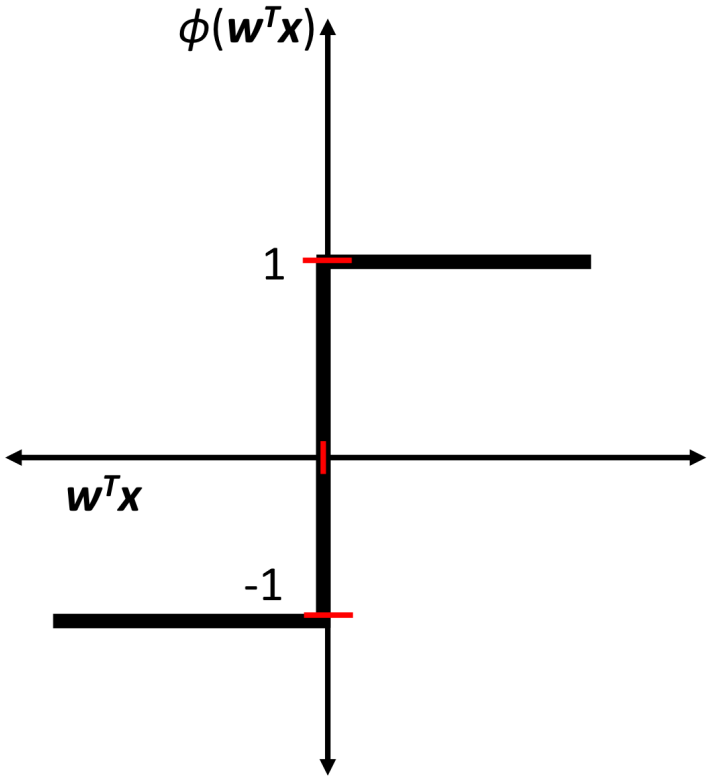
$$\phi(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ -1 & \text{otherwise .} \end{cases}$$

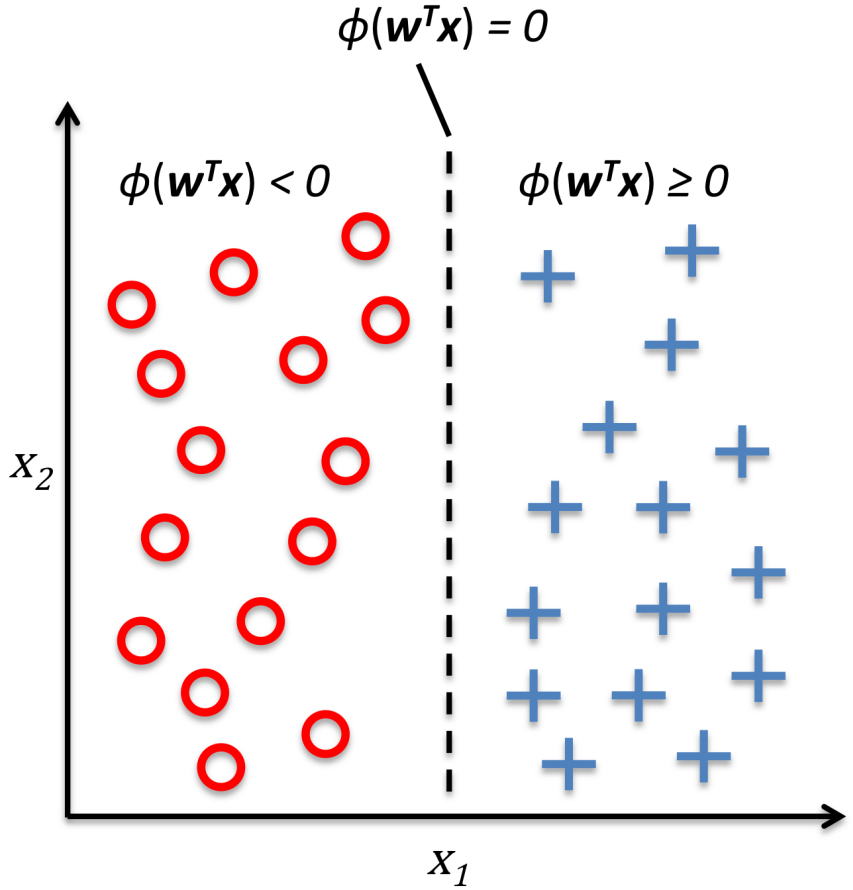
Vector dot product

$$z = \mathbf{w}^{\mathbf{T}}\mathbf{x} = \sum_{j=0}^{m} \mathbf{w_j x_j}$$

$$\begin{bmatrix} 1 & 2 & 3 \end{bmatrix} \times \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} = 1 \times 4 + 2 \times 5 + 3 \times 6 = 32.$$

Input squashed into a binary output





Rosenblatt perceptron algorithm

1. Initialize the weights to 0 or small random numbers.
2. For each training sample $\mathbf{x}^{(i)}$, perform the following steps:
   1. Compute the output value $\hat{y}$.
   2. Update the weights.

Weight update

Weight update rule:

$$w_j := w_j + \Delta w_j$$

Perceptron learning rule:

$$\Delta w_j = \eta \left(y^{(i)} - \hat{y}^{(i)} \right) x_j^{(i)}$$

Where η is the learning rate (a constant between 0.0 and 1.0), $y^{(i)}$ is the true class label of the ith training sample, and $\hat{y}^{(i)}$ is the predicted class label.

Update rule examples

Correct prediction, weights unchanged:

$$\Delta w_j = \eta\Big(-1 - -1 \Big) x_j^{(i)} = 0$$

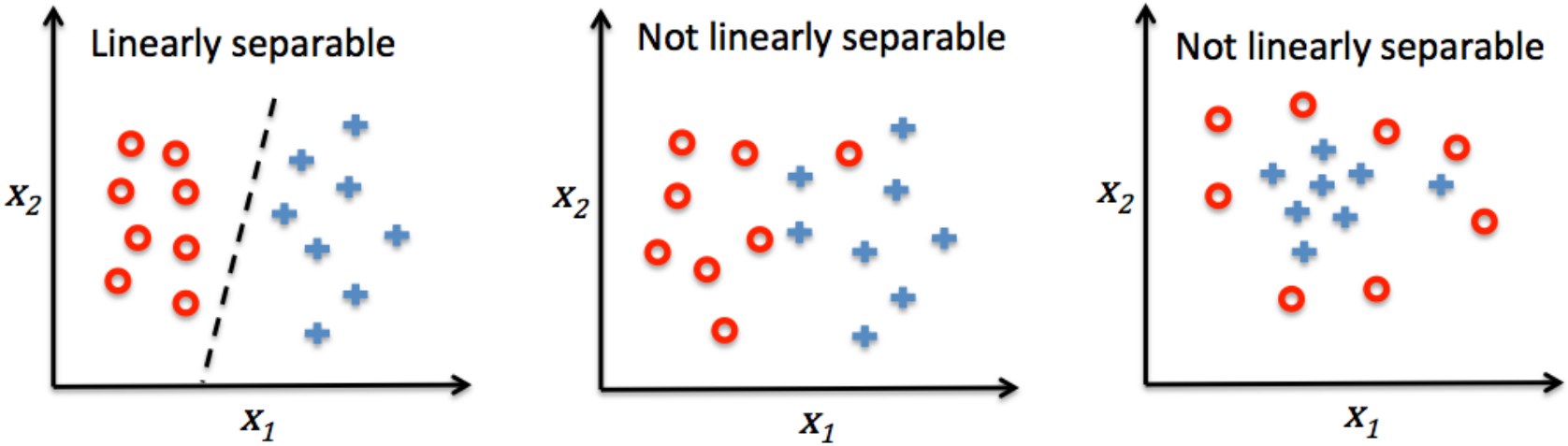
$$\Delta w_j = \eta\Big(1 - 1 \Big) x_j^{(i)} = 0$$

Wrong prediction, weights pushed towards the positive or negative class:

$$\Delta w_j = \eta\Big(1 - -1 \Big) x_j^{(i)} = \eta(2) x_j^{(i)}$$

$$\Delta w_j = \eta\Big(-1 - 1 \Big) x_j^{(i)} = \eta(-2) x_j^{(i)}$$

Linear separability



Convergence

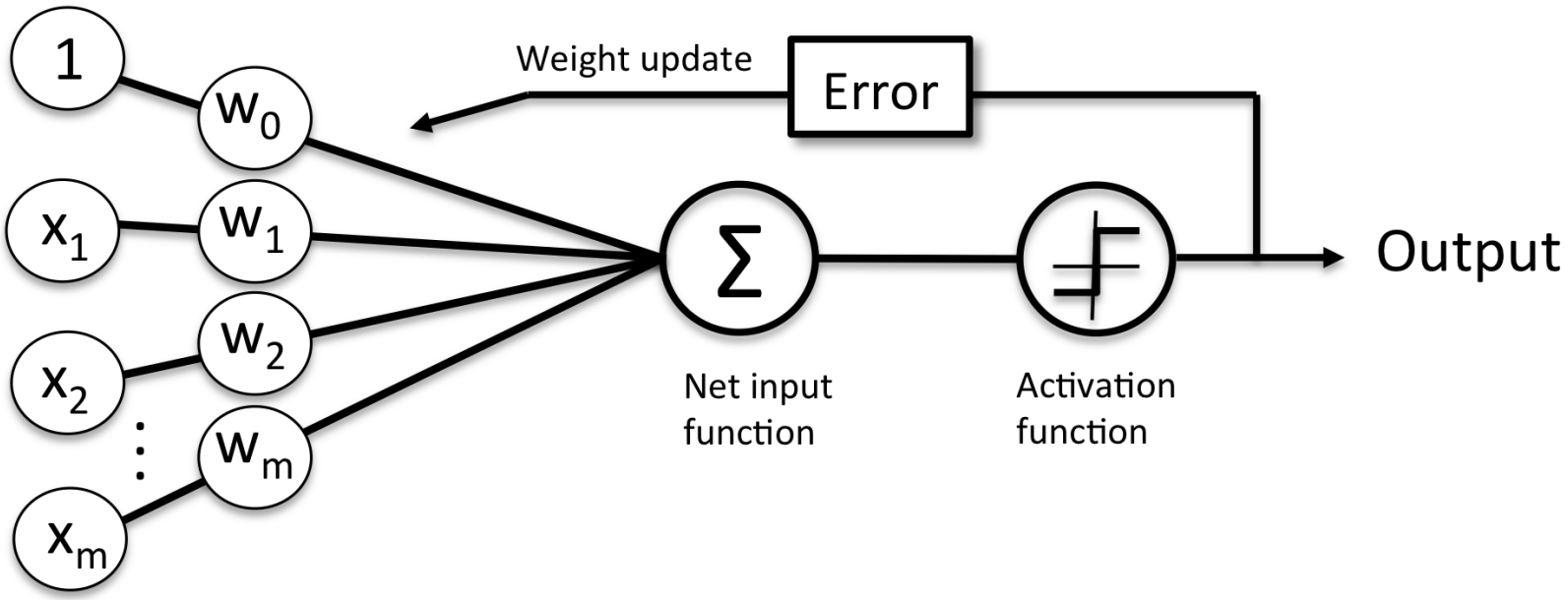
Convergence guaranteed if

- The two classess linearly separable
- Learning rate is sufficiently small

If classes cannot be seprated:

- Set a maximum number of passes over the training dataset (epochs)
- Set a threshold for the number of tolerated misclassifications
- Otherwise, it will never stop updating weights (converge)

Linear separability



Perceptron implementation

- iPython notebook on github

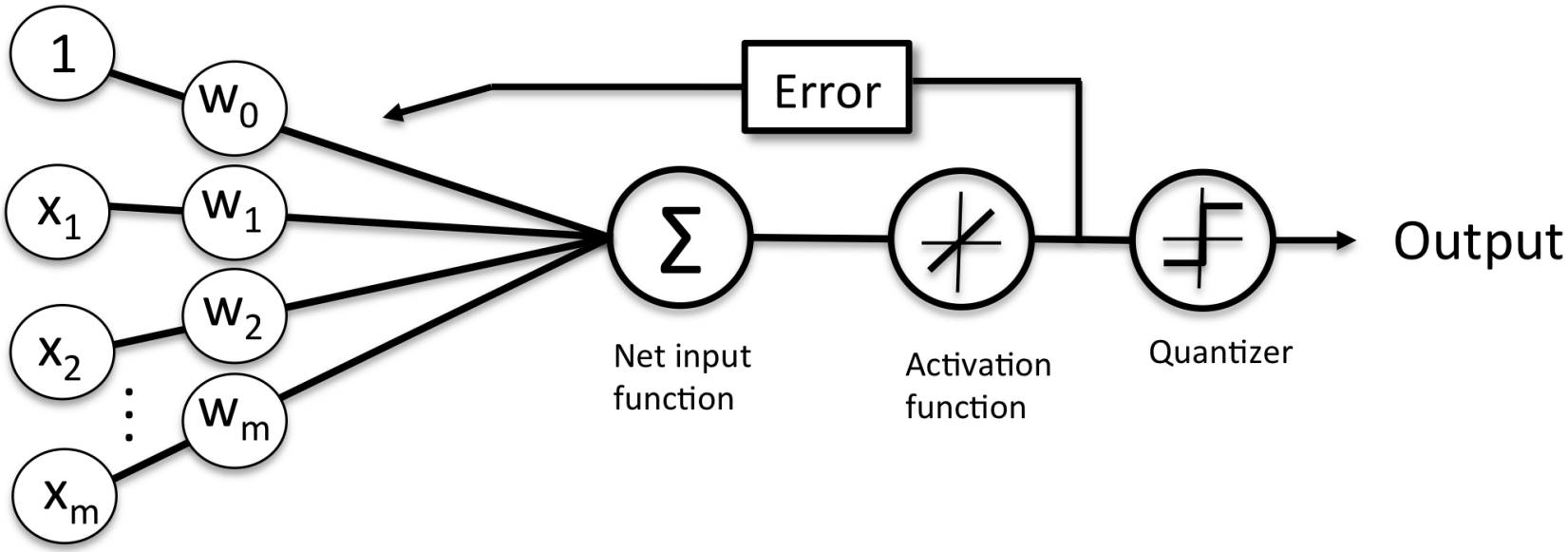
ADAPtive LInear NEuron (Adaline)

- Weights updated based on a linear activation function
- Remember that perceptron used a unit step function
- $\phi(z)$ is simply the identity function of the net input

$$\phi(\mathbf{w}^T\mathbf{x}) = \mathbf{w}^T\mathbf{x}$$

- A quantizer is then used to predict class label

Adaline: notice the difference with perceptron



Cost functions

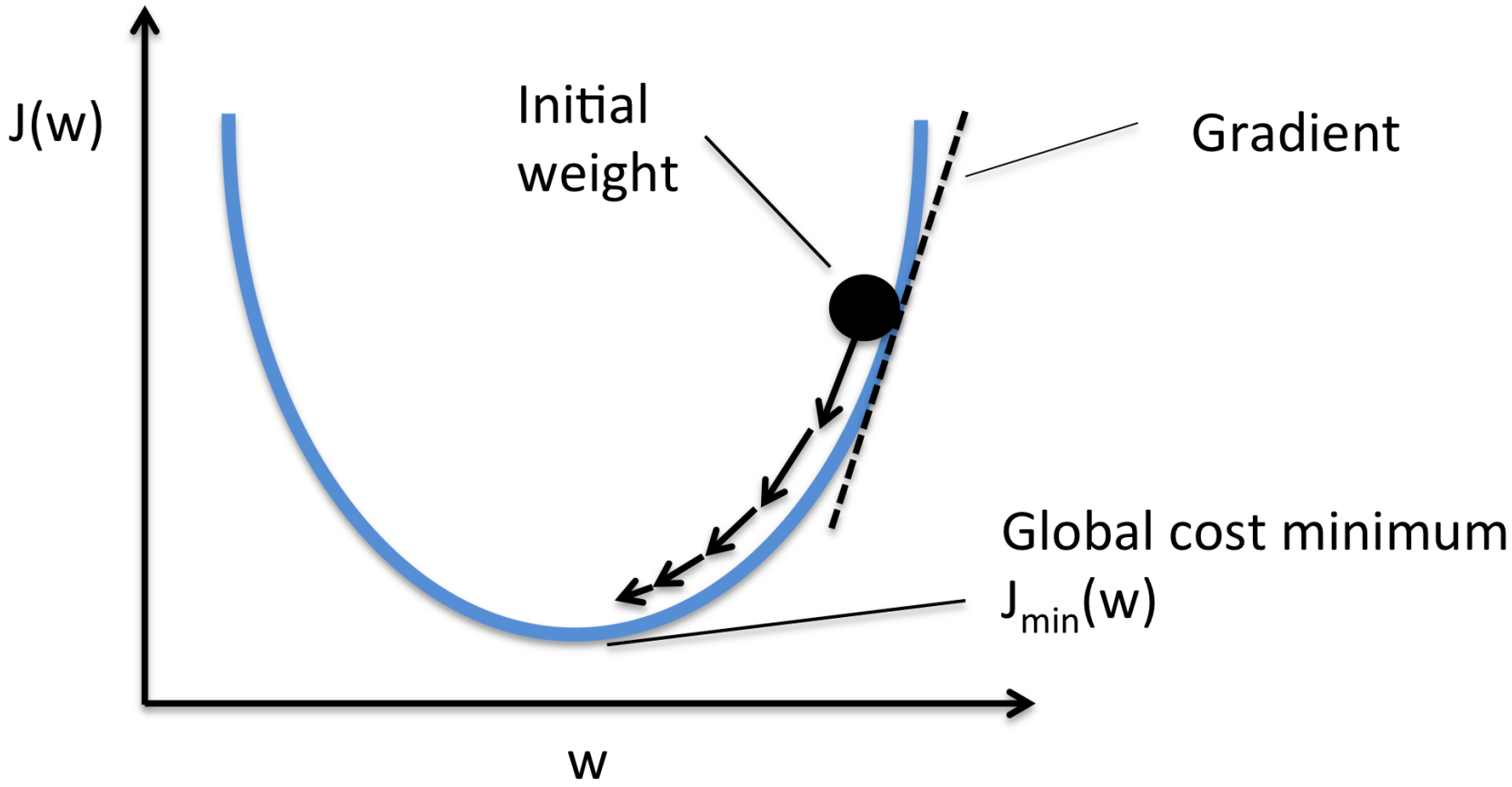
- ML algorithms often define an *objective* function
- This function is optimized during learning
- It is often a *cost* function we want to minimize
- Adaline uses a cost function $J(\cdot)$
- Learns weights as the sum of squared errors (SSE)

$$J(\mathbf{w}) = \frac{1}{2} \sum_i \left(y^{(i)} - \phi\left(z^{(i)}\right) \right)^2$$

Advantages of Adaline cost function

- The linear activation function is differentiable
- Unlike the unit step function
- It is convex
- Can use *gradient descent* to learn the weights

Gradient Descent



Gradient Descent

- Weights updated by taking small steps
- Step size determined by learning rate
- Take a step away from the gradient $\nabla J(\mathbf{w})$ of the cost function

$$\mathbf{w} := \mathbf{w} + \Delta\mathbf{w}.$$

- The weight change is defined as follows:

$$\Delta\mathbf{w} = -\eta\nabla J(\mathbf{w})$$

Gradient computation

To compute the gradient of the cost function, we need to compute the partial derivative of the cost function with respect to each weight w_j,

$$\frac{\partial J}{\partial w_j} = -\sum_i \Big(y^{(i)} - \phi\big(z^{(i)}\big)\Big) x_j^{(i)},$$

Weight update of weight w_j

$$\Delta w_j = -\eta \frac{\partial J}{\partial w_j} = \eta \sum_i \Big(y^{(i)} - \phi\big(z^{(i)}\big)\Big) x_j^{(i)}$$

We update all weights simultaneously, so Adaline learning rule becomes

$$\mathbf{w} := \mathbf{w} + \Delta \mathbf{w}.$$

Partial derivatives

$$\frac{\partial J}{\partial w_j} = \frac{\partial}{\partial w_j}\frac{1}{2}\sum_i \left(y^{(i)} - \phi\left(z^{(i)}\right)\right)^2$$

$$= \frac{1}{2}\frac{\partial}{\partial w_j}\sum_i \left(y^{(i)} - \phi\left(z^{(i)}\right)\right)^2$$

$$= \frac{1}{2}\sum_i 2\left(y^{(i)} - \phi(z^{(i)})\right)\frac{\partial}{\partial w_j}\left(y^{(i)} - \phi(z^{(i)})\right)$$

$$= \sum_i \left(y^{(i)} - \phi(z^{(i)})\right)\frac{\partial}{\partial w_j}\left(y^{(i)} - \sum_i \left(w_j^{(i)} x_j^{(i)}\right)\right)$$

$$= \sum_i \left(y^{(i)} - \phi\left(z^{(i)}\right)\right)\left(-x_j^{(i)}\right)$$

$$= -\sum_i \left(y^{(i)} - \phi\left(z^{(i)}\right)\right)x_j^{(i)}$$

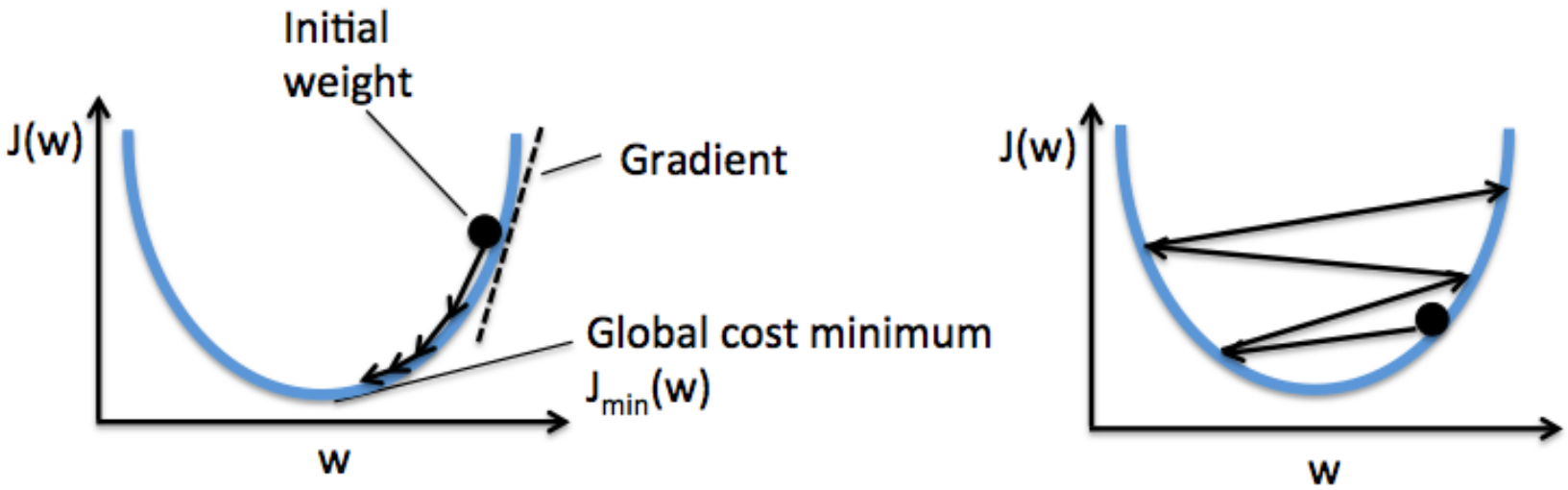
Adaline learning rule vs. Perceptron rule

- Looks identical
- $\phi(z^{(i)})$ with $z^{(i)} = \mathbf{w}^T \mathbf{x}^{(i)}$ is a real number
- And not an integer class label as in Perceptron
- The weight update is done based on *all* samples in training set
- Perceptron updates weights incrementally after each sample
- This approach is known as "batch" gradient descent

Perceptron implementation

- iPython notebook on github

Lessons learned



- Learning rate too high: error becomes larger (overshoots global min)
- Learning rate too low: takes many epochs to converge
- Feature normalization

Stochastic gradient descent (SGD)

- Large dataset with millions of data points ("big data")
- Batch gradient descent costly
- Need to compute the error for the entire dataset ...
- ... to take one step towards the global minimum!

$$\Delta \mathbf{w} = \eta \sum_i \left(y^{(i)} - \phi\left(z^{(i)}\right) \right) \mathbf{x}^{(i)}.$$

- SGD updates the weights incrementally for each training sample

$$\Delta \mathbf{w} = \eta \left(y^{(i)} - \phi\left(z^{(i)}\right) \right) \mathbf{x}^{(i)}.$$

SGD details

- Approximation of gradient descent
- Reaches convergence faster because of frequent weight updates
- Important to present data in random order
- Learning rate often gradually decreased (adaptive learning rate)
- Can be used for online learning
- Middle ground between SGD and batch GD is known as *mini-batch learning*
  - E.g. 50 examples at a time
  - Can use vector/matrix operations rather than loops as in SGD
  - Vectorized operations highly efficient