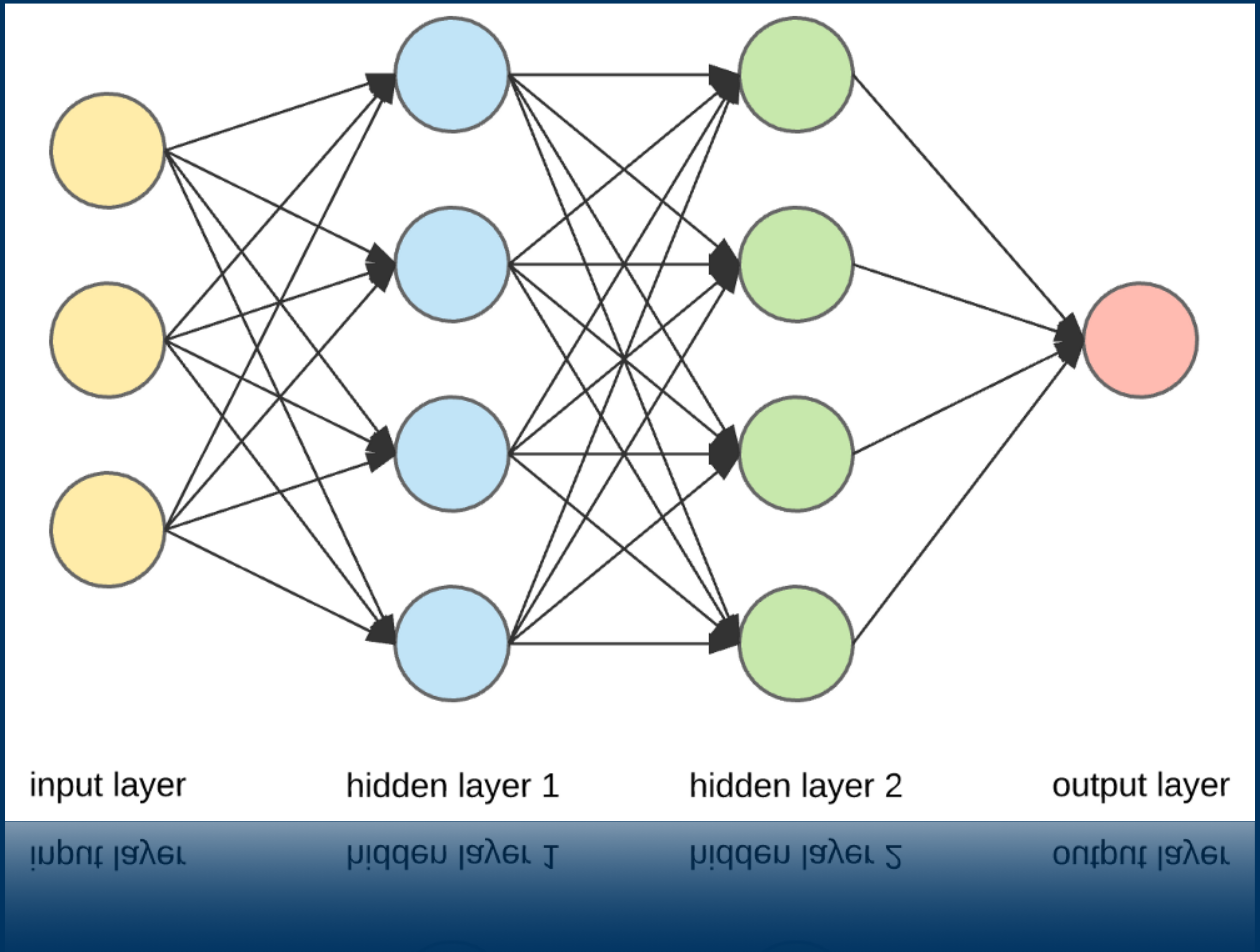


Neural Networks II

CSCI-P556 Applied Machine Learning
Lecture 14

D.S. Williamson

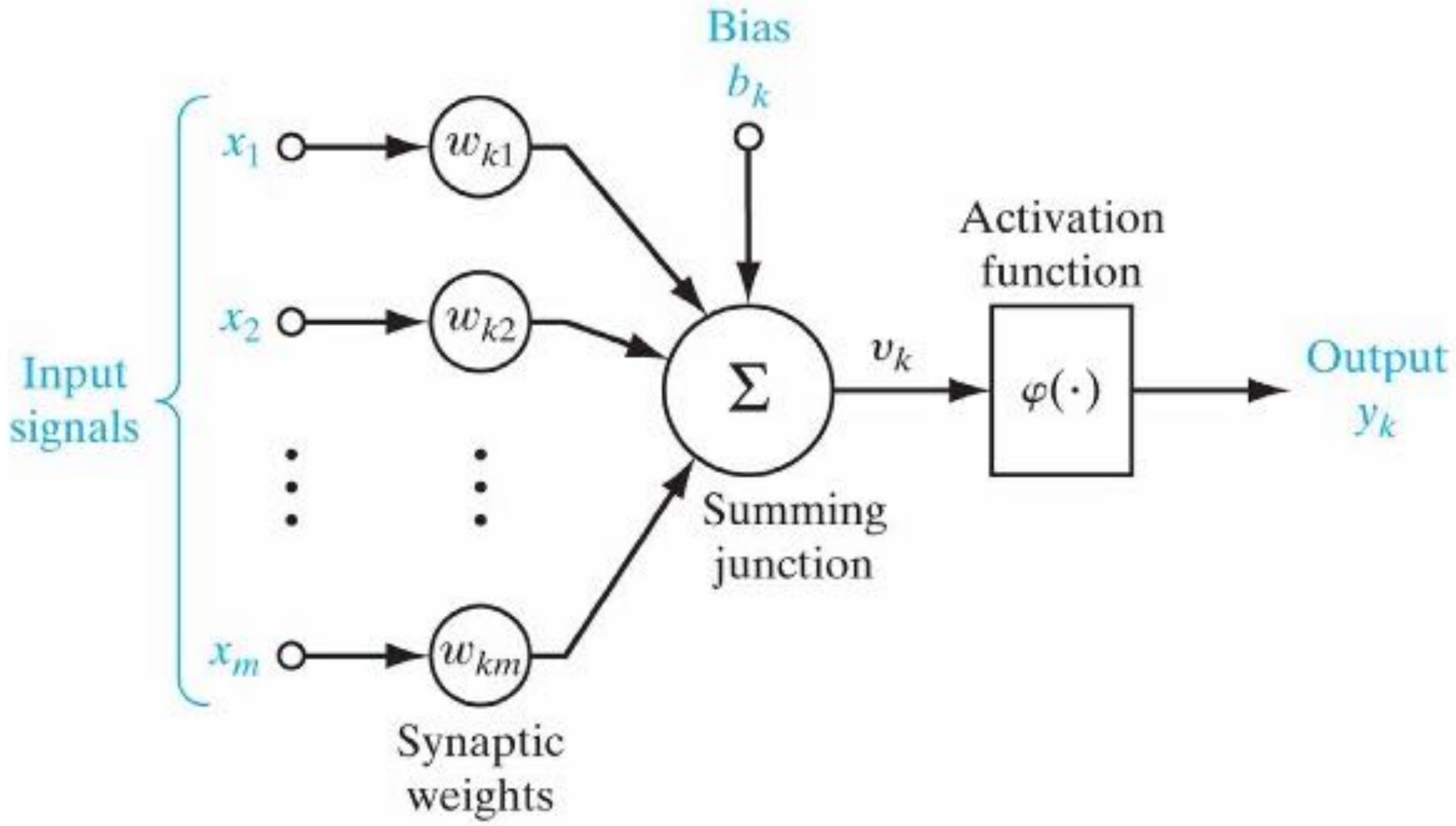
Agenda and Learning Outcomes

Today's Topic(s)

- **Topic(s): Neural Networks**
  - Multi-layer Perceptrons (MLP)
  - Deep Neural Networks
  - Backpropagation
- **Announcements**

Recall: Perceptron Neuron Model

Modified version of McCulloch-Pitts neuron



- **Perceptrons** use ***real-valued inputs***.
- Perceptrons are also used for learning.
- Invented by Rosenblatt in 1957
- Useful for binary classification

$$x_i \in \mathbb{R}$$ Real-valued inputs

$$v = \sum_{i=1}^{m} w_i x_i + b$$ Activation potential

$$y = \phi(v)$$ Output

$$\phi(v) = \begin{cases} 1, & \text{if } v \geq 0 \\ -1, & \text{if } v < 0 \end{cases}$$ Activation function

Recall: Decision Boundary

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

Perceptrons as classifiers

- The ***decision boundary*** of a perceptron is the line (or hyperplane) where the activation potential equals 0. This is based on the activation function of a perceptron
- For a 2-D input space with a bias: $$g(x_1, x_2) = w_1 x_1 + w_2 x_2 + b = 0$$

=> After re-writing the equation we can see that it follows the equation of a line

$$x_2 = -\frac{w_1}{w_2} x_1 - \frac{b}{w_2}$$

- The discriminant function is a line with slope $-w_1/w_2$ and intercept $-b/w_2$
- The distance of the function to the origin is $|b|/||\mathbf{w}||$, where

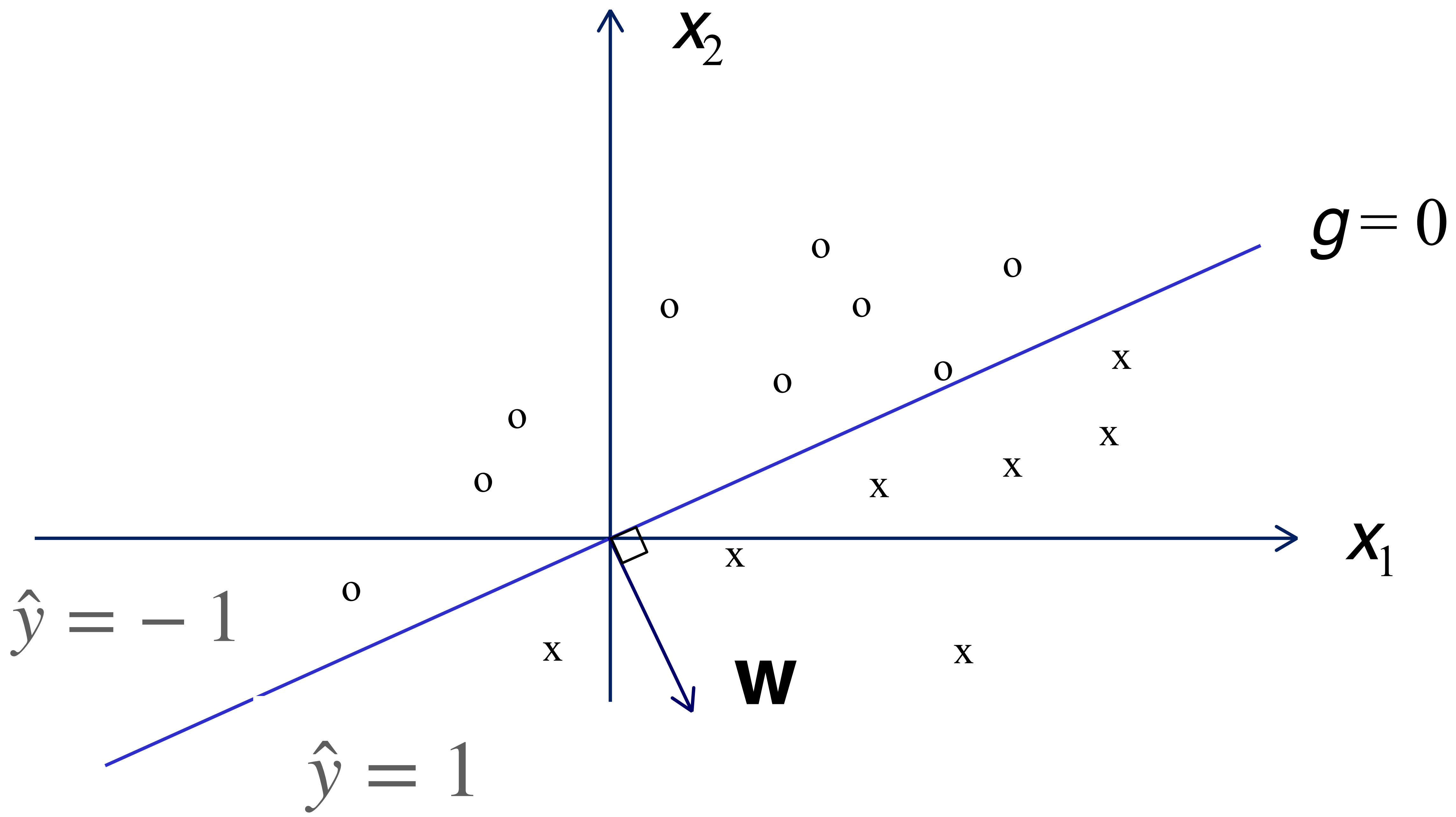
$$||\boldsymbol{w}|| = \sqrt{w_1^2 + w_2^2}$$

Recall: Decision Boundary

Perceptrons as classifiers

$$x_2 = -\frac{w_1}{w_2}x_1 - \frac{b}{w_2}$$

- For an m-dimensional input space, the decision boundary is an (m-1)-dimensional hyperplane perpendicular to **w**.
  - By definition, the weight vector is orthogonal to the decision boundary. **Why**? Recall: inner product
- The hyperplane separates the input space into two halves
  - One half having $\hat{y}$ = 1
  - The other half having $\hat{y}$ = -1
- When b=0, the hyperplane goes through the origin



Recall: Perceptron Learning Rule: Finding Weights

Single Perceptron, Multiple inputs

- How do we (iteratively) change the weights if they are too small or too large?
  - Weights must be initialized (more on this next week)

$$\mathbf{w}^{n+1} = \mathbf{w}^n + \nabla(\mathbf{w})$$
$$= \mathbf{w}^n + \eta(y - \hat{y})\mathbf{x}$$

$n:$ iteration number

$\eta:$ step size or learning rate

Actual output

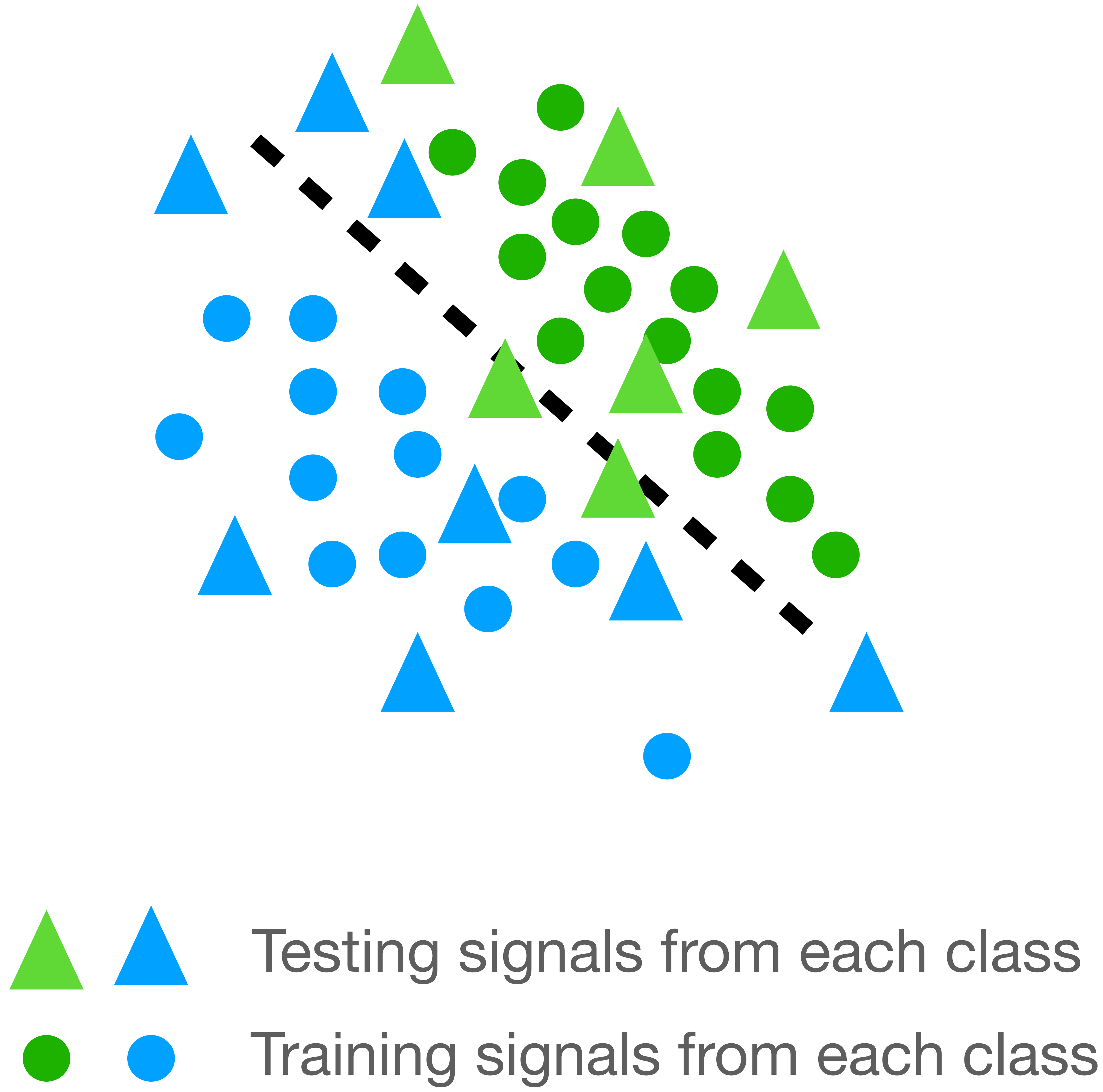
Desired output

- Note:
  - The outputs are bipolar {-1,1}
  - Thus, [y-$\hat{y}$] is either 0 (correct), -2 (too strong), or 2 (too weak)

Generalization Once Trained

Perceptrons during testing

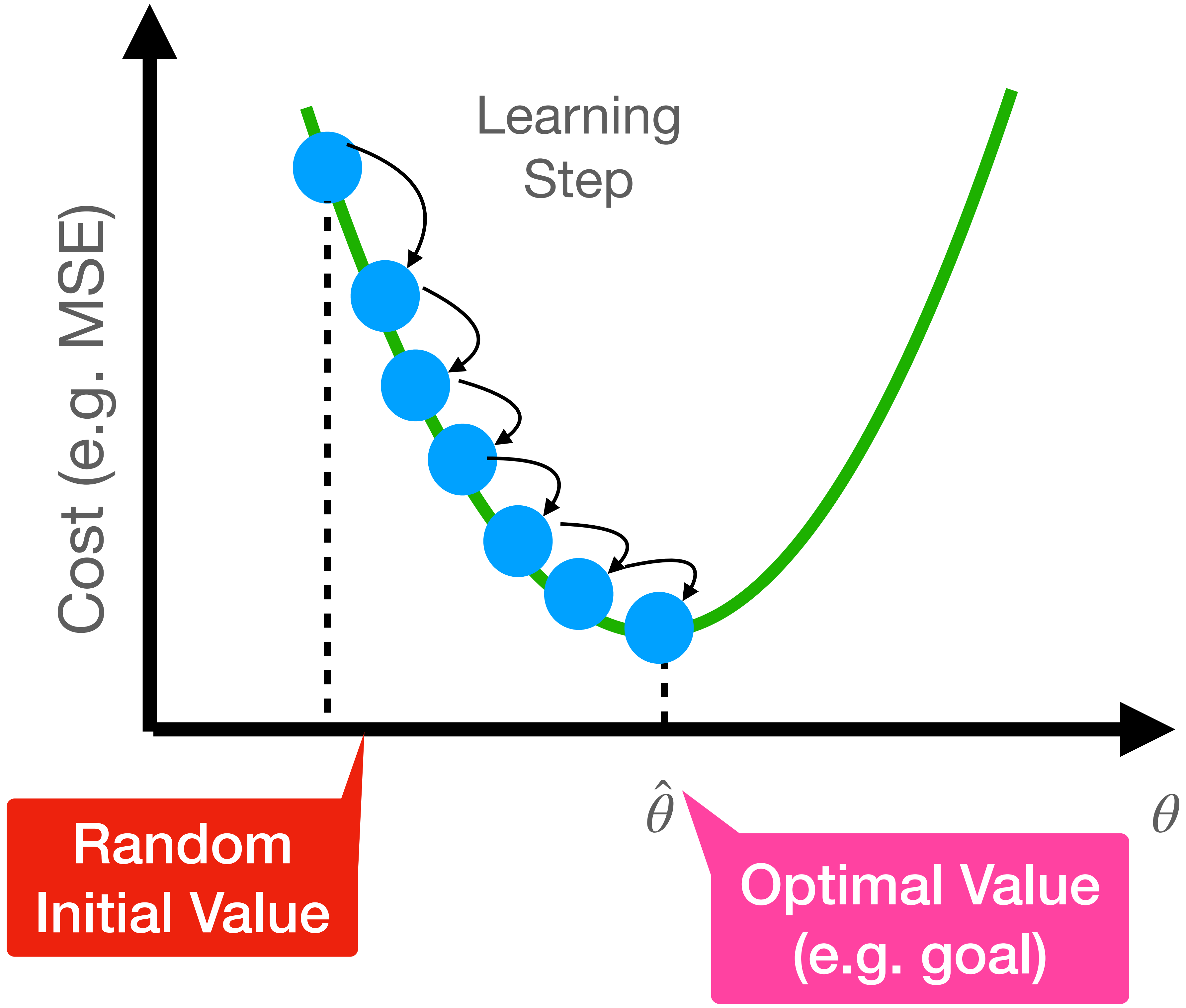
- Recall the definition of ***generalization***
  - **Definition**: Performance of a learning machine on test patterns not seen (or used) during training.
- Perceptrons generalize by deriving a decision boundary in the input space.
  - The selection of training patterns is thus important for generalization
  - The solution weight vector is not unique. There are infinite possible solutions and decision boundaries.



Gradient Descent vs. Perceptron Learning Rule

The math is the same

- ***Perceptron learning*** is for McCulloch-Pitts neurons (with real inputs), which are ***nonlinear***
  - Gradient descent (as discussed) is for linear neurons (e.g. linear regression)
  - Perceptron learning is for classification
  - Linear regression learning via gradient descent is for estimation (or regression)



Perceptron Learning

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

$$v = \sum_{i=1}^{m} w_i x_i + b \qquad y = \phi(v)$$

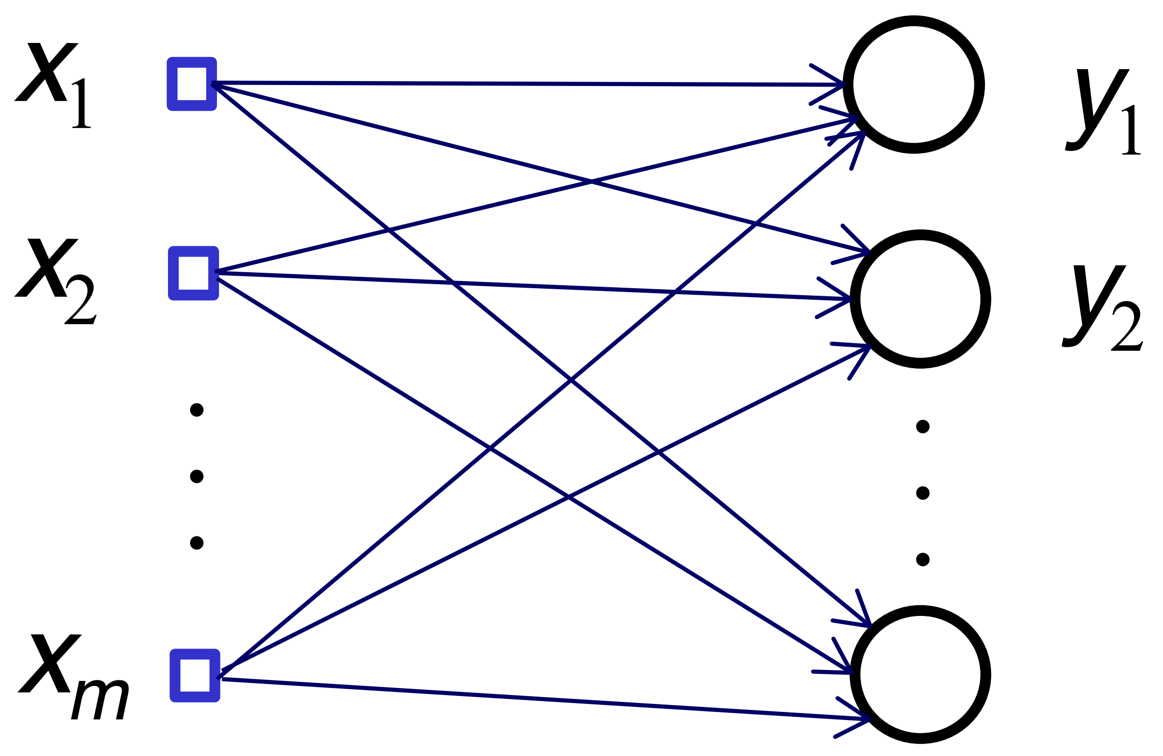
Linear Regression

$$y = \sum_{i=1}^{m} w_i x_i + b \qquad \phi(v) = v$$

Perceptrons for Multi-dimensional outputs

For classification or regression

- Multiple perceptrons can be used when performing multi-class classification (one for each class) or multi-dimensional estimation
  - **Classification**: Perceptron output is 1 when input is from the corresponding class. Its output is 0 otherwise. Each perceptron forms it's own decision boundary
  - **Regression:** Each perception corresponds to one of the output dimensions
- When these perceptrons have the same inputs (but with different weights), this stacking of perceptrons is called a ***layer***

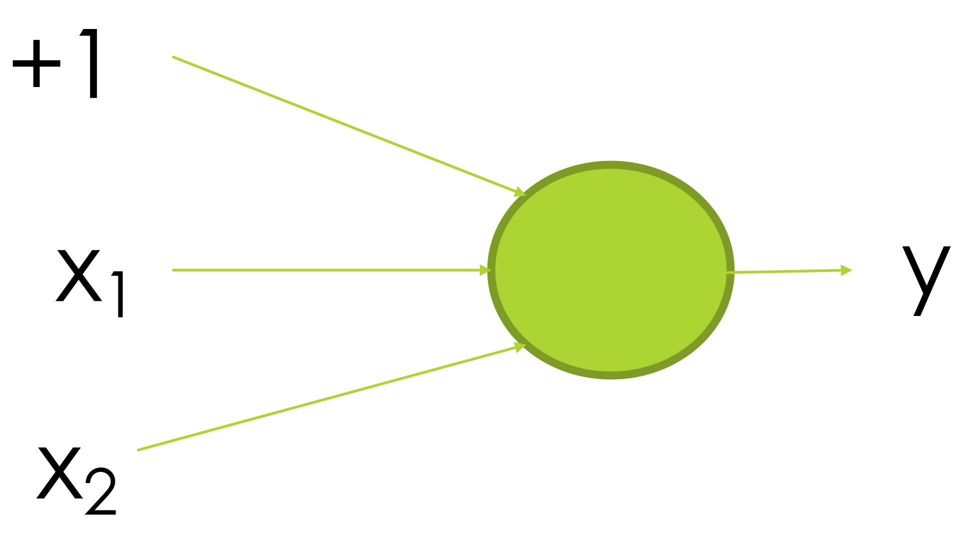


A limitation of single-layer perceptrons

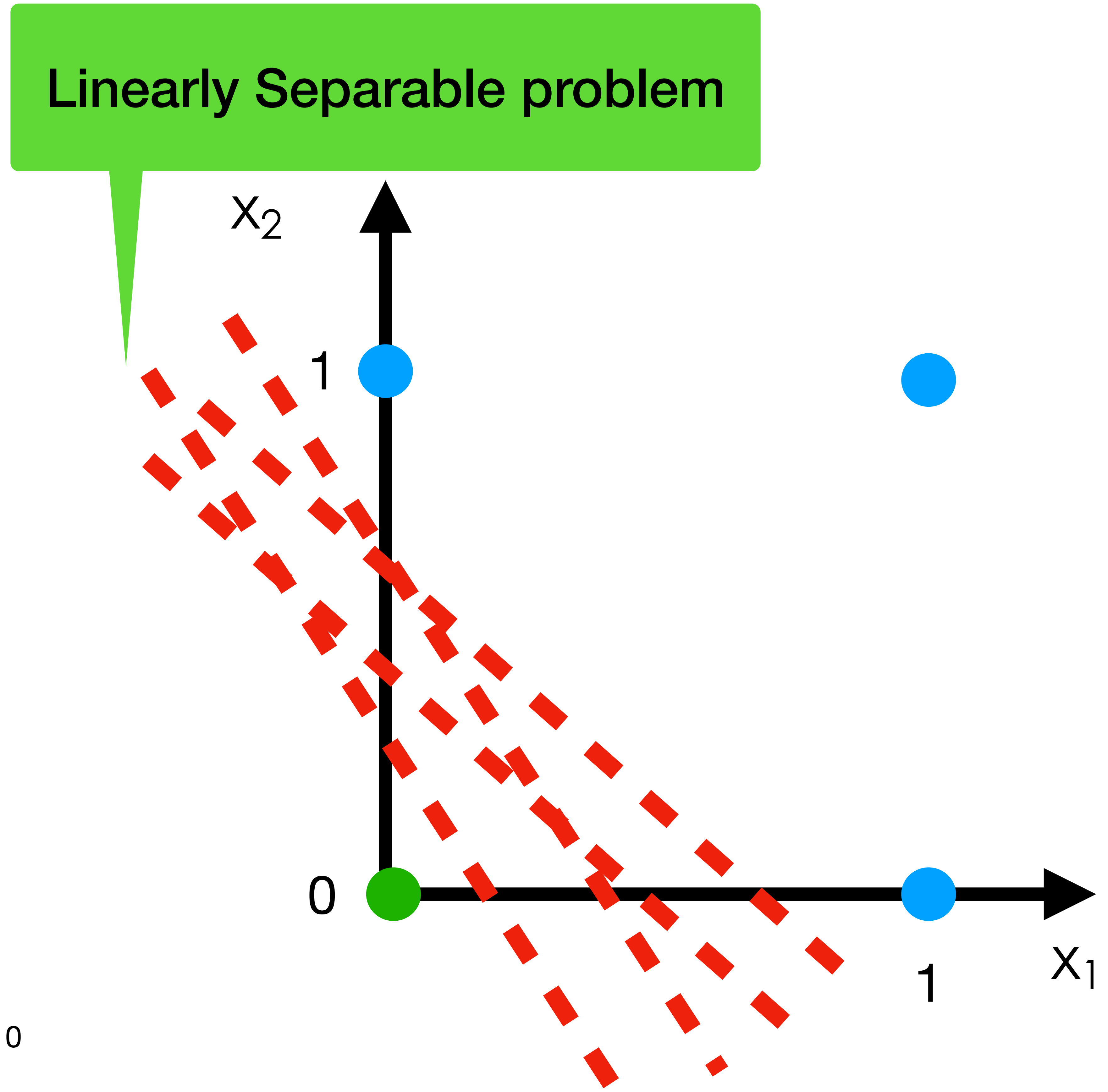
Logic Gate Example: OR Gate

- Single-layer perceptron networks can be used to solve multi-class classification problems, but they are not as useful for problems that are linearly inseparable or linearly-separable problems that require multiple boundaries per class

OR Function



x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	1

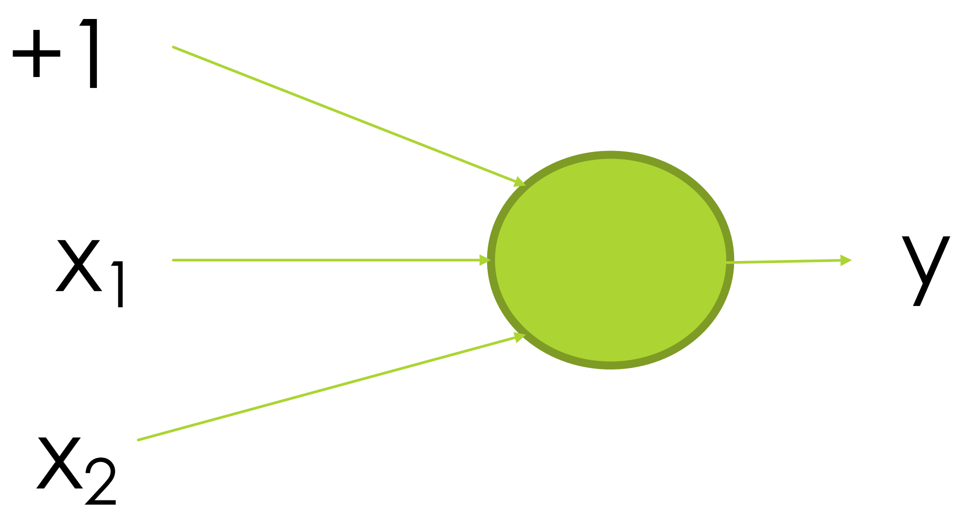


A limitation of single-layer perceptrons

Logic Gate Example: XOR Gate

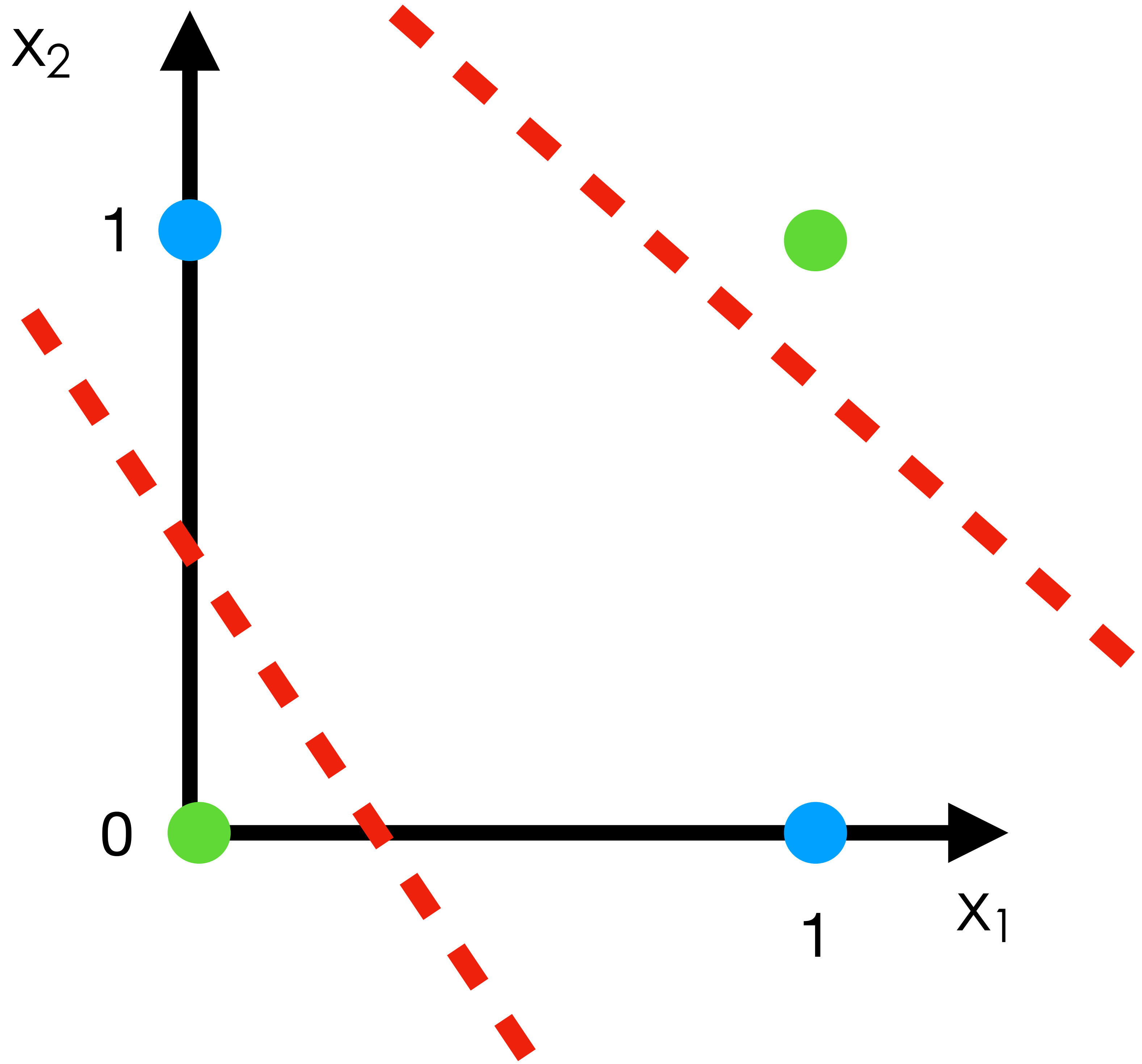
- Single-layer perceptron networks can be used to solve multi-class classification problems, but they are not as useful for problems that are linearly inseparable or linearly-separable problems that require multiple boundaries per class

XOR Function



x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0

A single (layer) perceptron cannot solve this problem



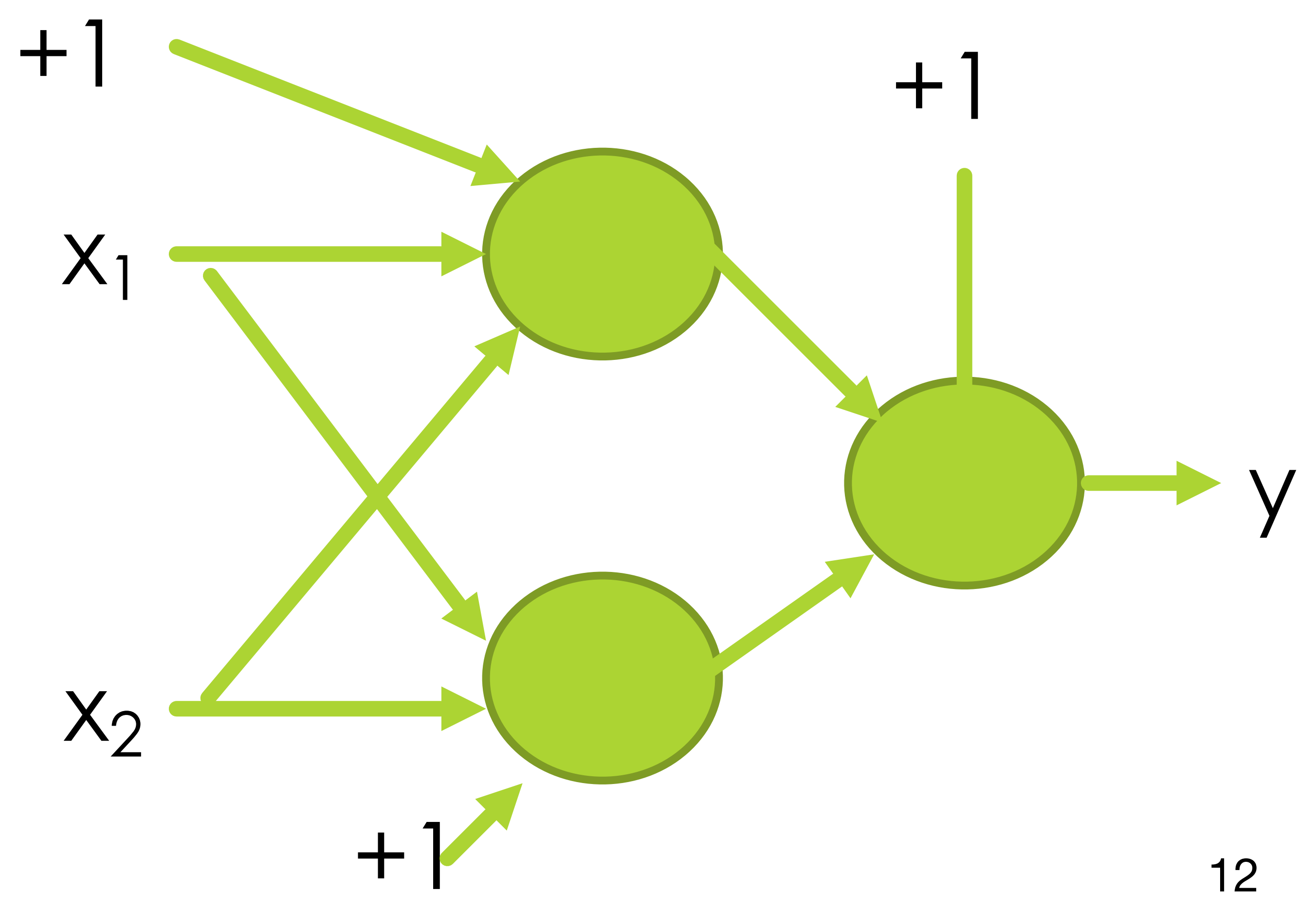
The Case for Multi-Layered Perceptrons (MLP)

Logic Gate Example

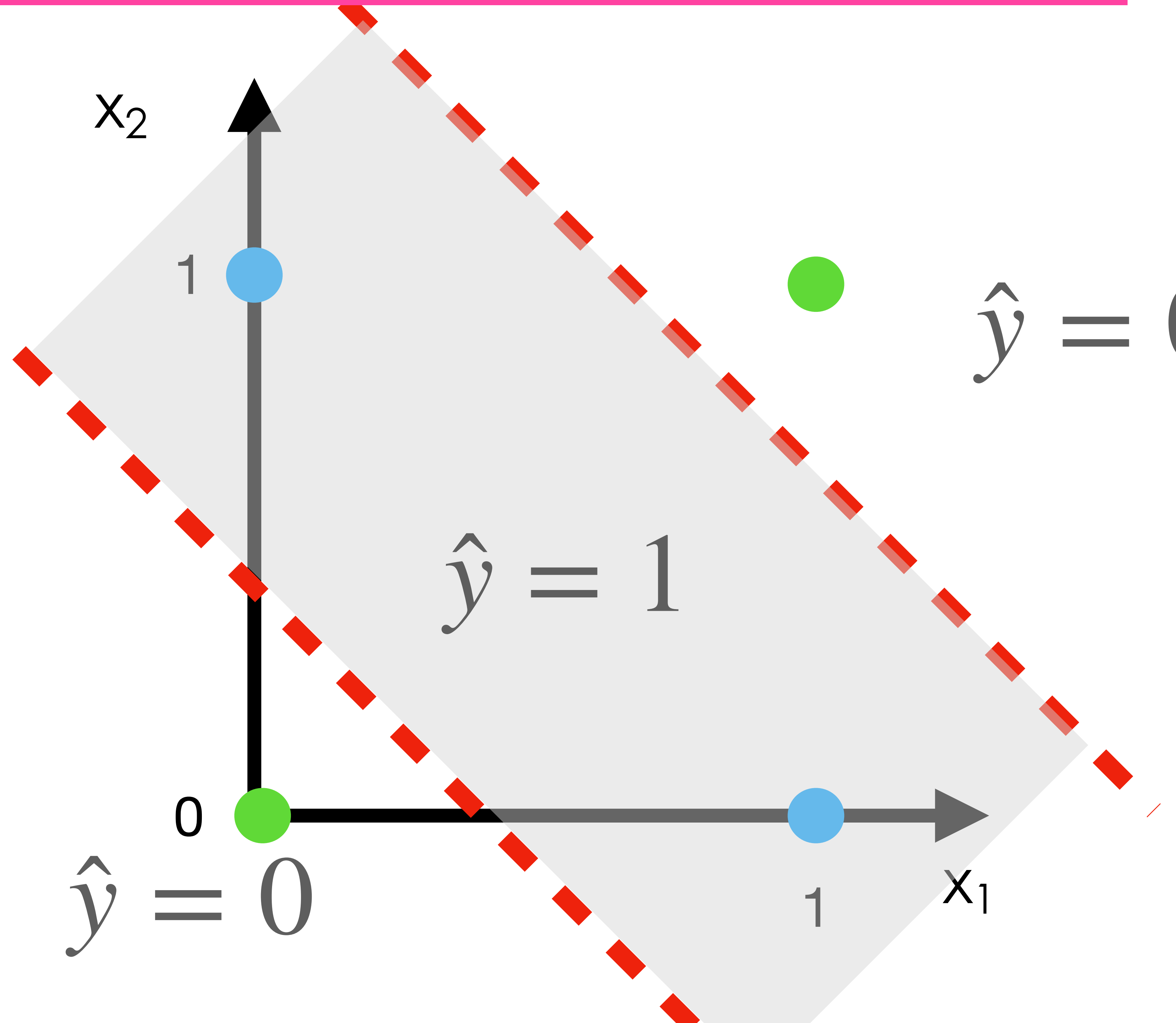
- Adding layers to a network can help solve more complicated problems. The resulting neural network is called a ***Multi-Layer Perceptron (MLP)***

XOR Function

x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0



The decision boundary becomes a decision region

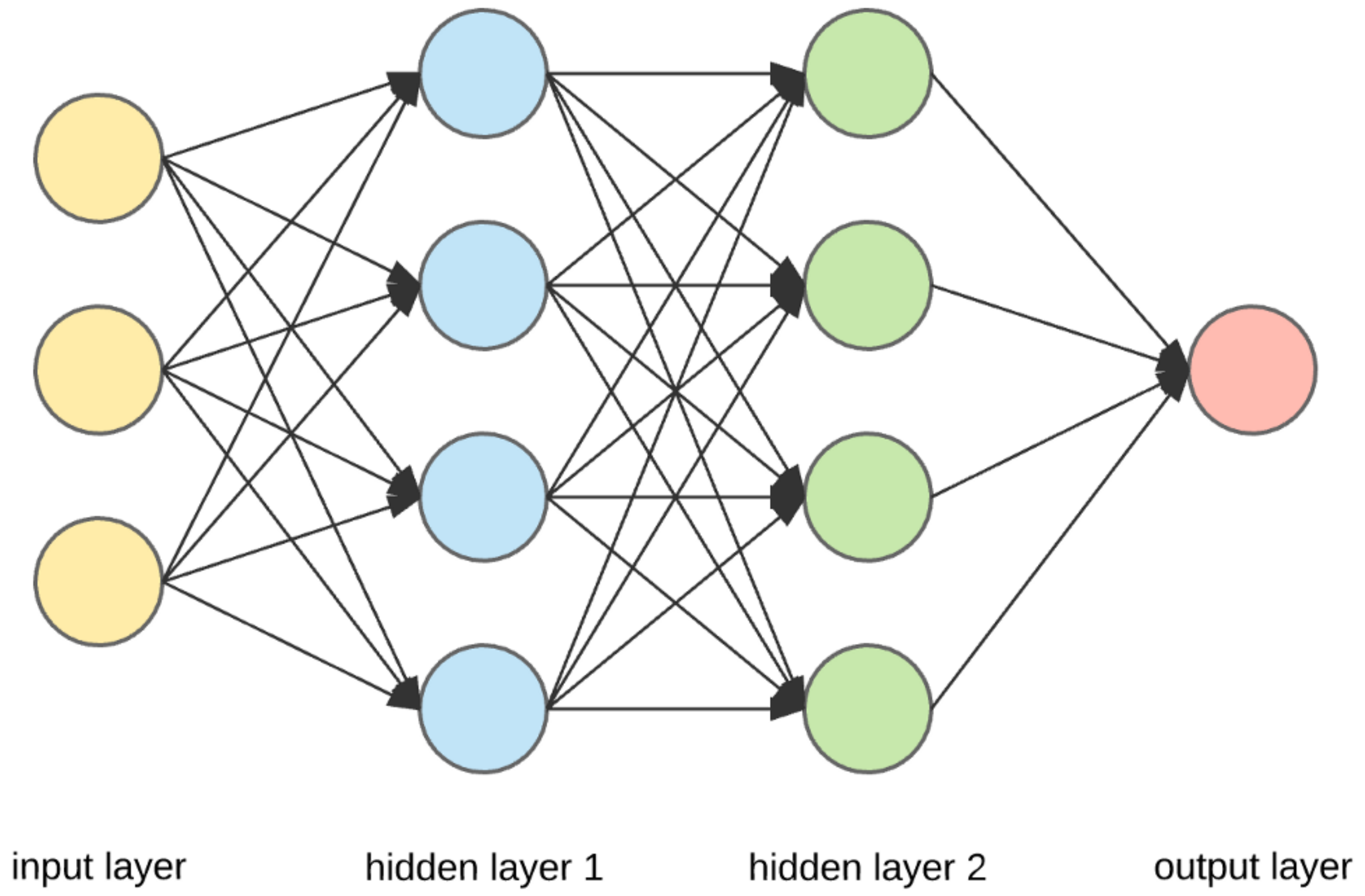


Multi-Layer Perceptron (MLP)

Components of the MLP

- **Input layer**: not really a layer, but serves to represent the inputs to a network
- **Hidden layers**: Layers where the output goes to another layer of neurons
- **Output layer**: Final layer of network, where output(s) are computed

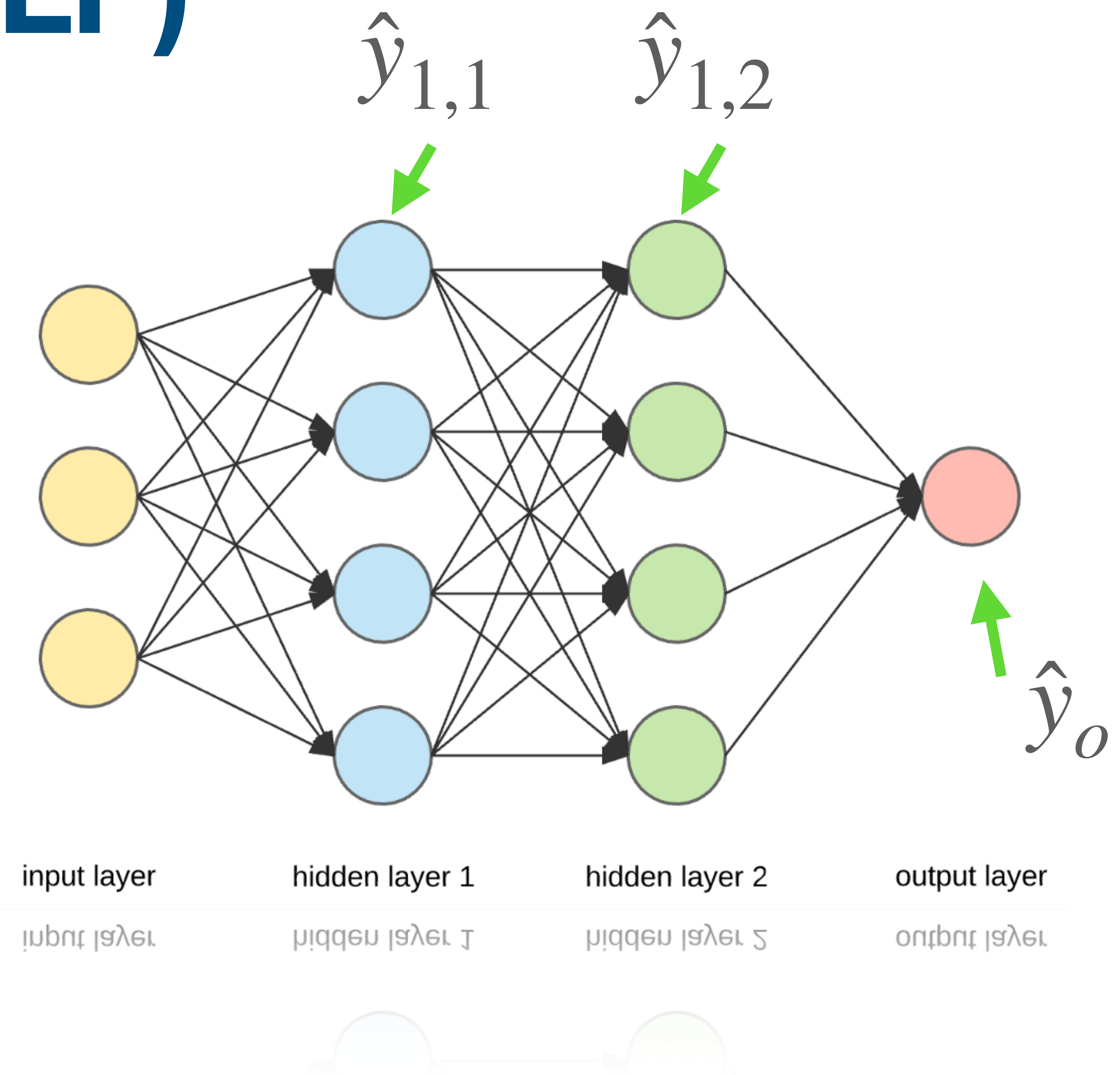
- ***Deep neural networks(DNN)*** have two or more hidden layers (or three or more layers, excluding the input layer)
  - This is an example of a three-layer DNN. The input layer is not counted.



Multi-Layer Perceptron (MLP)

Computing Output(s): Forward Pass

- The output(s) of the network is(are) computed in a layer-wise fashion. This is known as the ***forward pass***
    - The output from layer one is first computed and this becomes the input to the next layer
    - This continues until the output(s) is(are) computed



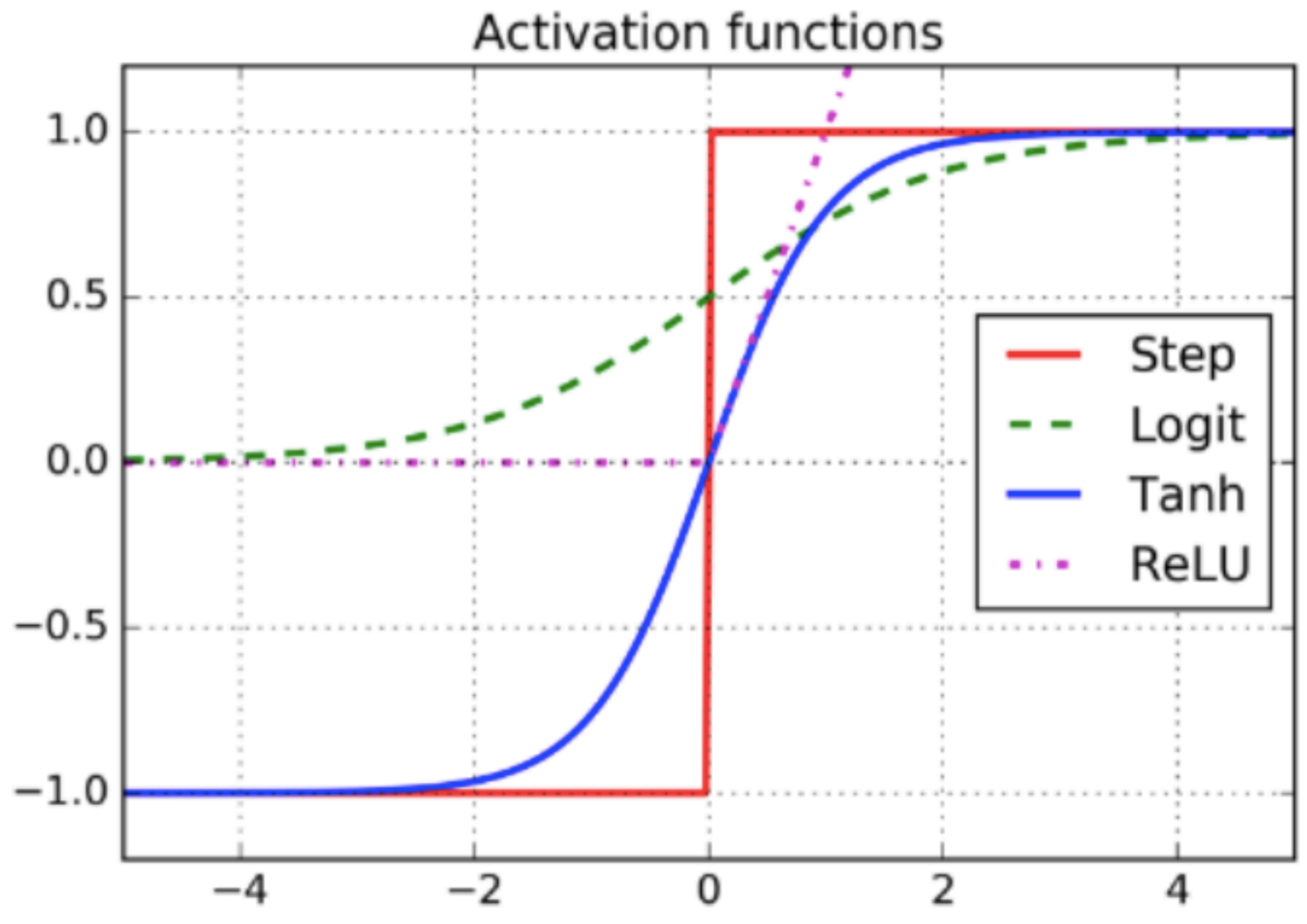
$$\hat{y}_{1,1} = \phi(\mathbf{w}_{1,1}^T \mathbf{x})$$

$$\hat{y}_{1,2} = \phi(\mathbf{w}_{1,2}^T \hat{\mathbf{y}}_1) \qquad \hat{y}_o = \phi(\mathbf{w}_o^T \mathbf{y}_2)$$

Deep Neural Networks

Distinction with MLPs: Activation Functions

- The sign (or step) function of MLPs is mostly useful for classification problems. It also is not as useful for more complicated problems.
- To address these problems, other activation functions are often used in DNNs. These activation functions all use the activation potential as originally defined, as their input
  - **Sigmoid (or logit)**: $\phi(v) = 1/(1 + e^{-v})$
  - **Hyperbolic Tangent (tanh)**: $\phi(v) = 2/(1 + e^{-2v}) - 1$
  - **Rectified Linear (ReLU)**: $\phi(v) = \max(0, v)$
  - **Linear**: $\phi(v) = v$
- Different activation functions may be used in different layers (not required).



DNN Weight Learning

DNNs are supervised learning algorithms

- **Goal**: Find the weights that minimize the error (often MSE) between true and predicted values using a training set.
- During the training phase, the ***back propagation*** algorithm is used to find these weights
- **General idea of back propagation**:
    - For each training sample (e.g. input), compute the output using the forward pass
    - Compute the estimation/prediction error
    - Sequentially go through each layer (in reverse order) to measure the error contribution from each connection
    - Update the weights based on the error contribution to reduce the error (e.g. gradient descent)

DNN Weight Learning

Graphical depiction of backpropagation

- <u>**General idea of back propagation**</u>:
  - For each training sample (e.g. input), compute the output using the forward pass
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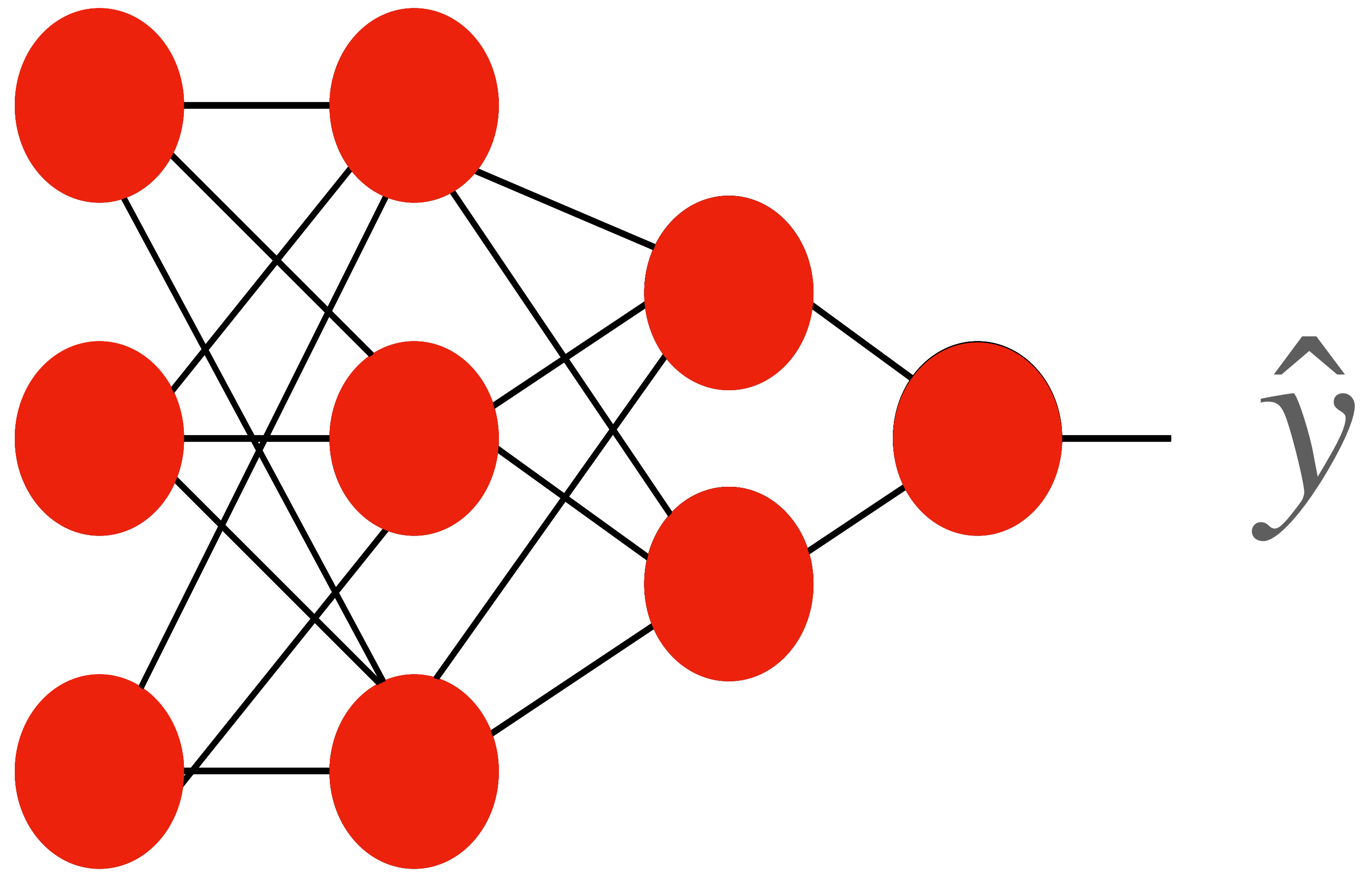

Compute Forward Pass of DNN to get output from input

DNN Weight Learning

Graphical depiction of backpropagation

- **<u>General idea of back propagation</u>**:
    - For each training sample (e.g. input), compute the output using the forward pass
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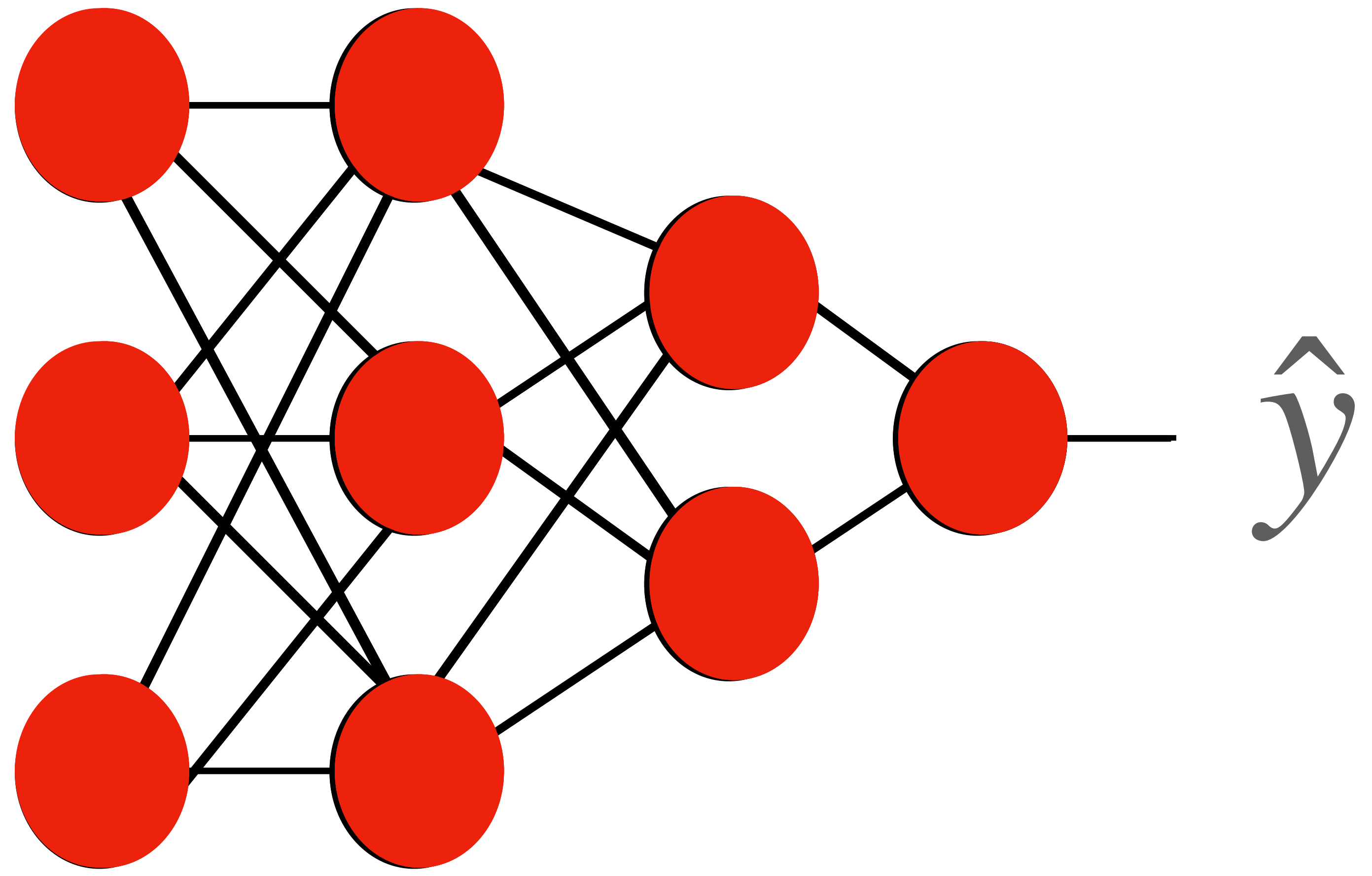

Compute output error

$$y - \hat{y}$$

DNN Weight Learning

Graphical depiction of backpropagation

- <u>**General idea of back propagation**</u>:
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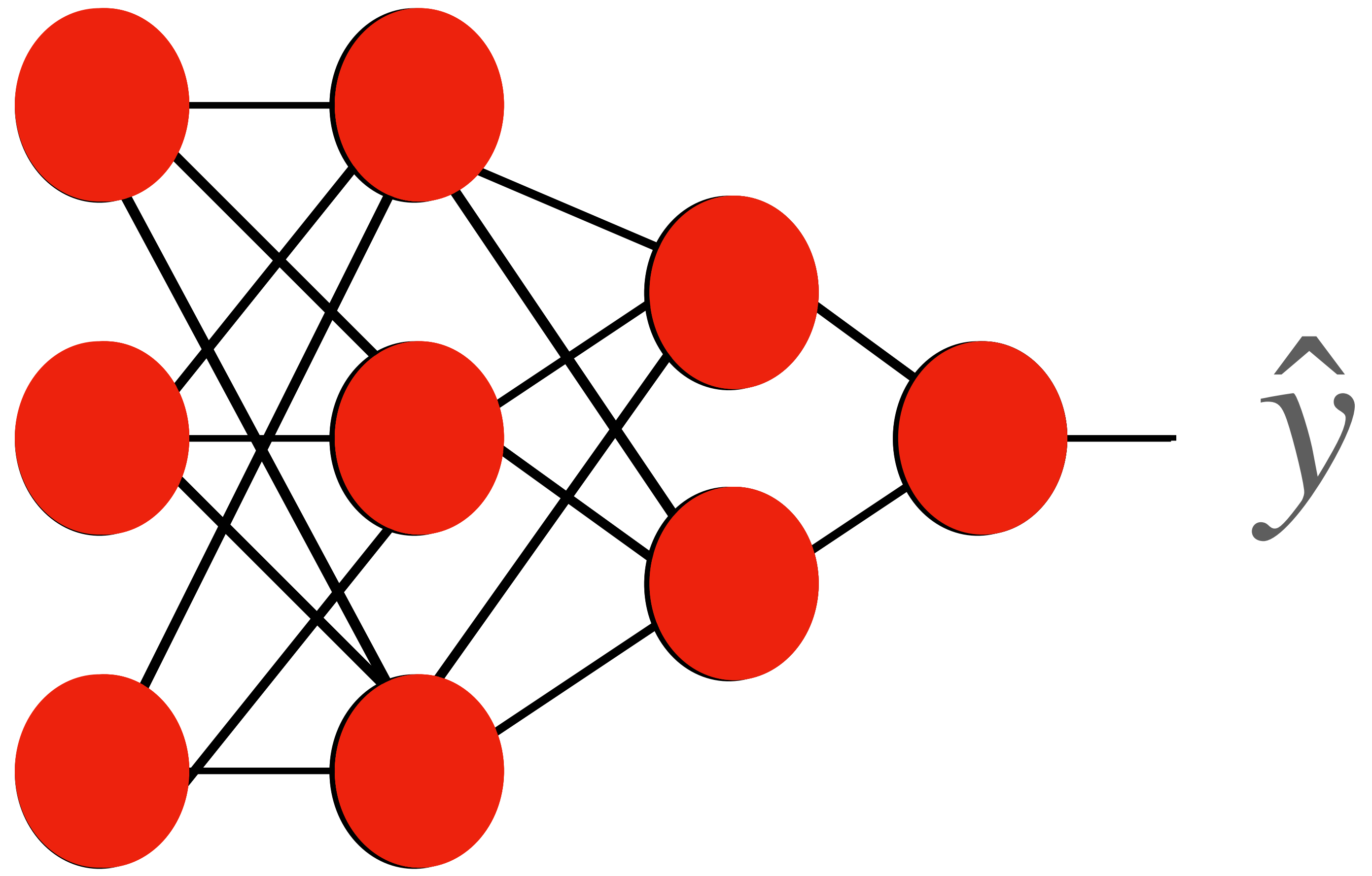

Compute contribution from each neuron in each layer

δ_k

DNN Weight Learning

Graphical depiction of backpropagation

- **<u>General idea of back propagation</u>**:
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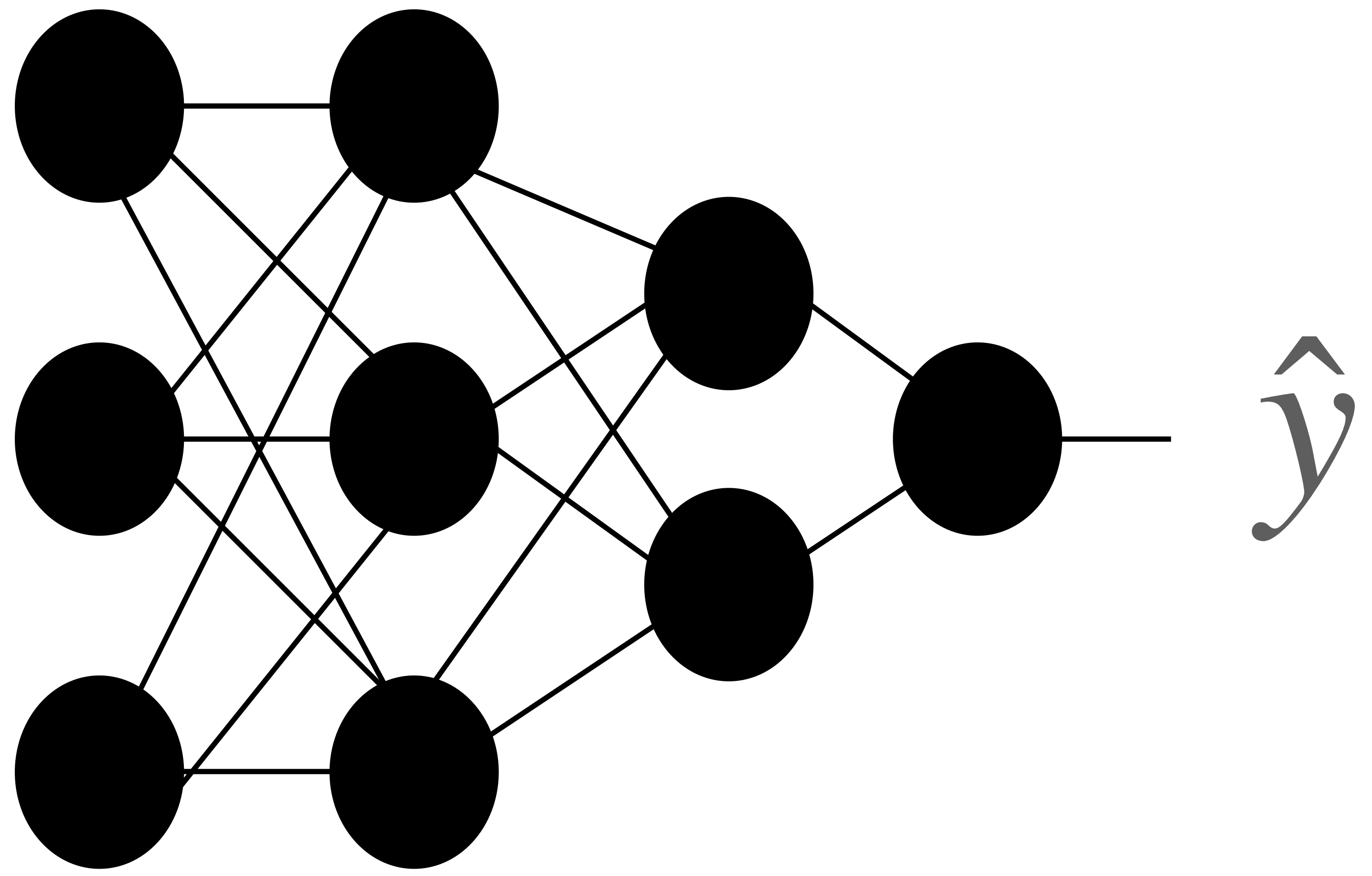
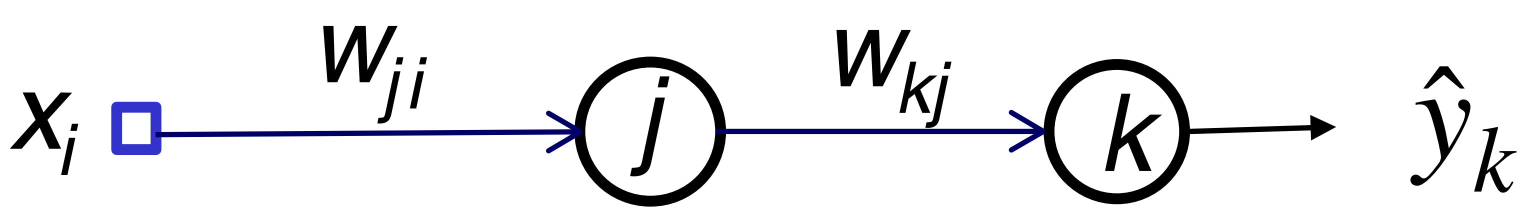


Update weights based on error and (weighted) contributions for each neuron and layer

$$\mathbf{w}_k = \mathbf{w}_k - \eta \nabla E(w)$$

Mathematics behind Backpropagation

Simplified DNN

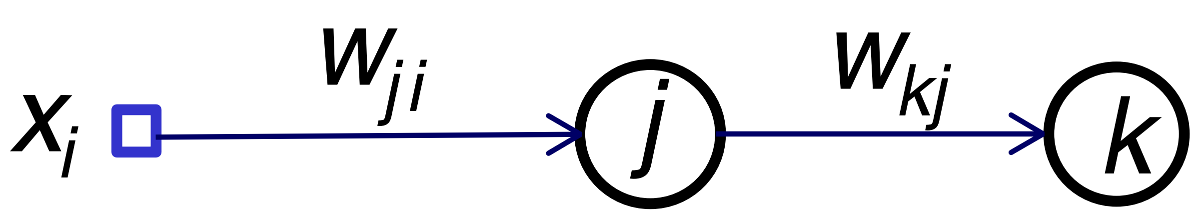


- Notation for one hidden layer
  - Weight(s) for the k-th neuron in the output layer are denoted as $\mathbf{w}_{kj}$
  - Weight(s) for the j-th neuron in the hidden layer are denoted as $\mathbf{w}_{ji}$
- **Iterative weight update equations based on MSE loss function each iteration performs both in an interlaced manner** (e.g. output update, hidden layer update, output update, hidden layer update, out…)
  - **Output layer (delta rule)**: $\mathbf{w}_{kj}(n+1) = \mathbf{w}_{kj}(n) + \eta e_k(n)\phi'(v_k)\hat{y}_j(n) = \mathbf{w}_{kj}(n) + \eta\delta_k(n)\hat{y}_j(n)$
  - ***Hidden layer (generalized delta rule)***:

$$\mathbf{w}_{ji}(n+1) = \mathbf{w}_{ji}(n) + \eta\phi'(v_j(n))\left[\sum_k \delta_k(n) w_{kj}(n)\right]\mathbf{x}_i(n) = \mathbf{w}_{ji}(n) + \eta\delta_j(n)\mathbf{x}_i(n)$$

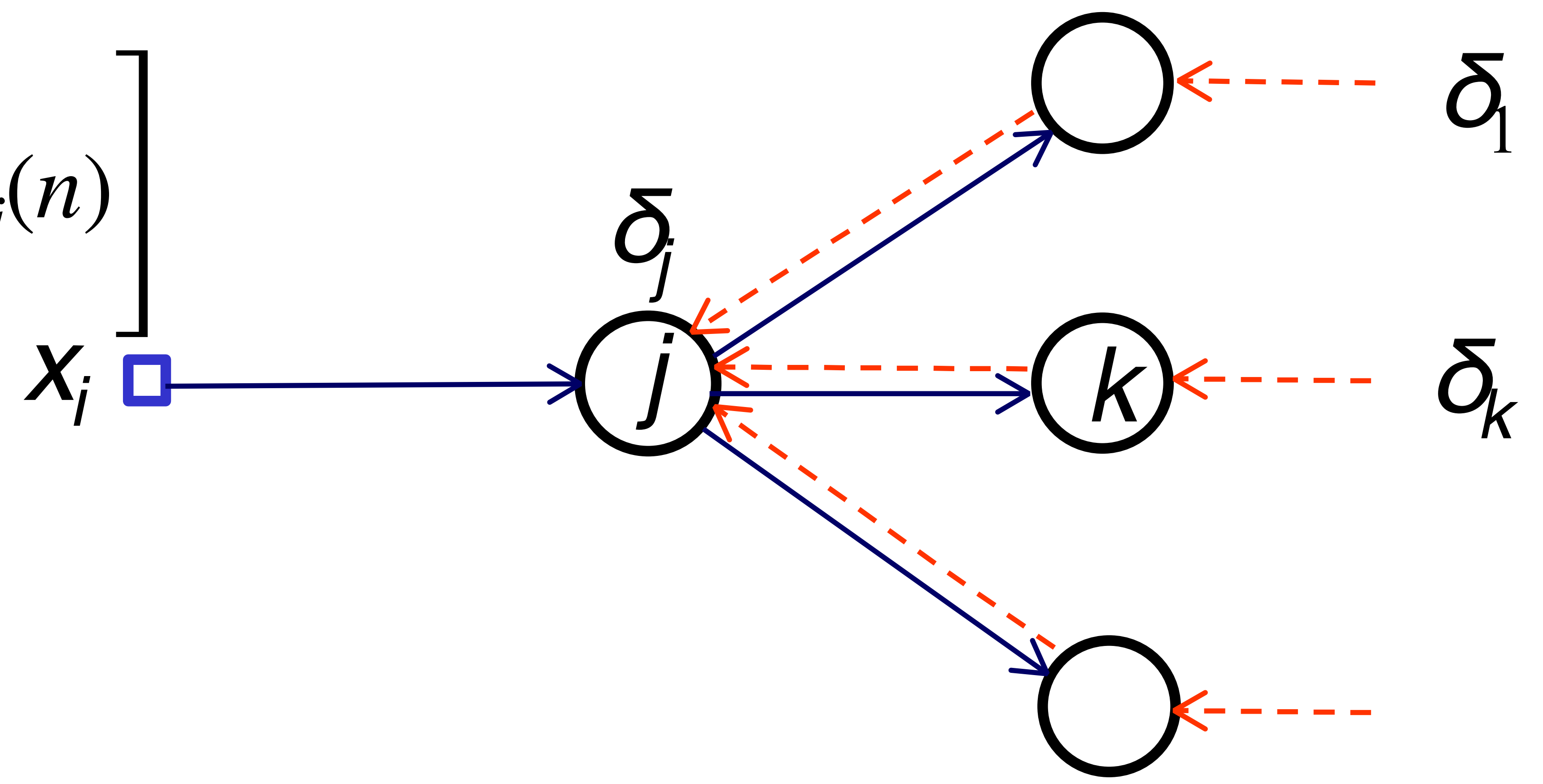
Backpropagation

Illustration of delta rules



- Illustration of the generalized δ rule,

$$\delta_j(n) = \phi'(v_j(n))\left[\sum_k \delta_k(n) w_{kj}(n)\right]$$



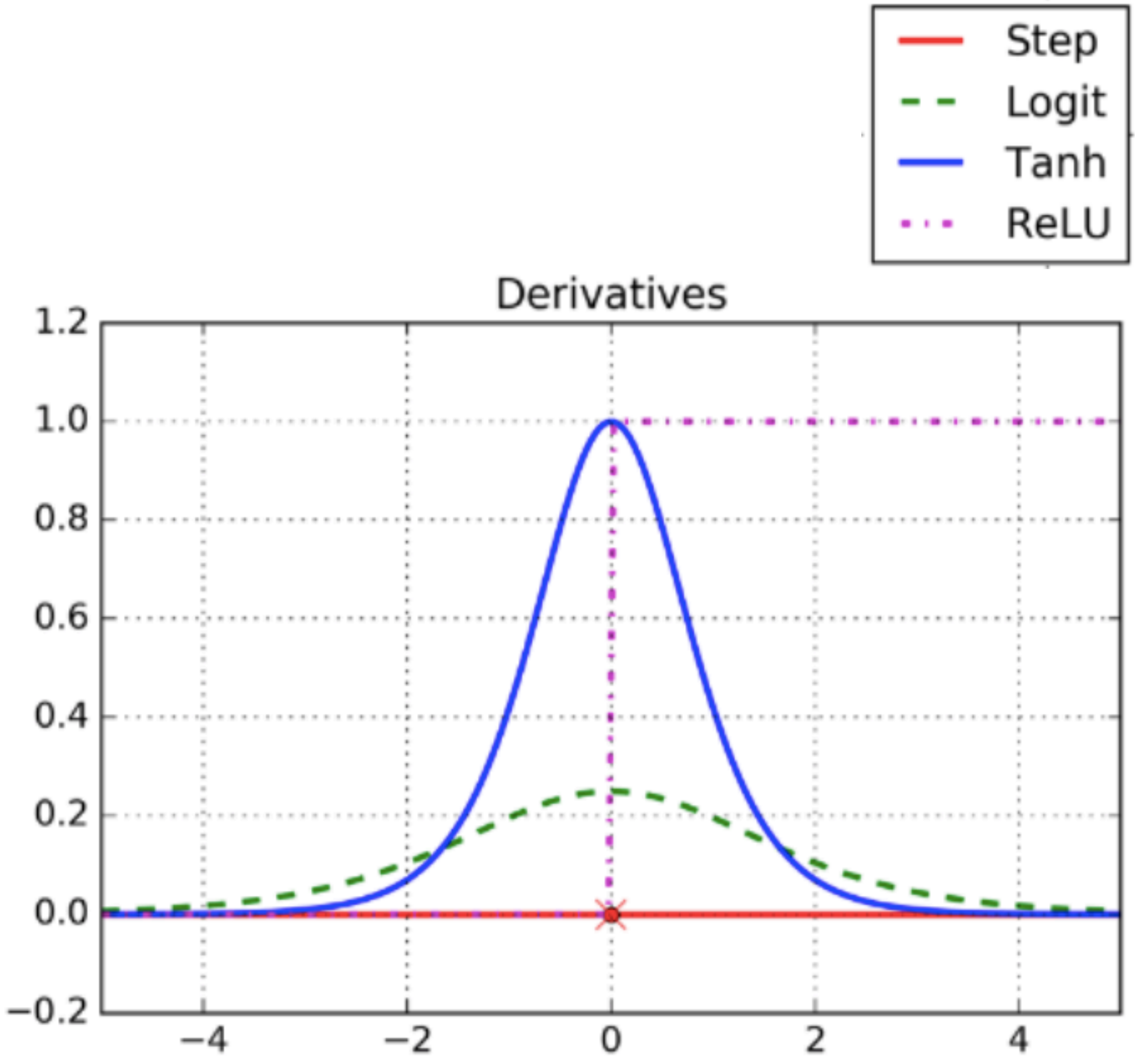
$$\delta_k(n) = (y_k - \hat{y}_k)\phi'(v_k) = e_k(n)\phi'(v_k)$$

- The ***generalized*** δ ***rule*** gives a solution to the credit (blame) assignment problem (e.g. which neuron is most responsible for the error).
- The updates depend on the partial derivative of the activation function $\phi'(v)$
- Updates can be done using Stochastic or Mini-batch gradient descent

Derivatives of activation functions

Needed for weight update

- Plot of partial derivatives for different activation functions



- For a logistic sigmoid for ϕ

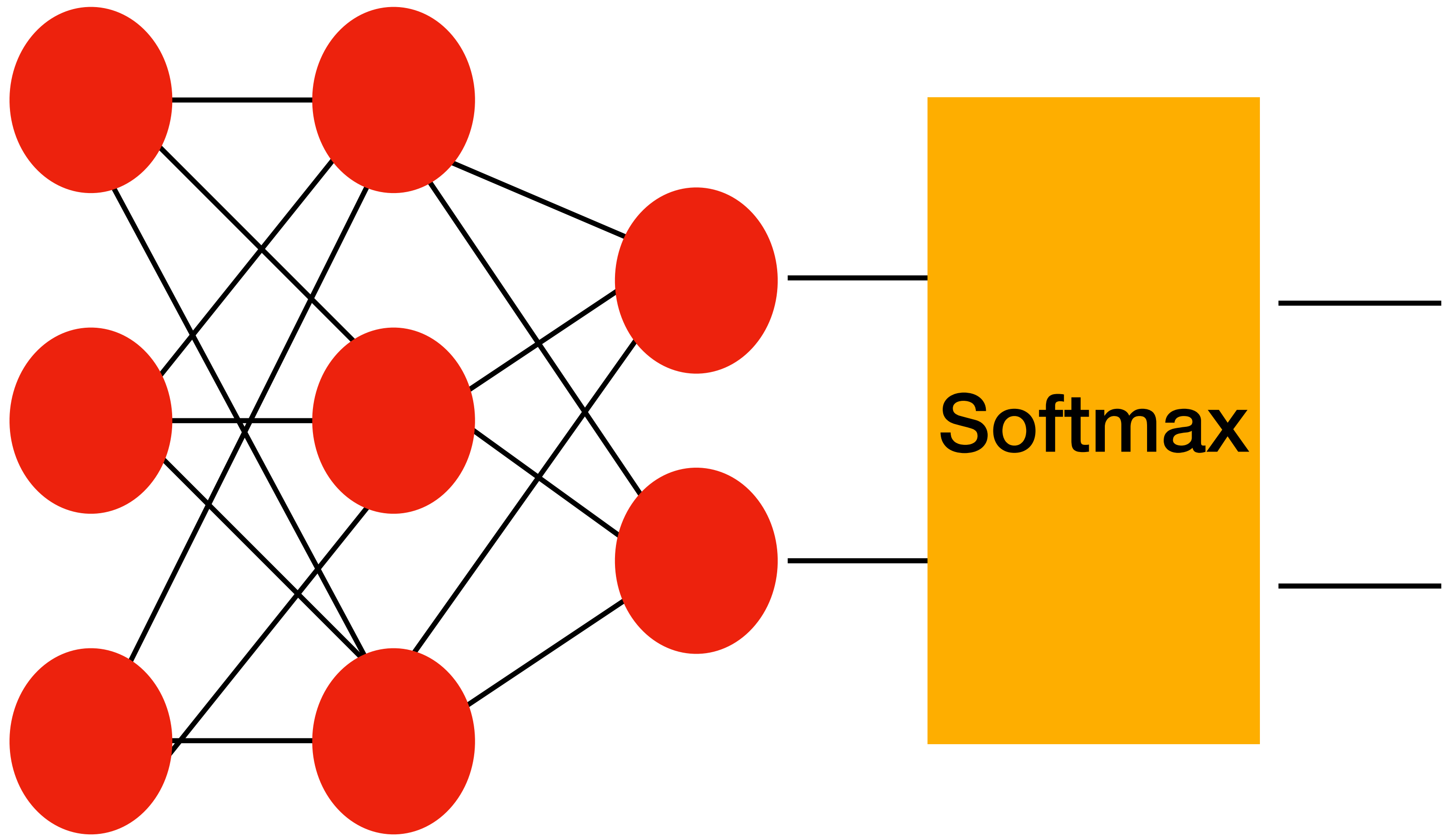
$$\phi(v) = \frac{1}{1 + e^{-v}} \quad => \quad \phi'(v) = \phi(v)[1 - \phi(v)]$$

DNNs as Multi-Class Classifiers

Softmax layer

- The prior approach assumes that the DNN is being trained to solve a regression problem. What happens if we need to solve a classification problem?
- For binary classification, we can merely threshold the output neuron, as was shown previously for Linear Regression
- For multi-class classification (when the classes are exclusive), each neuron in the output layer corresponds to a single class.
  - The output layer is then modified to replace the individual activation functions with a shared ***soft-max function***
  - Outputs represent estimated probability of the corresponding class

$$\hat{y}_i = p_{y_i} = \phi_k(v) = \frac{e^{v_k}}{\sum_{j=1}^{K} e^{v_j}}$$



Cross Entropy Loss to train network

$$L_{ce} = -\sum_{i=1}^{m} y_i \log(p_{y_i})$$

Next Class: Neural Networks III

Training a DNN

A Python Example using TensorFlow

- MNIST Digit Recognition Example
- Other considerations during training