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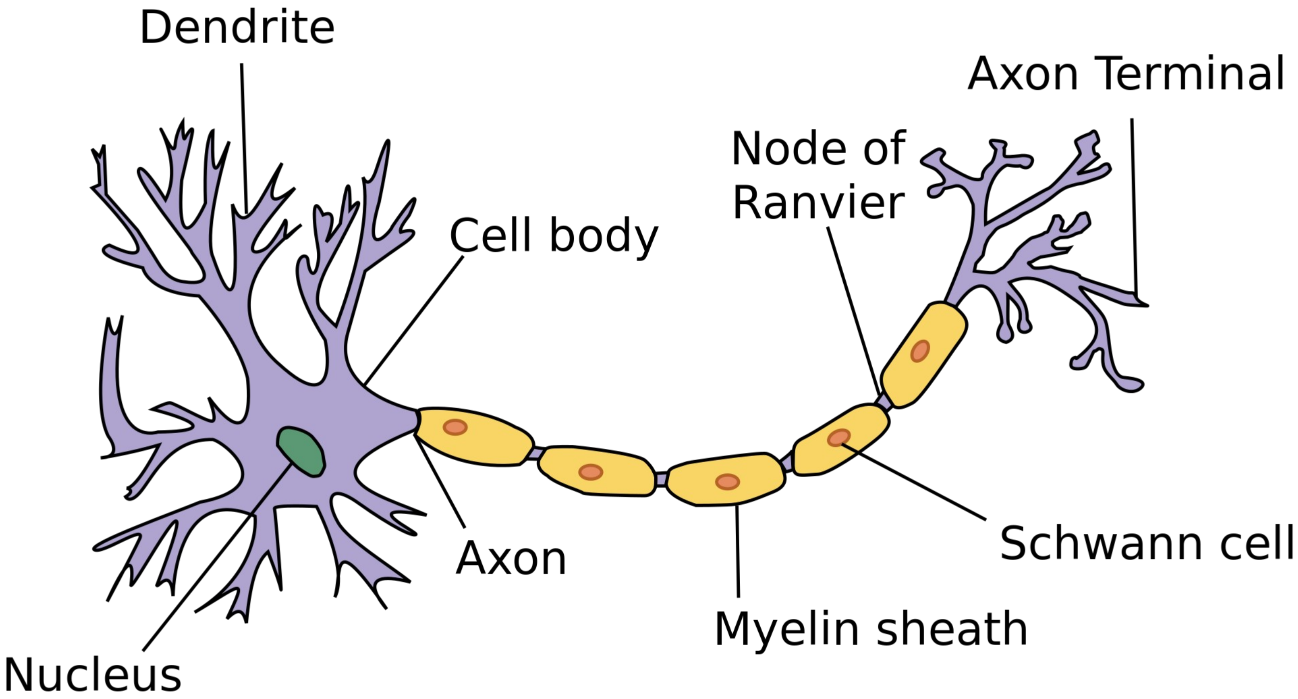
Basic theory of Feed-forward Neural Networks

NATIONAL BIOINFORMATICS
INFRASTRUCTURE SWEDEN

Resources

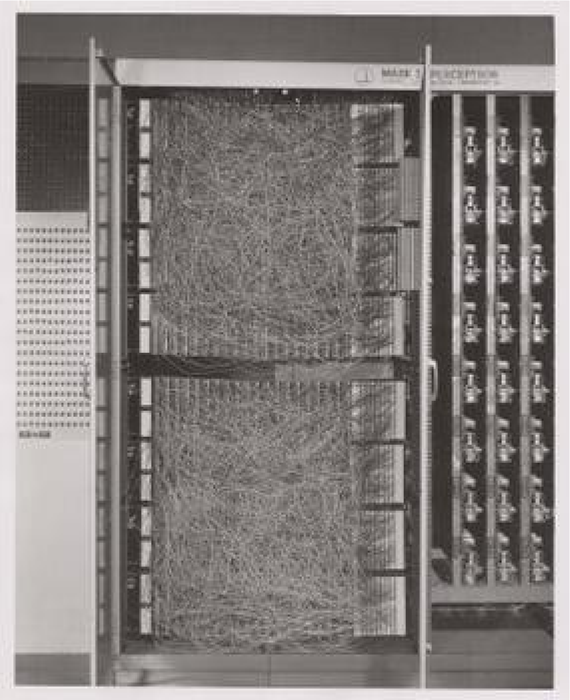
- MIT lectures on Deep Learning (http://introtodeeplearning.com/)
- TensorFlow Playground (https://playground.tensorflow.org)
- Keras Docs (https://keras.io)

This is a neuron

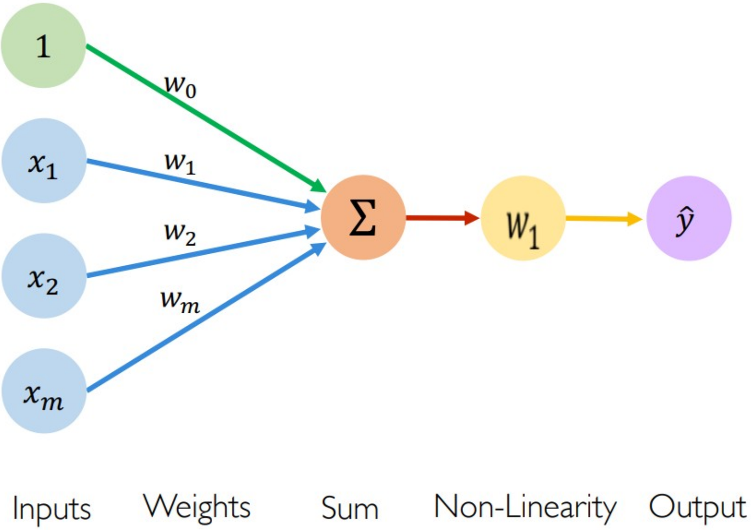


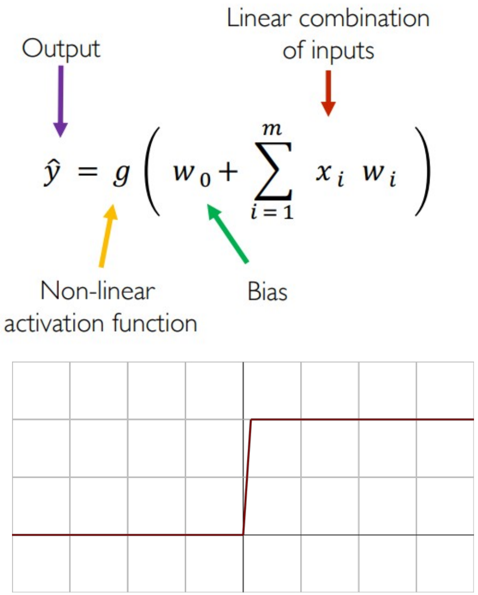
wikipedia.org

This is a perceptron (1958)



Mark I Perceptron machine
wikipedia.org





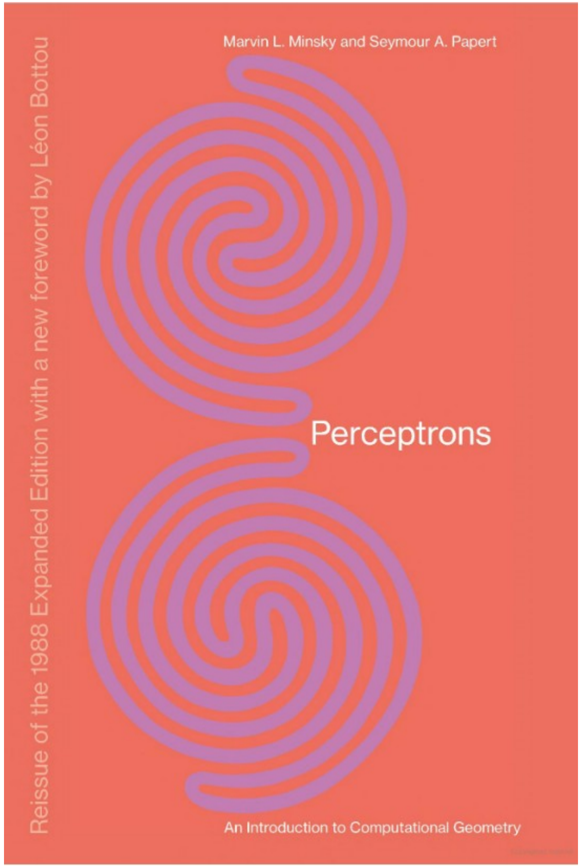
MIT “Intro to Deep Learning”

Perceptrons caused excitement

- *"the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence."*

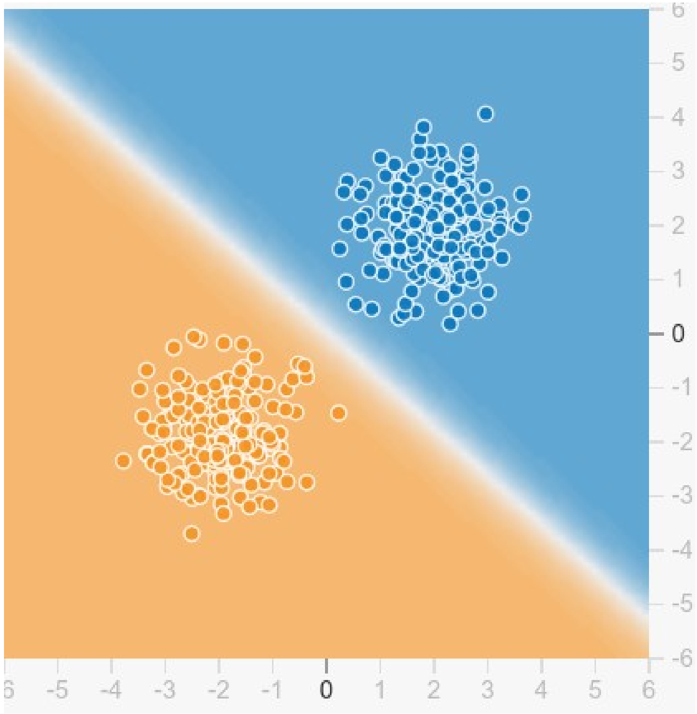
The New York Times

Perceptrons can only learn linearly separable classes



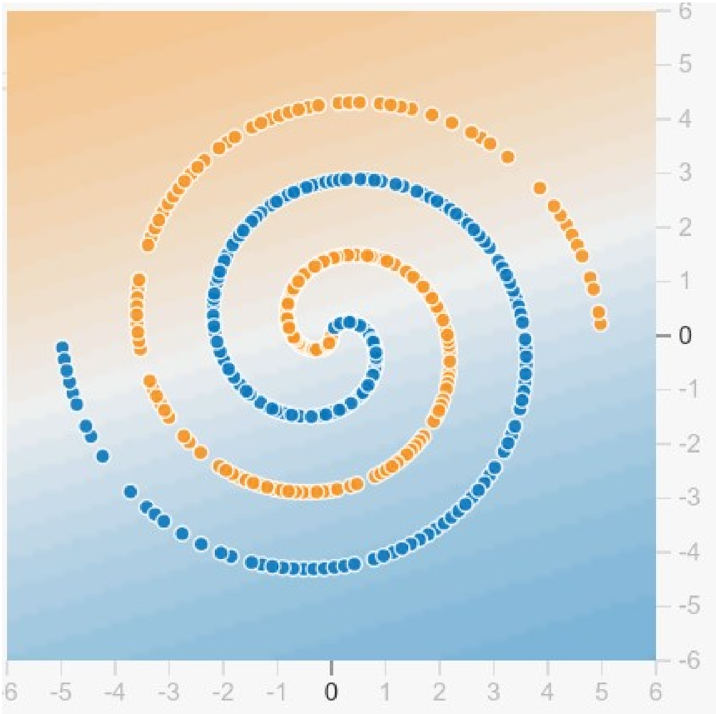
Minsky and Papert, 1969

Perceptrons can only learn linearly separable classes



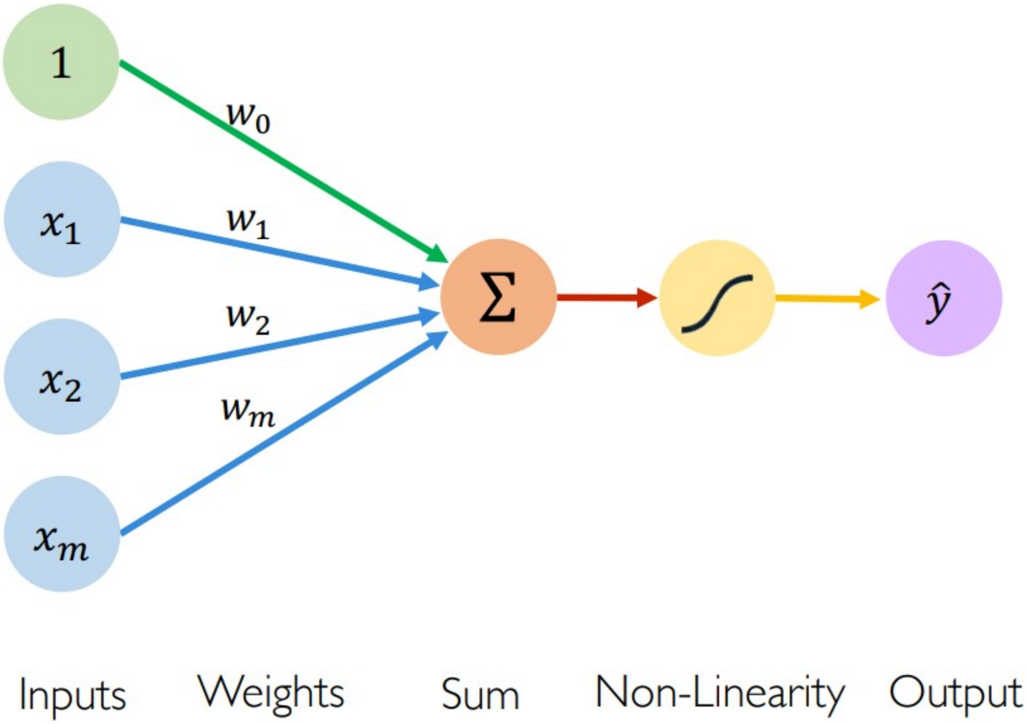
TensorFlow Playground

But sometimes you want to model non-linear functions



How do we make this non-linear then?
Two ingredients to add

1: Differentiable, non-linear activation functions

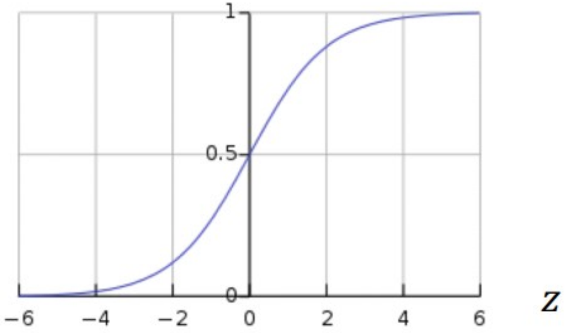


Activation Functions

$$\hat{y} = g\left(w_0 + \boldsymbol{X}^T \boldsymbol{W} \right)$$

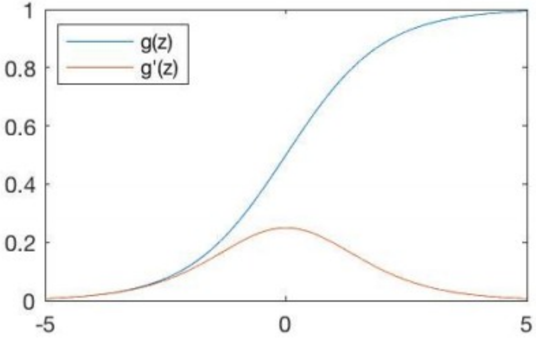
- Example: sigmoid function

$$g(z) = \sigma(z) = \frac{1}{1 + e^{-z}}$$



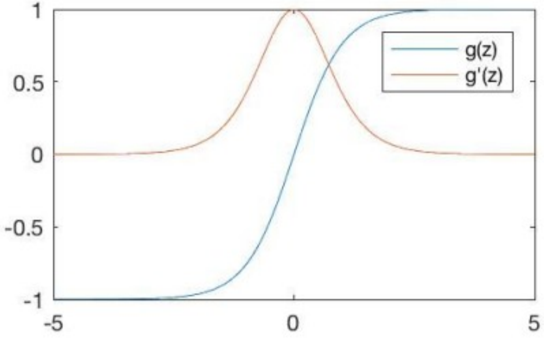
Common activation functions

Sigmoid Function	Hyperbolic Tangent	Rectified Linear Unit (ReLU)



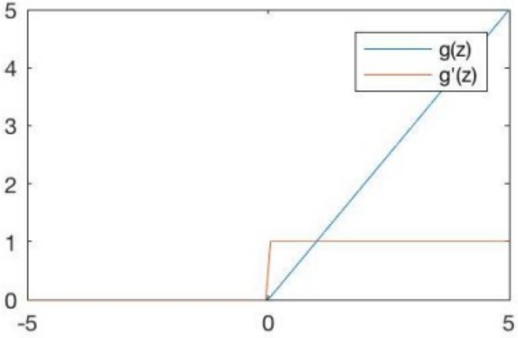
$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$



$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$



$$g(z) = \max(0, z)$$

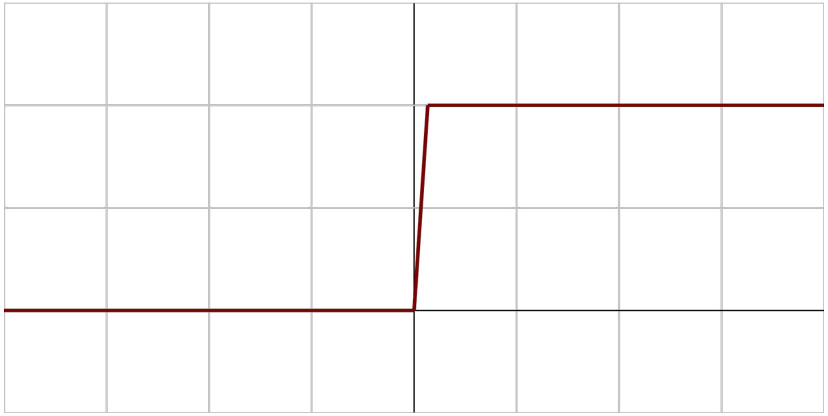
$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

Special case: softmax

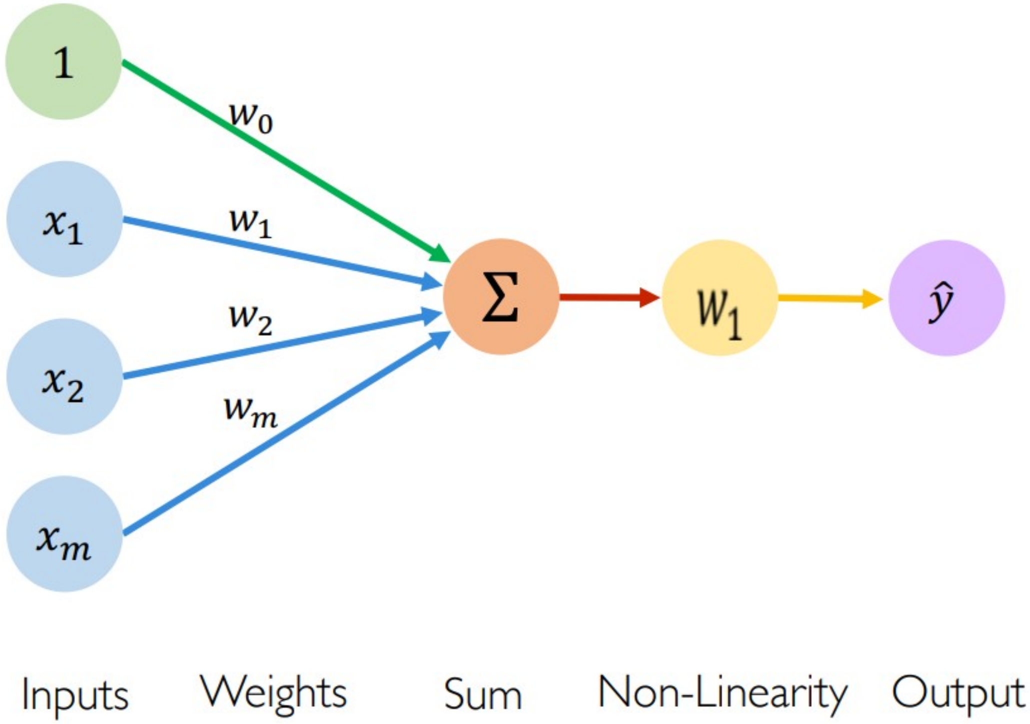
- Used in classification problems
- Given k classes, it decides which one is more likely
- One output per class, each output is assigned a probability from 0 to 1
- The sum of probabilities for all outputs is 1

$$g(z)_j = \frac{e^{z_j}}{\sum_{k=1}^{k} e^{z_k}} \; for\; j = 1, \ldots, k$$

Wait a second, the perceptron already has a non-linear (step) activation function!



This is a perceptron



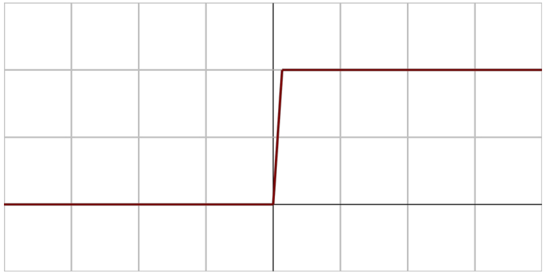
Output

Linear combination of inputs

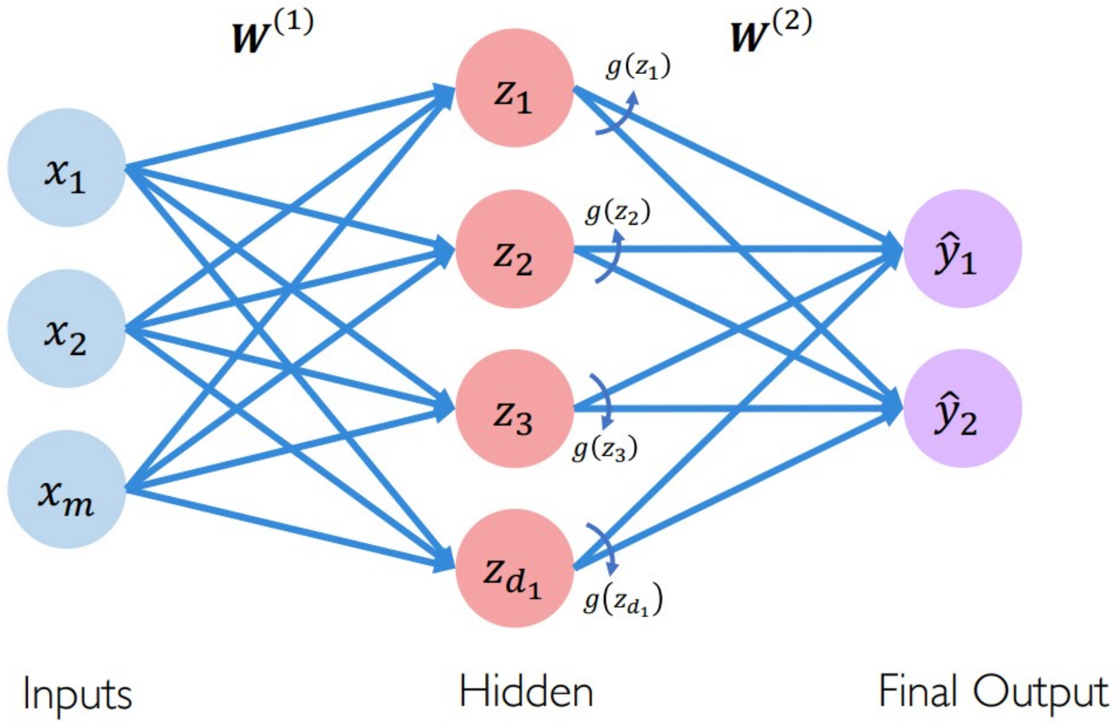
$$\hat{y} = g\left(w_0 + \sum_{i=1}^{m} x_i \, w_i \right)$$

Bias

activation function

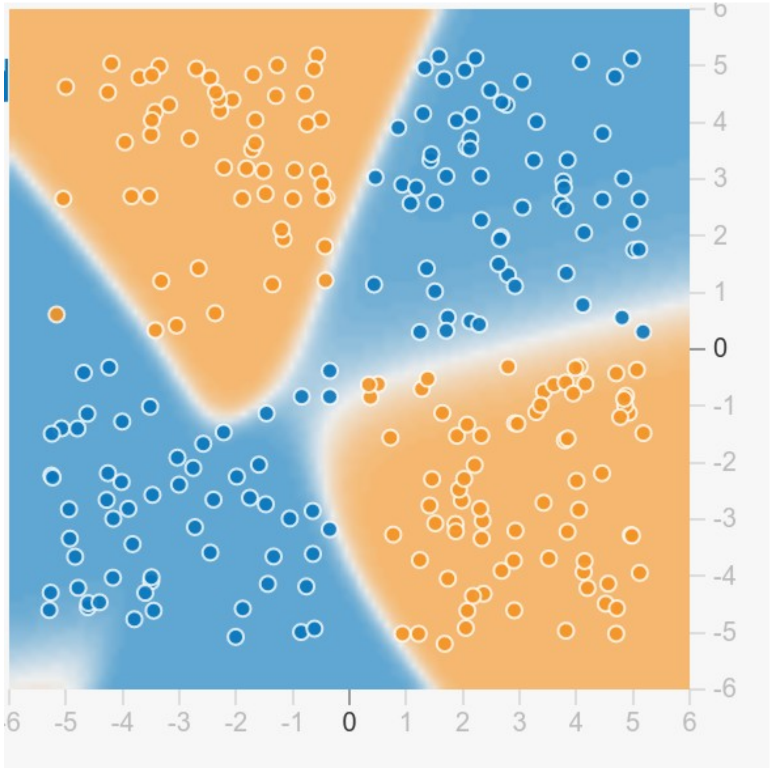


2: Multi-layer Perceptron (1986)

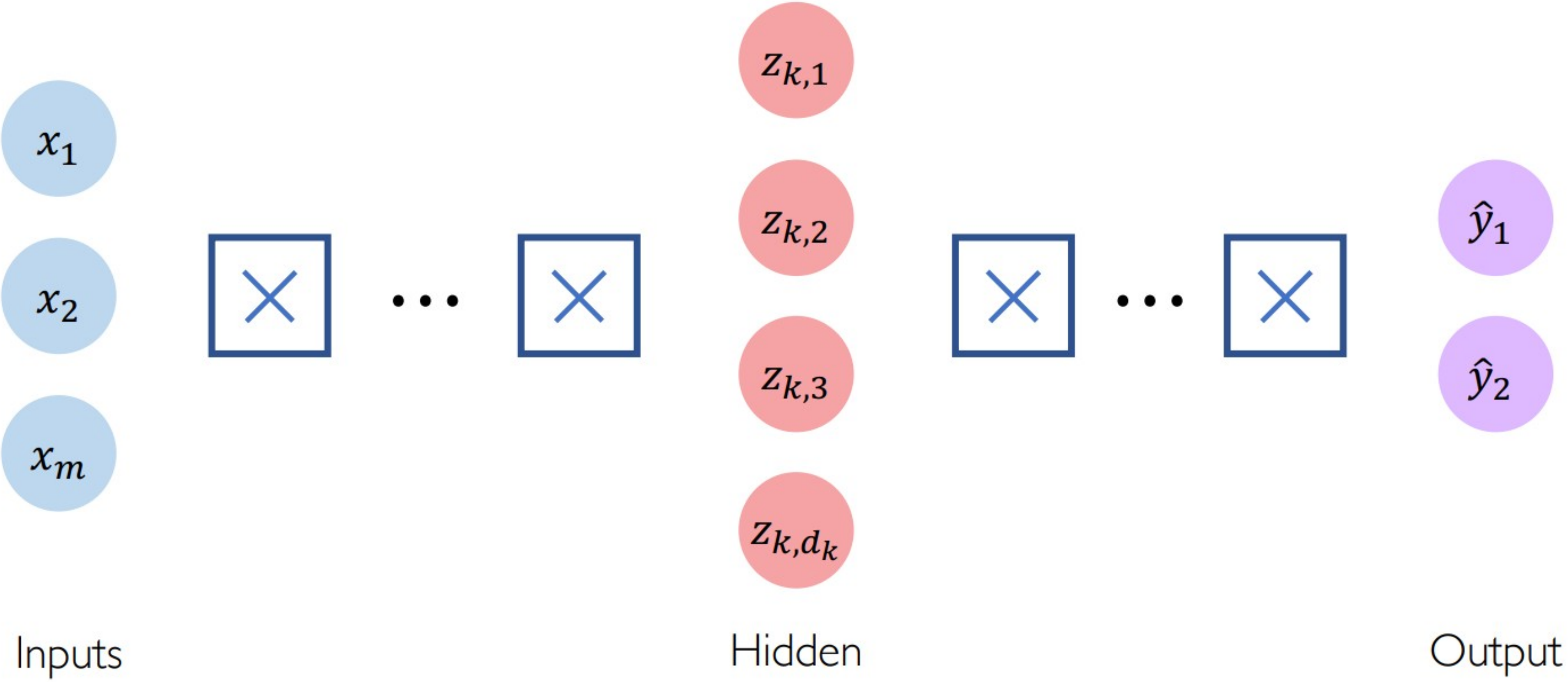


$$z_i = w_{0,i}^{(1)} + \sum_{j=1}^{m} x_j\, w_{j,i}^{(1)} \qquad \hat{y}_i = g\left(w_{0,i}^{(2)} + \sum_{j=1}^{d_1} z_j\, w_{j,i}^{(2)}\right)$$

Now we're getting somewhere

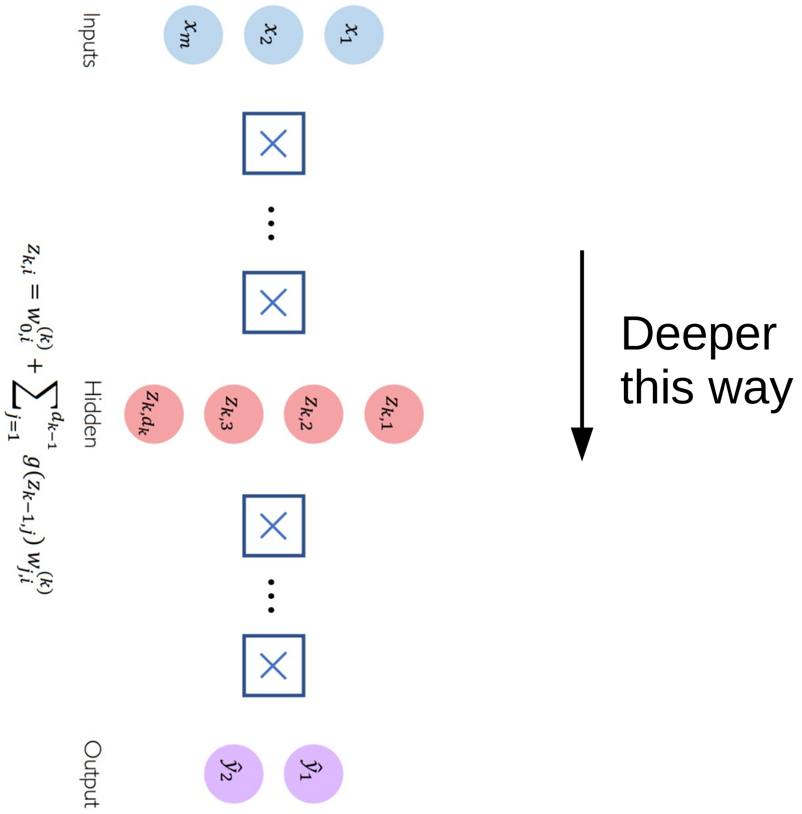


Why stop at one hidden layer?

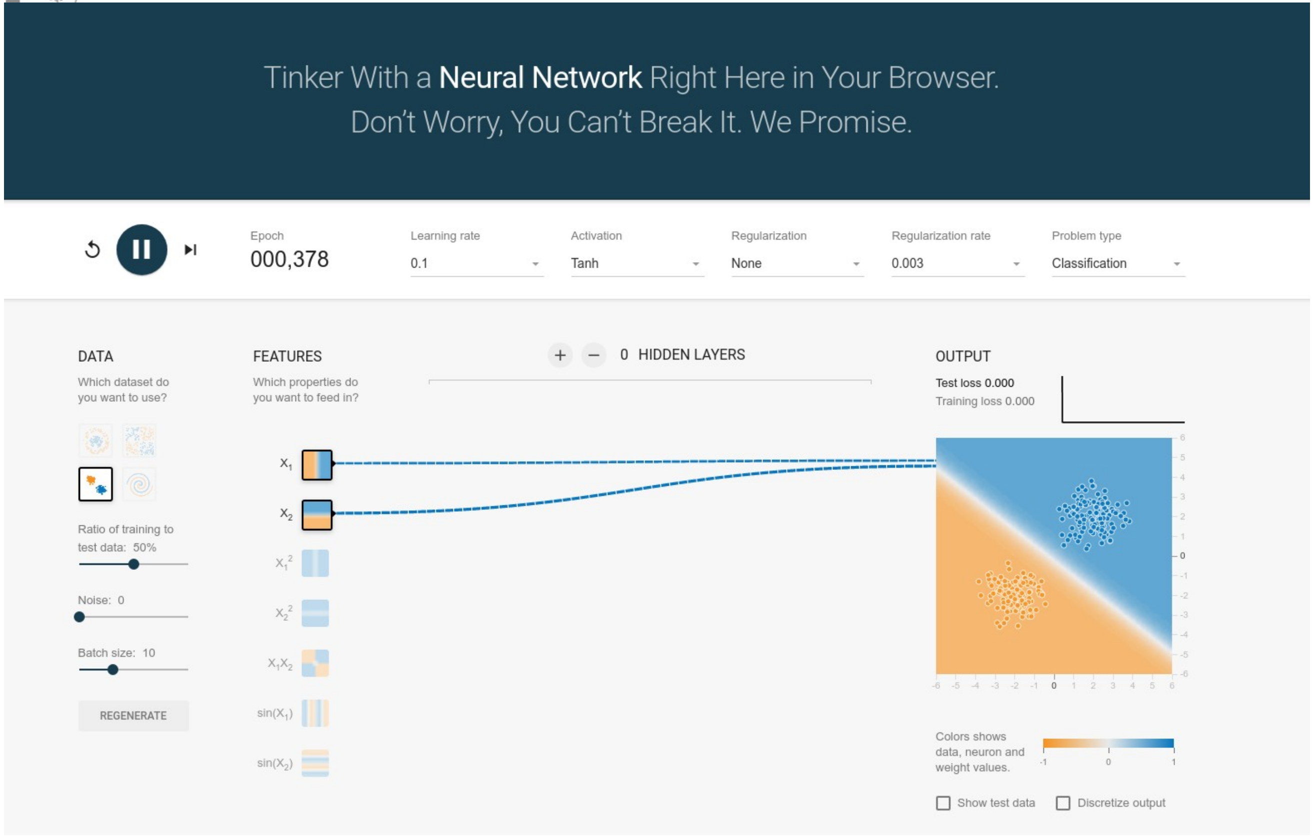


$$z_{k,i} = w_{0,i}^{(k)} + \sum_{j=1}^{d_{k-1}} g(z_{k-1,j})\, w_{j,i}^{(k)}$$

Deep Networks are simply NNs with multiple hidden layers



https://playground.tensorflow.org



Let's review:

- Perceptron
- XOR problem
- Activations
- Multi-layer perceptron

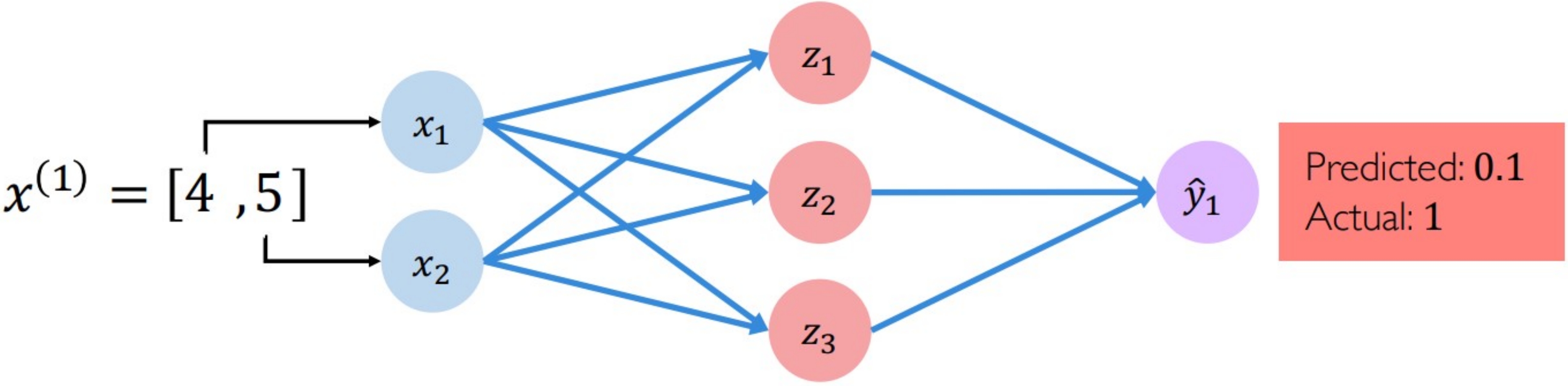
How do we decide which weights are optimal?

- A linear regressor's weights (coefficients) are calculated in closed form

- This can't be done if you have hidden layers and non-linear activations

How do we decide which weights are optimal?

The ***loss*** *of our network measures the cost incurred from incorrect predictions*

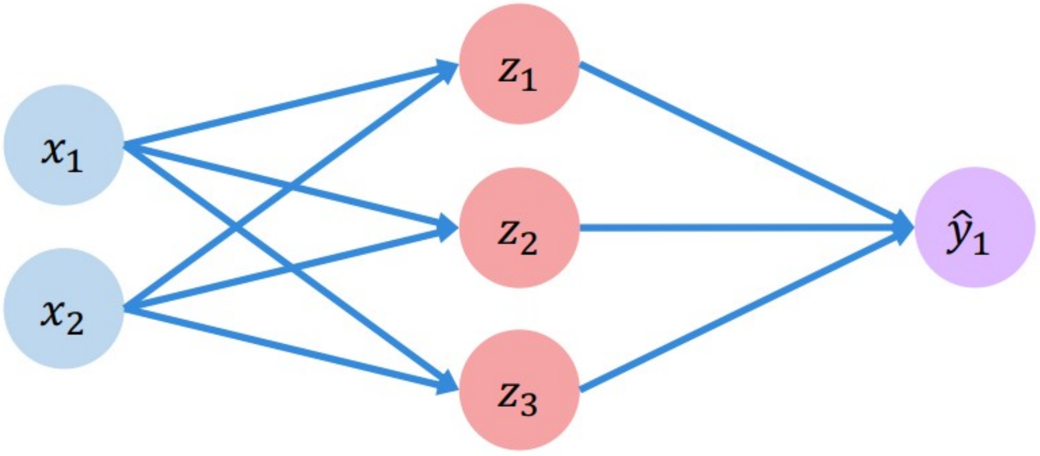


$$\mathcal{L}\Big(\underbrace{f\big(x^{(i)}; \boldsymbol{W}\big)}_{\text{Predicted}}, \underbrace{y^{(i)}}_{\text{Actual}}\Big)$$

How do we decide which weights are optimal?

*The **empirical loss** measures the total loss over our entire dataset*

$$\boldsymbol{X} = \begin{bmatrix} 4, & 5 \\ 2, & 1 \\ 5, & 8 \\ \vdots & \vdots \end{bmatrix}$$



$$f(x) = \begin{bmatrix} 0.1 \\ 0.8 \\ 0.6 \\ \vdots \end{bmatrix} \qquad y = \begin{bmatrix} 1 \\ 0 \\ 1 \\ \vdots \end{bmatrix}$$

$$J(\boldsymbol{W}) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}\Big(\underbrace{f\big(x^{(i)}; \boldsymbol{W}\big)}_{\text{Predicted}}, \underbrace{y^{(i)}}_{\text{Actual}}\Big)$$

Also known as:

- Objective function
- Cost function
- Empirical Risk

Lower loss => better predictions

We want to find the network weights that ***achieve the lowest loss***

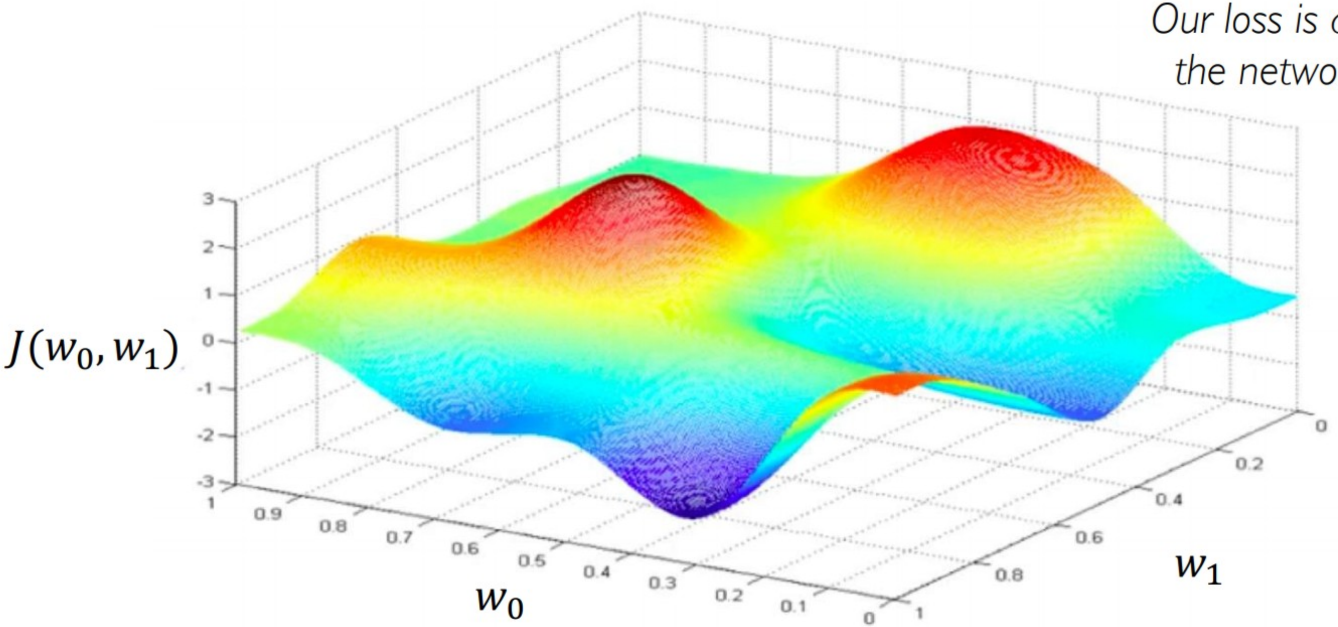
$$\boldsymbol{W}^* = \underset{\boldsymbol{W}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}\left(f\left(x^{(i)}; \boldsymbol{W}\right), y^{(i)}\right)$$

$$\boldsymbol{W}^* = \underset{\boldsymbol{W}}{\operatorname{argmin}}\, J(\boldsymbol{W})$$

Minimizing loss

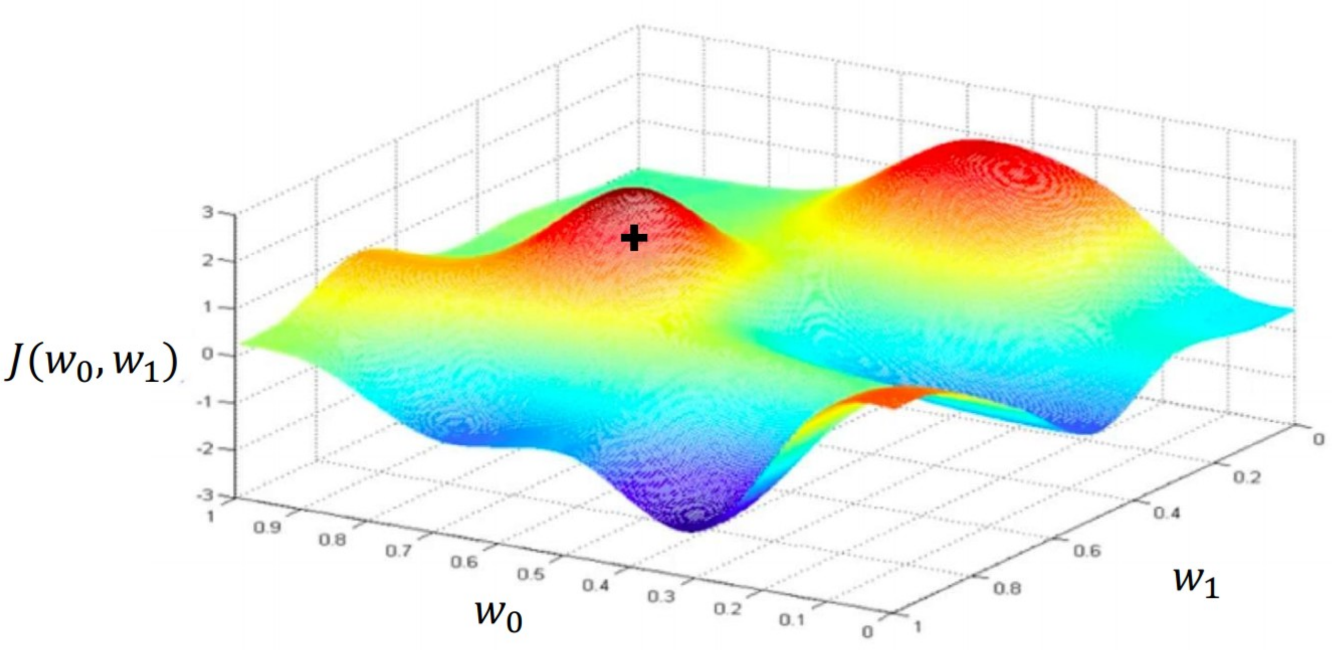
$$\boldsymbol{W}^* = \underset{\boldsymbol{W}}{\operatorname{argmin}}\, J(\boldsymbol{W})$$

Remember:
Our loss is a function of the network weights!



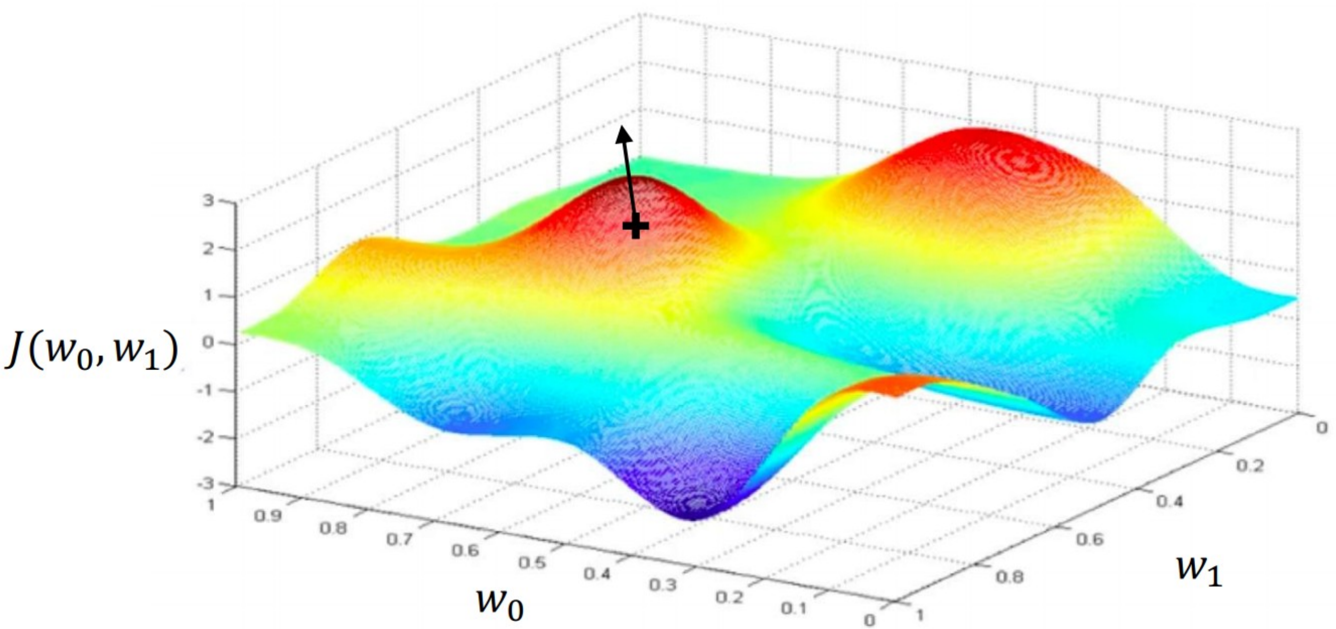
Minimizing loss

Randomly pick an initial (w_0, w_1)

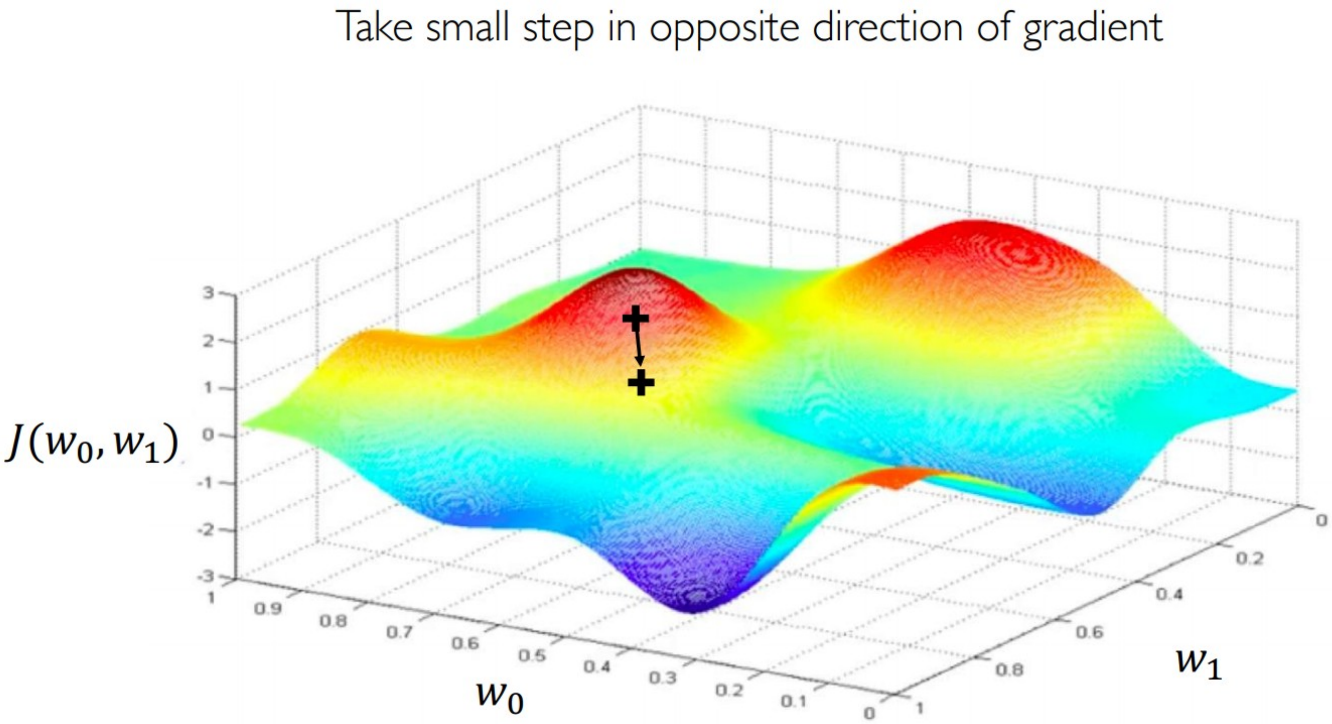


Minimizing loss

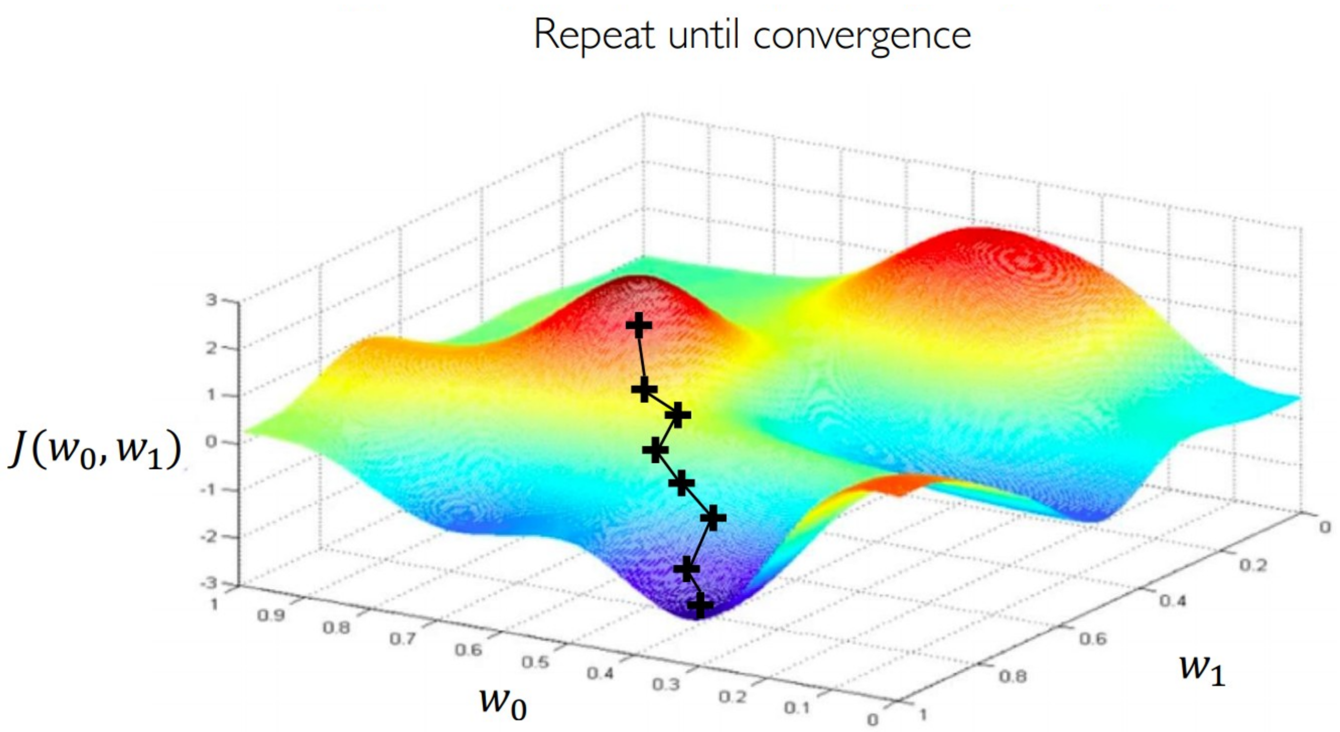
Compute gradient, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$



Minimizing loss



Minimizing loss



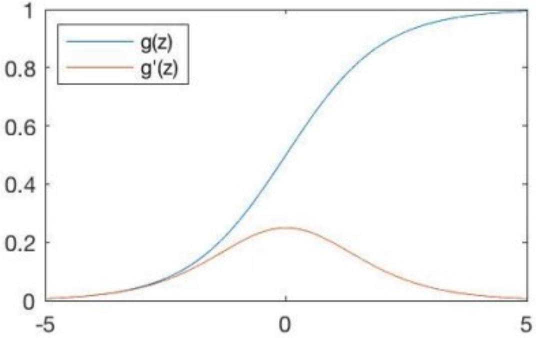
Gradient descent

Algorithm

1. Initialize weights randomly $\sim\mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Compute gradient, $\boxed{\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}}$
4. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5. Return weights

Activation functions have to be differentiable!

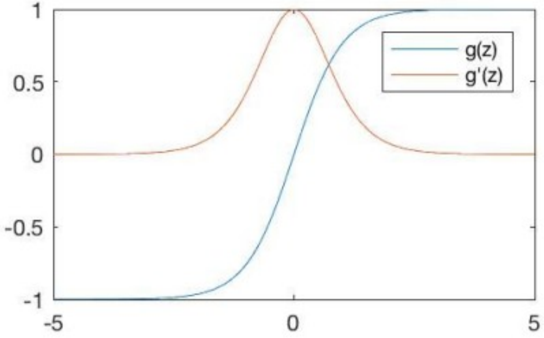
Sigmoid Function



$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

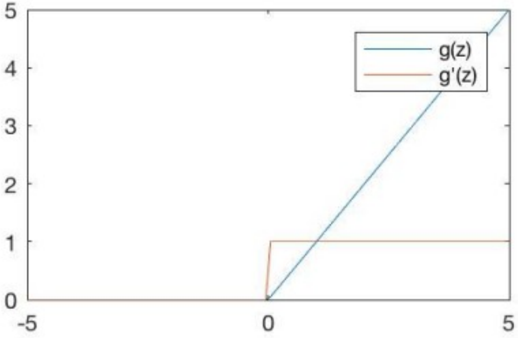
Hyperbolic Tangent



$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

Rectified Linear Unit (ReLU)



$$g(z) = \max(0, z)$$

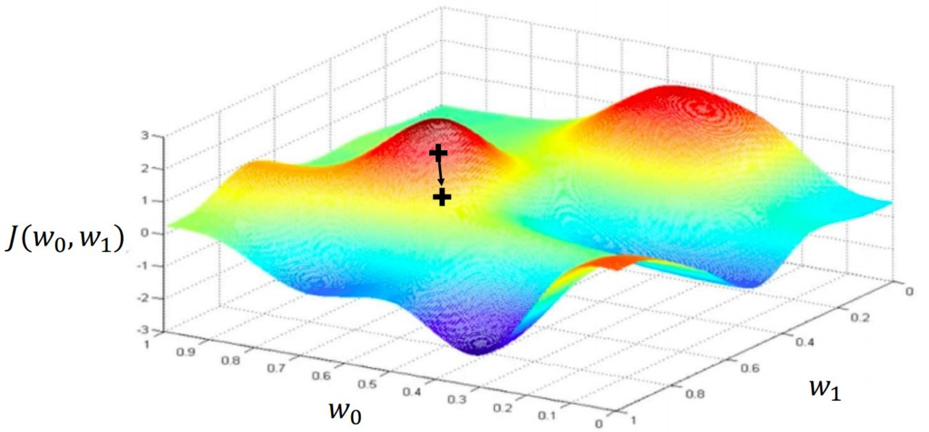
$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

The learning rate η

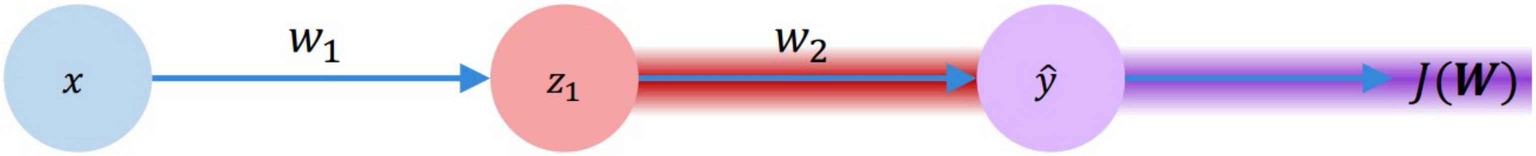
Algorithm

1. Initialize weights randomly $\sim\mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Compute gradient, $\boxed{\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}}$
4. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5. Return weights

Take small step in opposite direction of gradient

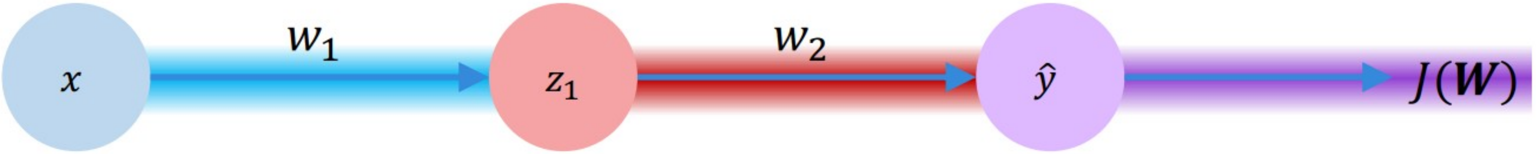


Backpropagation



$$\frac{\partial J(\boldsymbol{W})}{\partial w_2} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial w_2}$$

Backpropagation

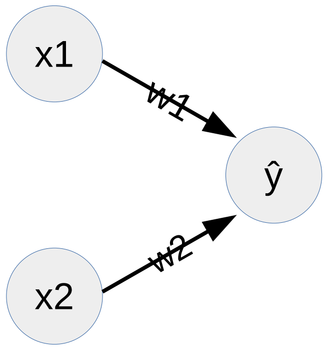


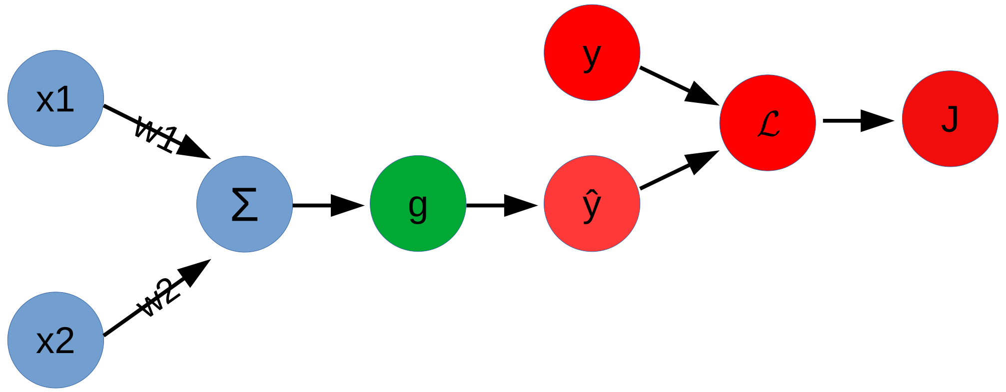
$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial w_1}$$

Backpropagation example, step by step:
https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

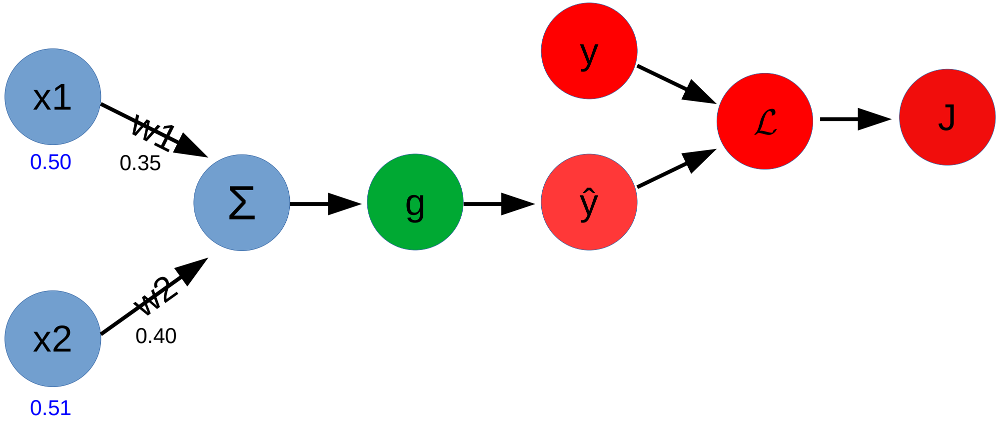
Practical example

- Simple network:
  - Two inputs [x1, x2]
  - Two weights [w1, w2]
  - No bias
  - Activation function g( )
  - One output ŷ
  - One label y
  - Loss function $\mathcal{L}(\ )$
  - Weight-dependent error J(W)





1. Forward pass

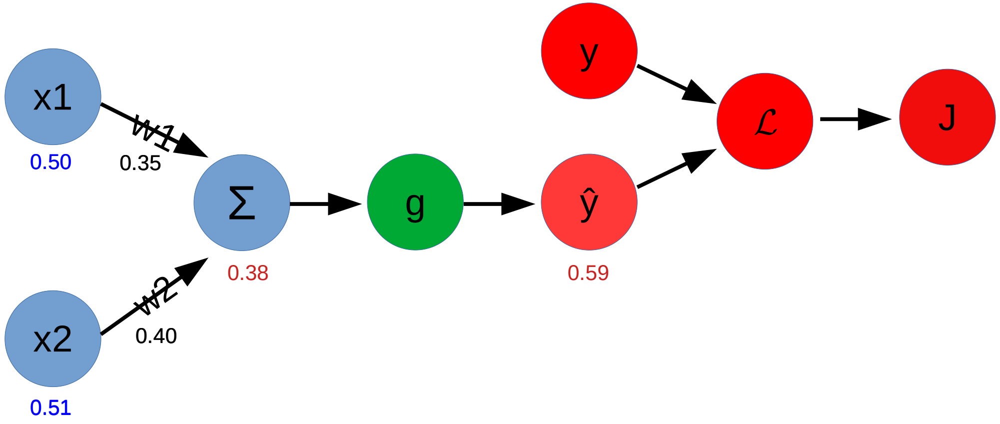


x1 = 0.50
x2 = 0.51

w1 = 0.35
w2 = 0.40

Σ = ?
ŷ = **g(Σ) =** $1/(1+e^{-\Sigma})$ = ?

1. Forward pass

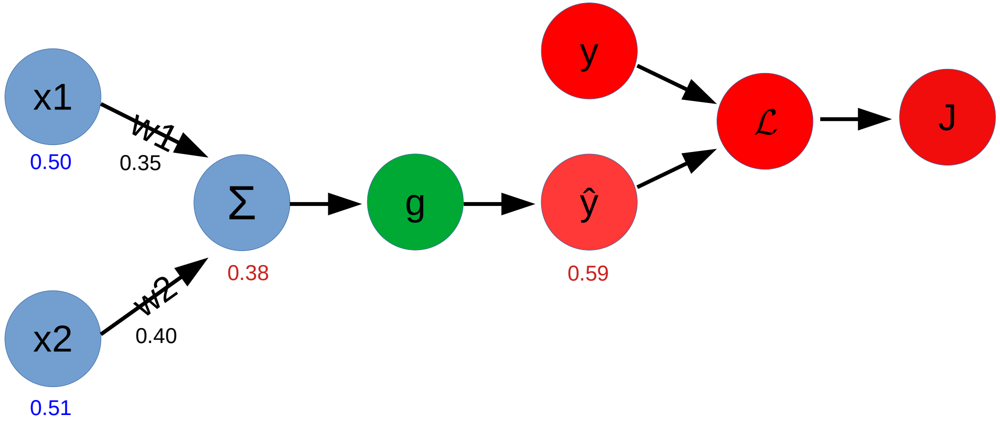


x1 = 0.50
x2 = 0.51

w1 = 0.35
w2 = 0.40

$\boldsymbol{\Sigma}$ = 0.35 * x1 + 0.4 * w2 = 0.38
$\boldsymbol{\hat{y}}$ = $g(\Sigma) = 1/(1+e^{-\Sigma})$ = 0.59

2. Calculate Loss



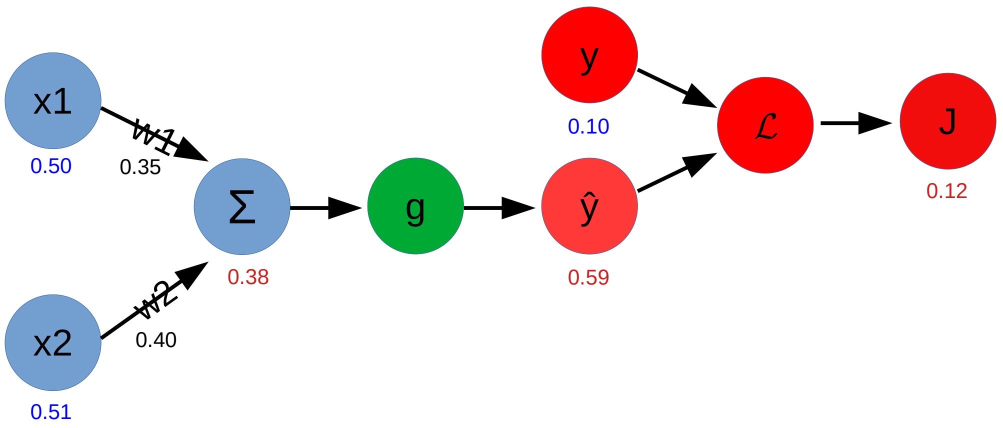
x1 = 0.50
x2 = 0.51

w1 = 0.35
w2 = 0.40

Σ = 0.35 * x1 + 0.4 * w2 = 0.38
ŷ = g(Σ) = $1/(1+e^{-\Sigma})$ = 0.59

Y = 0.10
J(W) = $\mathcal{L}(y, \hat{y}) = ½ * (y – \hat{y})^2$ = ?

2. Calculate Loss



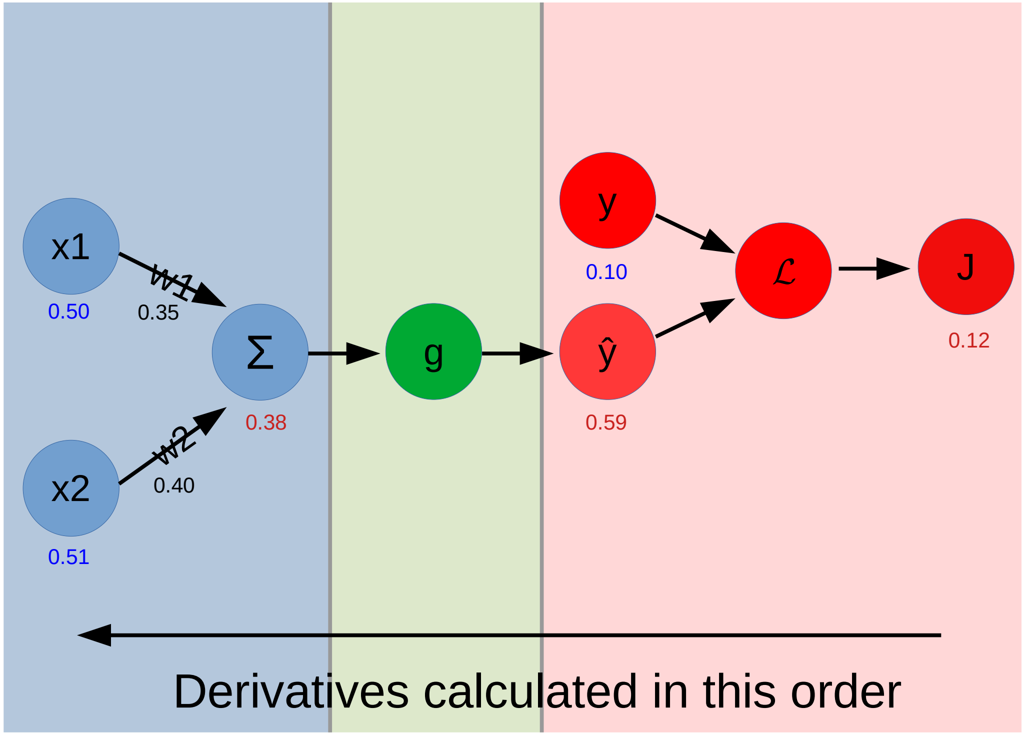
x1 = 0.50
x2 = 0.51

w1 = 0.35
w2 = 0.40

Σ = 0.35 * x1 + 0.4 * w2 = 0.38
ŷ = g(Σ) = $1/(1+e^{-\Sigma})$ = 0.59

Y = 0.10
J(W) = $\mathcal{L}(y, \hat{y}) = \frac{1}{2} * (y - \hat{y})^2$ = 0.12

3. Backpropagate the error



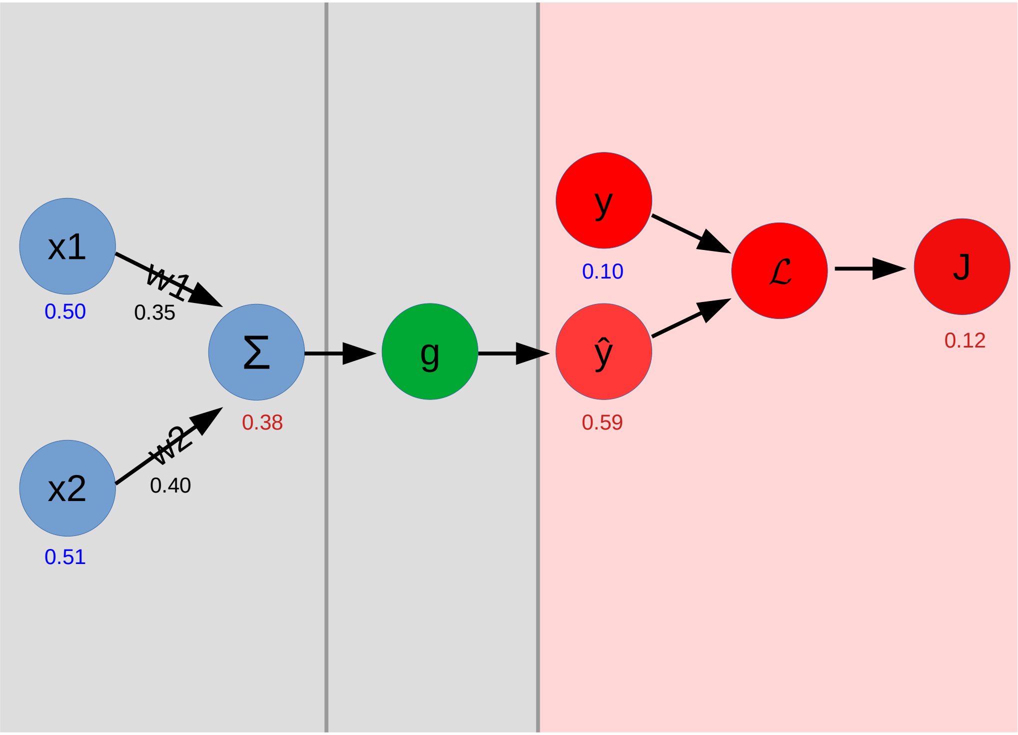
$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = \partial J(W) / \partial \hat{y}$ (loss)

$* \; \partial \hat{y} / \Sigma$ (activation)

$* \; \partial \Sigma / \partial w1$ (weight)

3. Backpropagate the error: loss



$$J(W) = \mathcal{L}(g(X * W))$$

$$\partial J(W)/\partial w1 = \partial J(W) / \partial \hat{y} \quad \text{(loss)}$$

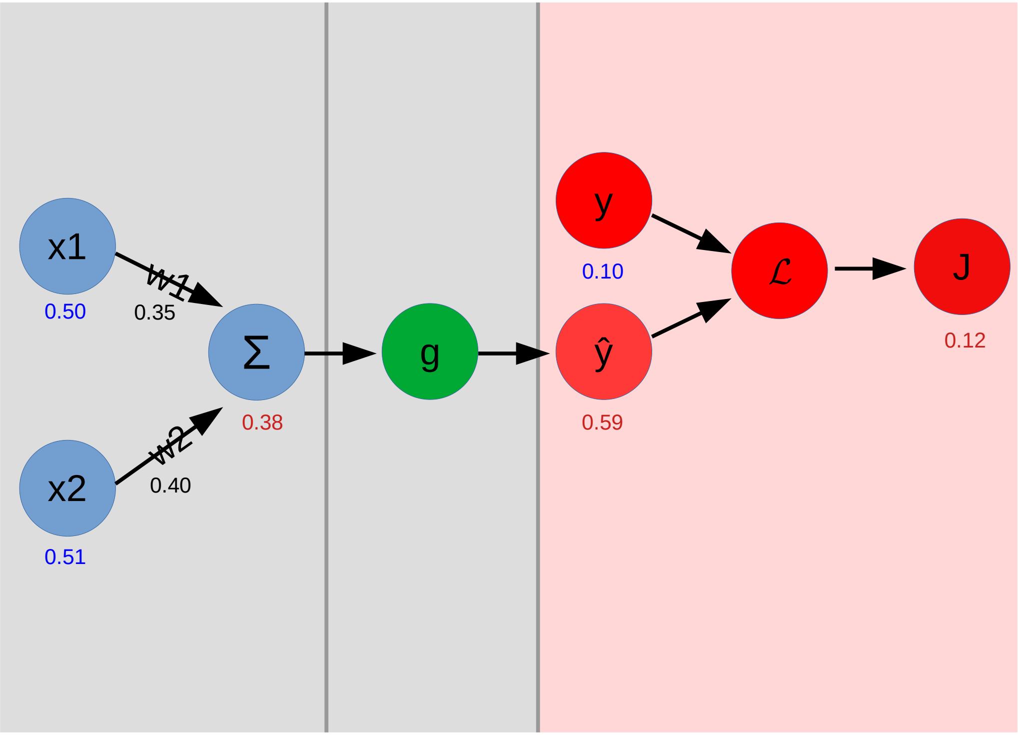
$$* \ \partial \hat{y} / \Sigma \quad \text{(activation)}$$

$$* \ \partial \Sigma / \partial w1 \quad \text{(weight)}$$

$$J(W) = \mathcal{L}(y, \hat{y}) = ½ * (y - \hat{y})^2$$

$$\partial J(W) / \partial \hat{y} = \partial \mathcal{L}(y, \hat{y}) / \partial \hat{y} = ?$$

3. Backpropagate the error: loss



$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = \partial J(W) / \partial \hat{y}$ (loss)

$* \ \partial \hat{y} / \Sigma$ (activation)

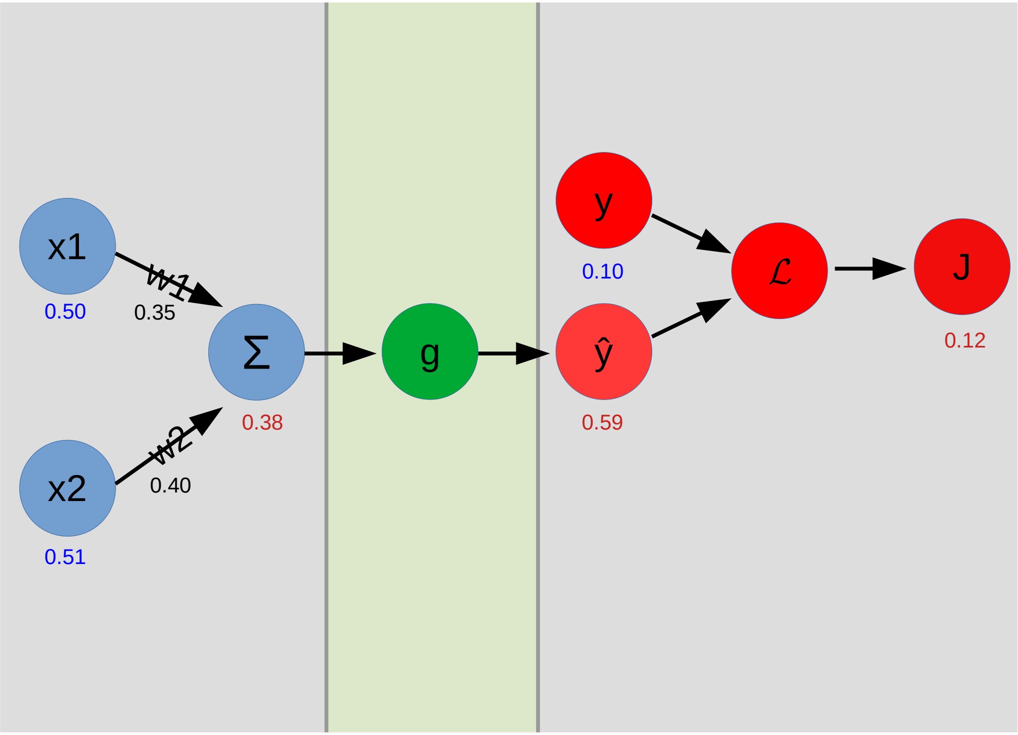
$* \ \partial \Sigma / \partial w1$ (weight)

$J(W) = \mathcal{L}(y, \hat{y}) = ½ * (y – \hat{y})^2$

$\partial J(W) / \partial \hat{y} = 2 * ½ * (y – \hat{y}) * -1$

$= -y + \hat{y} = -0.1 + 0.59 = 0.49$

3. Backpropagate the error: activation



$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = 0.49$ (loss)

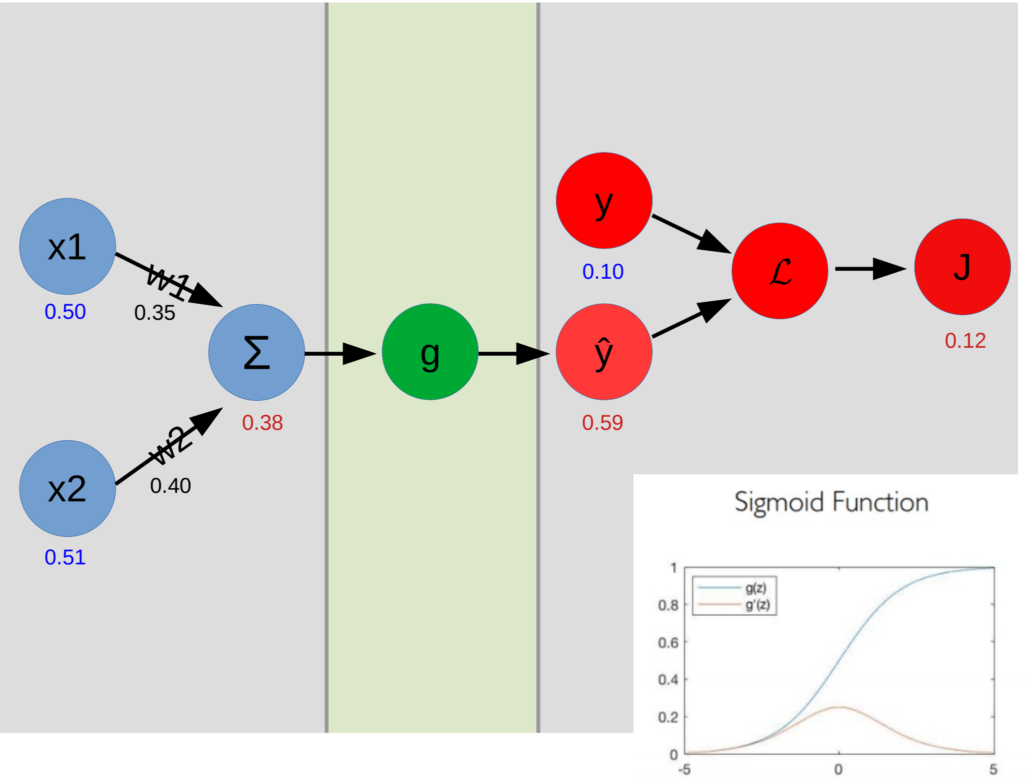
$* \, \partial \hat{y} / \partial \Sigma$ (activation)

$* \, \partial \Sigma / \partial w1$ (weight)

$\hat{\mathbf{y}} = g(\Sigma) = 1/(1+e^{-\Sigma})$

$\partial \hat{y} / \partial \Sigma = ?$

3. Backpropagate the error: activation



$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = 0.49$ (loss)

$* \ \partial \hat{y} / \partial \Sigma$ (activation)

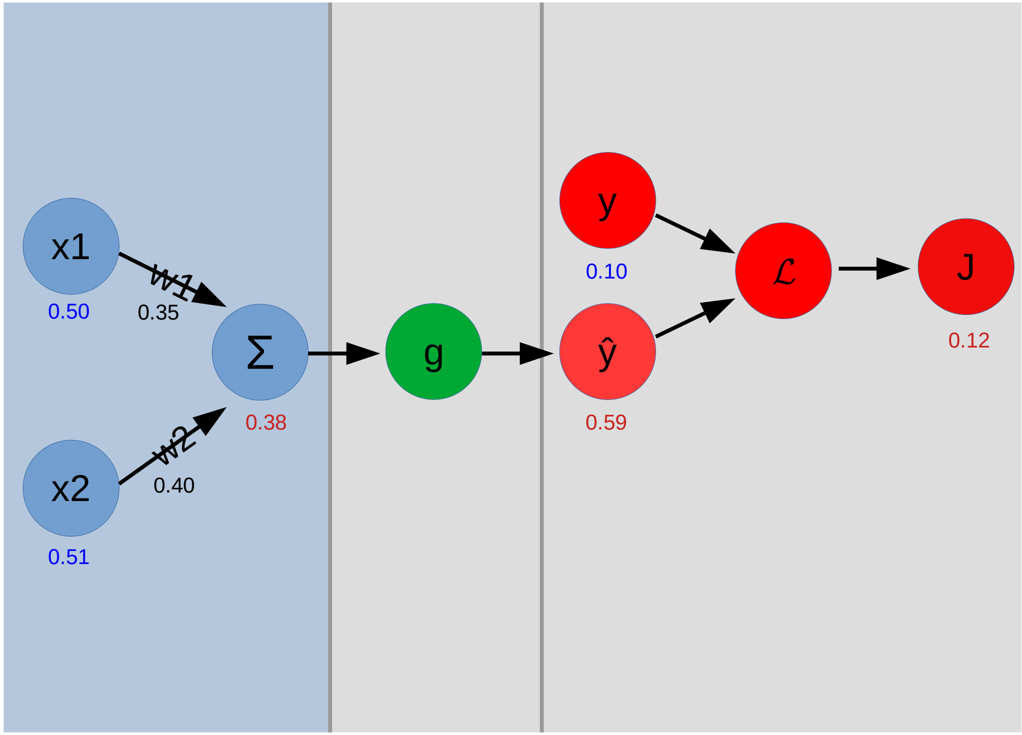
$* \ \partial \Sigma / \partial w1$ (weight)

$\hat{y} = g(\Sigma) = 1/(1+e^{-\Sigma})$

$\partial \hat{y} / \partial \Sigma = 1/(1+e^{-\Sigma}) * (1 - 1/(1+e^{-\Sigma}))$

$= 0.24$

3. Backpropagate the error: weight



$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = 0.49$ (loss)

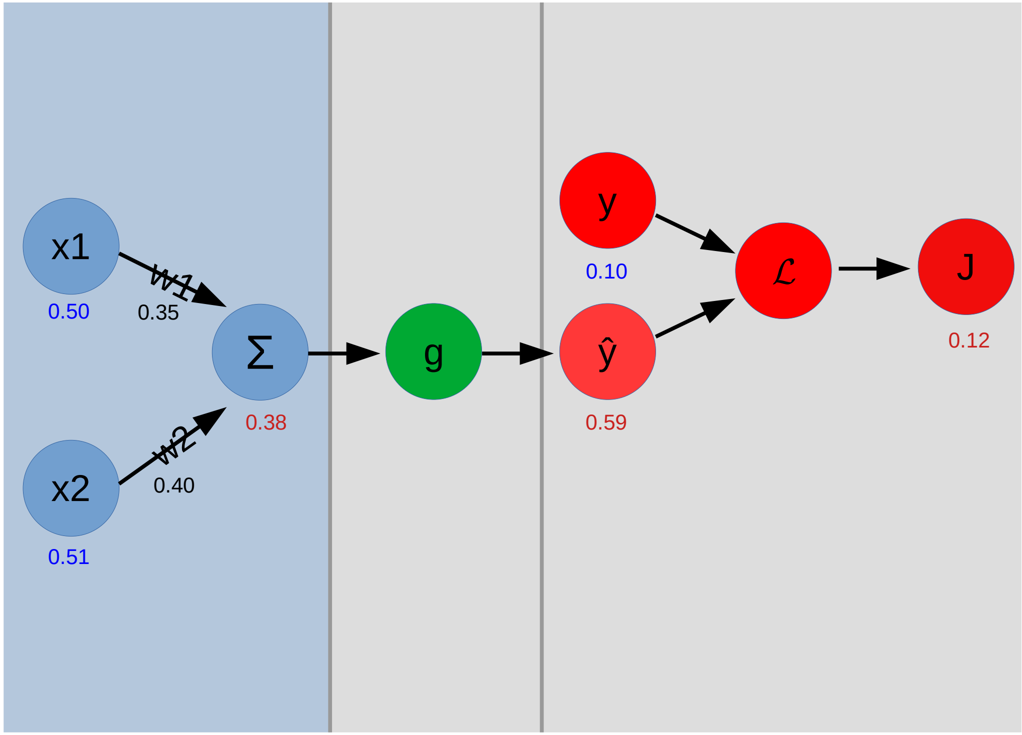
$* \ 0.24$ (activation)

$* \ \partial\Sigma / \partial w1$ (weight)

$\Sigma = X * W = x1 * w1 + x2 * w2$

$\partial\Sigma/\partial w1 = ?$

3. Backpropagate the error: weight



$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = 0.49$ (loss)

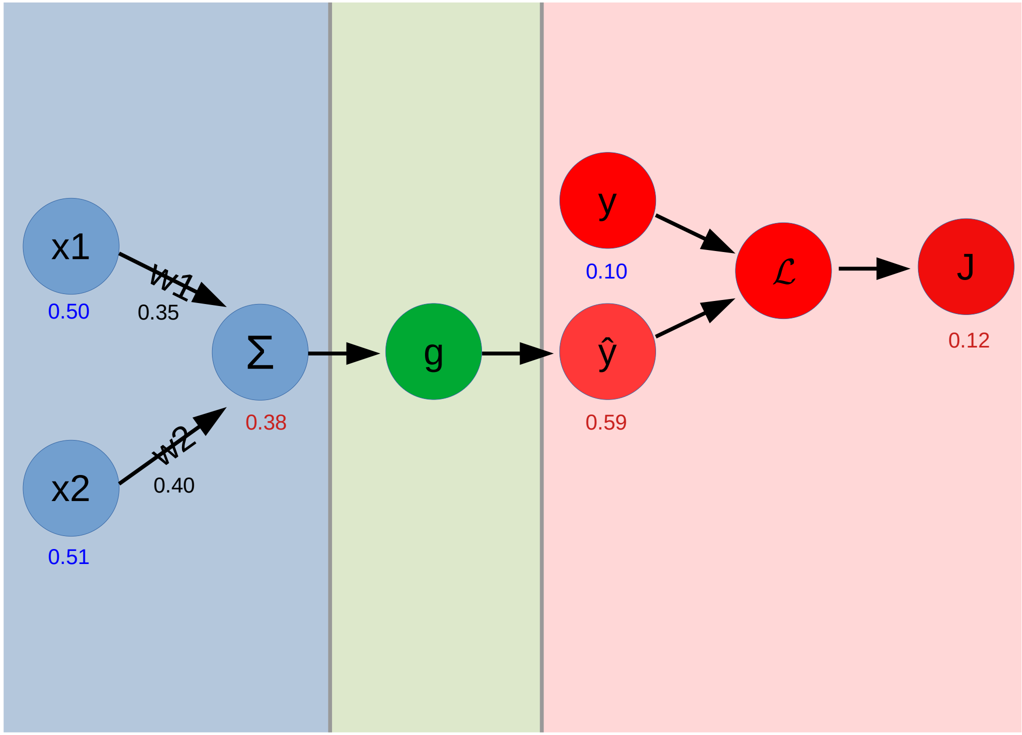
$* \ 0.24$ (activation)

$* \ \partial \Sigma / \partial w1$ (weight)

$\Sigma = X * W = x1 * w1 + x2 * w2$

$\partial \Sigma / \partial w1 = x1 + 0 = 0.5$

4. Weight update



$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = 0.49$ (loss)

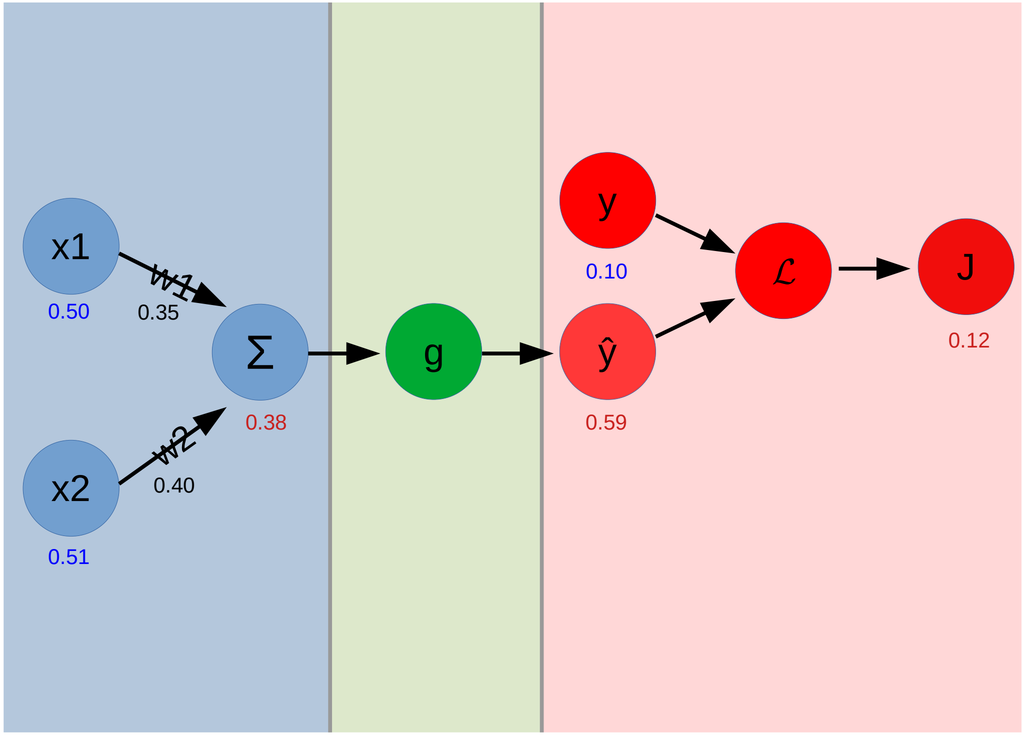
$* \ 0.24$ (activation)

$* \ 0.51$ (weight)

$= 0.06$ (gradient)

$w1' = ?$

4. Weight update



$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = 0.49$ (loss)

$* \; 0.24$ (activation)

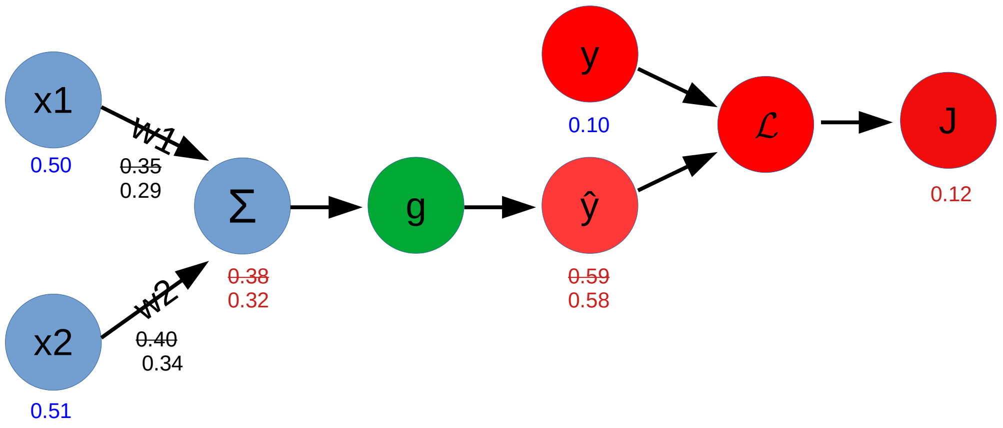
$* \; 0.51$ (weight)

$= 0.06$ (gradient)

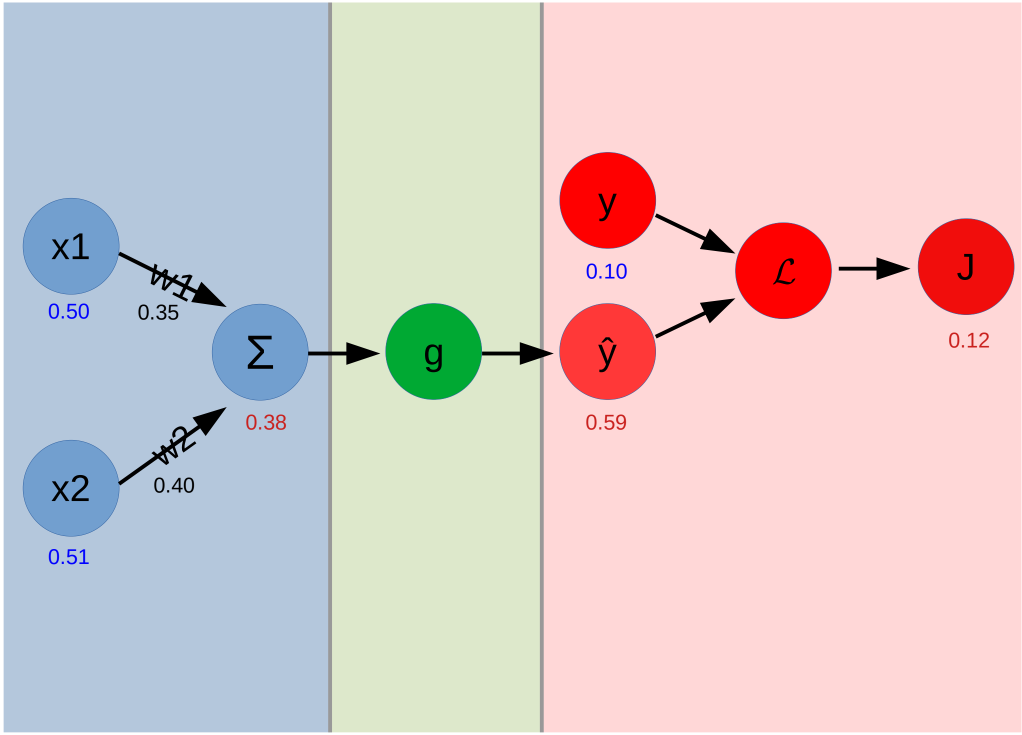
$w1' = w1 - \eta * 0.06 = 0.35 - 0.06 = 0.29$

Exercise

- Can you calculate the weight update for w2? How many new gradients do you need to calculate?
- What is the new predicted output? Has the error gone down?
- What if I had another layer before this one?



4. Weight update



$J(W) = \mathcal{L}(g(X * W))$

$\partial J(W)/\partial w1 = 0.49$ (loss)

$* \ 0.24$ (activation)

$* \ 0.51$ (weight)

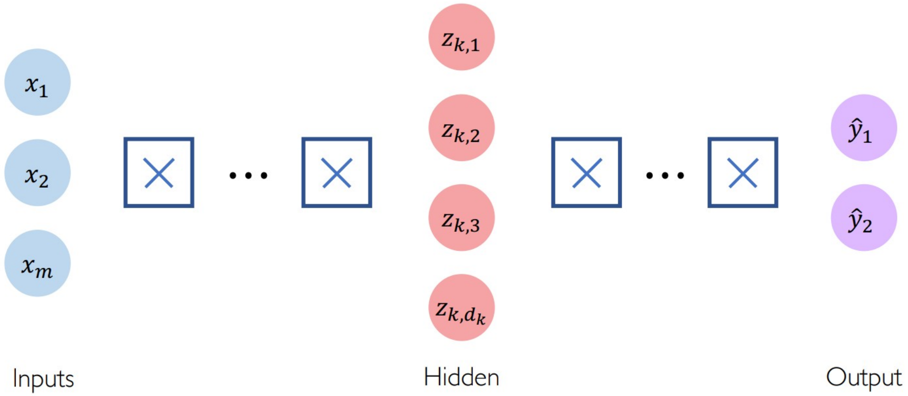
$= 0.06$ (gradient)

$w1' = w1 - \eta * 0.06 = 0.35 - 0.06 = 0.29$

$W2' = w2 - \eta * 0.06 = 0.4 - 0.06 = 0.34$

Gradient vanishing

- What happens if we backpropagate on a network with many (N > k > 1) hidden layers?



$$z_{k,i} = w_{0,i}^{(k)} + \sum_{j=1}^{d_{k-1}} g(z_{k-1,j})\, w_{j,i}^{(k)}$$

$$\partial J/\partial W1 = \partial J/\partial \hat{Y} * \partial \hat{Y}/\partial \Sigma_N * \partial \Sigma_N/\partial W_N * \ldots * \partial Z_k/\partial \Sigma_k * \partial \Sigma_k/\partial W_k * \ldots\ \partial Z_1/\partial \Sigma_1 * \partial \Sigma_1/\partial W_1$$

Gradient vanishing

- These are all “zero-point-somethings” multiplied by each other
- So the gradient becomes smaller by orders of magnitudes as we go back more and more layers until it’s so small that the network is stuck

$$\partial E/\partial W1 = \partial J/\partial \hat{Y} * \partial \hat{Y}/\partial \Sigma_N * \partial \Sigma_N/\partial W_N * ... * \partial Z_k/\partial \Sigma_k * \partial \Sigma_k/\partial W_k * \dots \partial Z_1/\partial \Sigma_1 * \partial \Sigma_1/\partial X_1 = O(10^{-N})$$

initial w1 = 0.5
optimal w1 = -0.2
5-layer gradient ~0.00001

How many iterations do we need to get from 0.5 to -0.2?