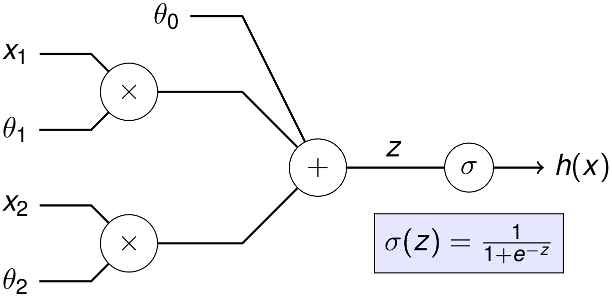
DD2418 Language Engineering
7a: Neural networks basics

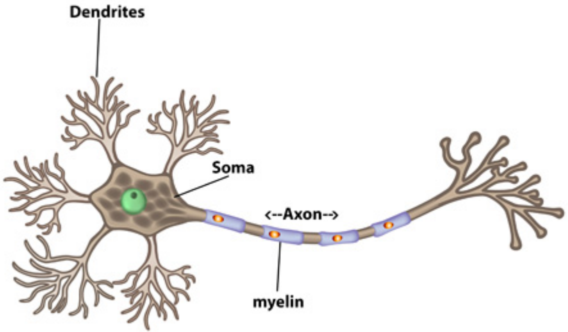
Johan Boye, KTH

Binary logistic regression

- Represent data as n-ary vectors of features $x = (x_1, \ldots, x_n)$.
- The model consists of weights $\theta_0, \theta_1, \ldots, \theta_n$.
- The result $h(x)$ is interpreted as the probability that x belongs to the positive class.

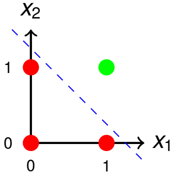


Biological inspiration: The neuron



An artificial neuron cannot compute XOR

AND is linearly separable:



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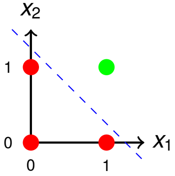
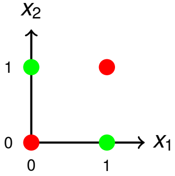


XOR is *not* linearly separable:



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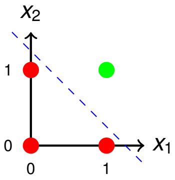

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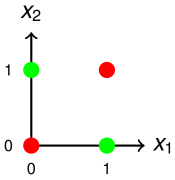
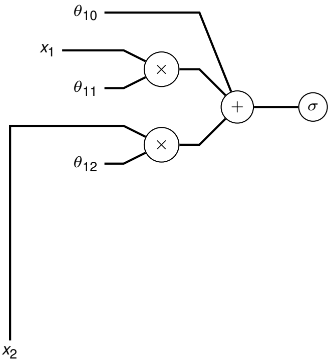
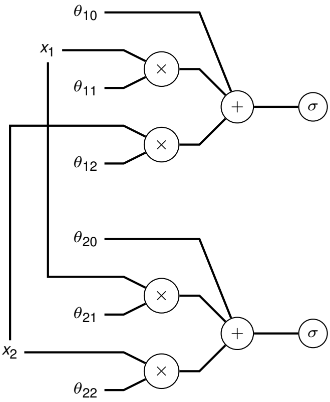


Solution: Use several connected artificial neurons.

Using three neurons



Using three neurons



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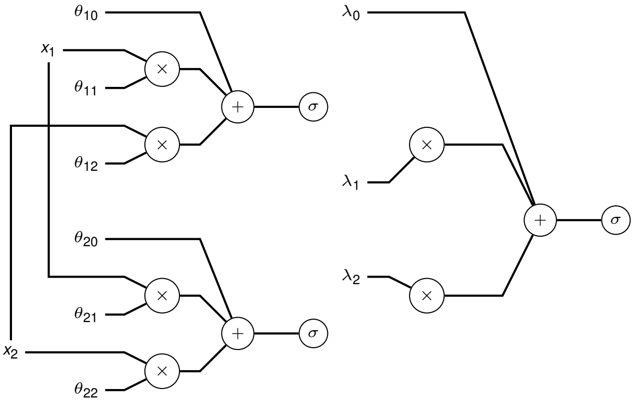
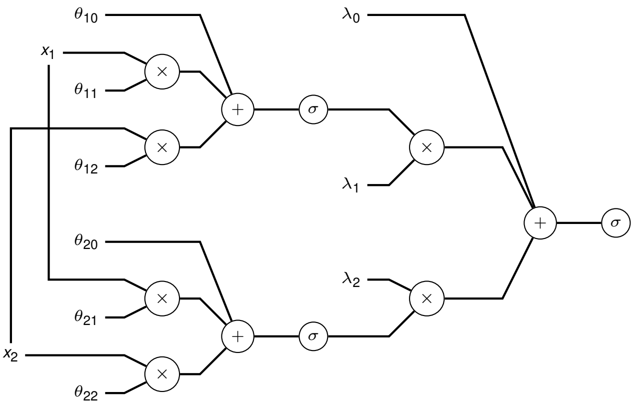
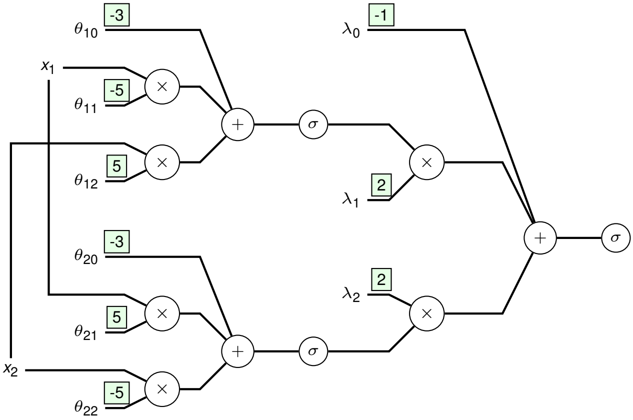


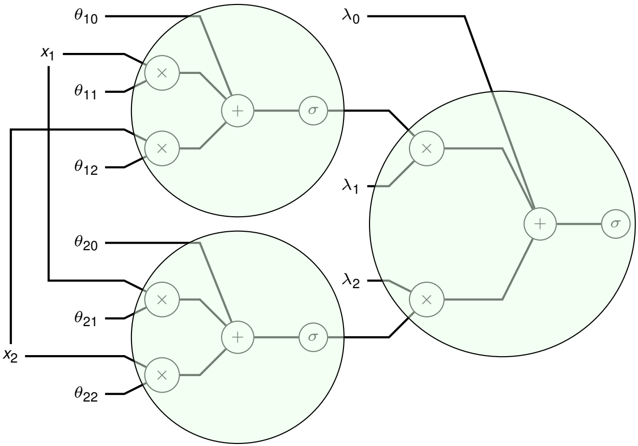
Using three neurons



Solving XOR using three neurons



Simplifying the picture



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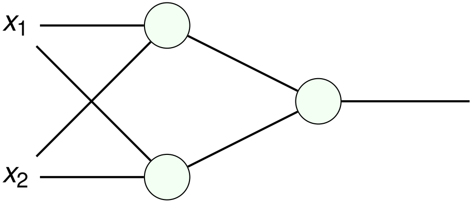

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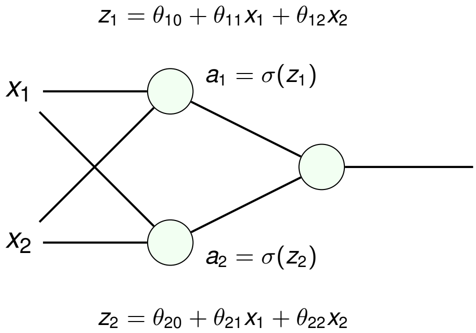

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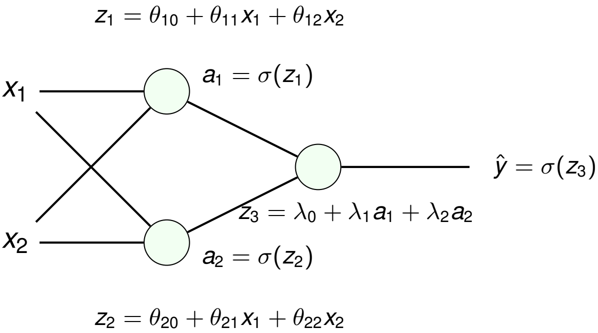
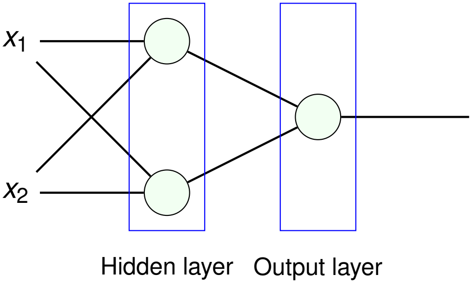
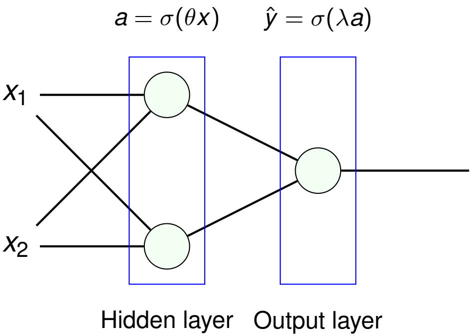


Layers



Vector notation

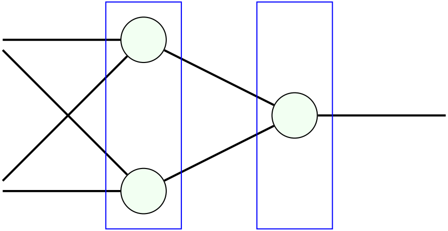


Example revisited

$$\theta = \begin{pmatrix} -3 & -5 & 5 \\ -3 & 5 & -5 \end{pmatrix}$$

$$\lambda = \begin{pmatrix} -1 & 2 & 2 \end{pmatrix}$$

$$x = \begin{pmatrix} 1 \\ x_1 \\ x_2 \end{pmatrix}$$

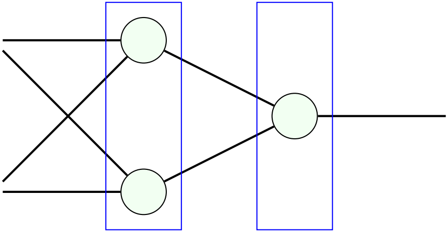


Alternative notation

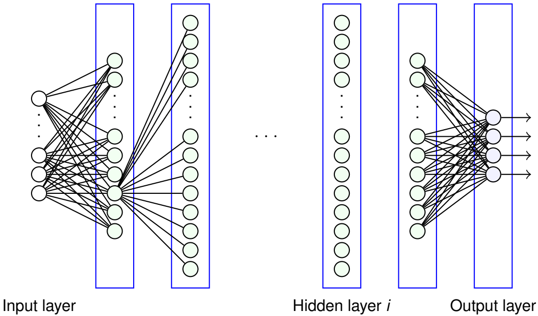
$$\theta = \begin{pmatrix} -5 & 5 \\ 5 & -5 \end{pmatrix} \quad b_\theta = \begin{pmatrix} -3 \\ -3 \end{pmatrix} \quad \lambda = \begin{pmatrix} 2 & 2 \end{pmatrix} \quad b_\lambda = -1$$

$$a = \sigma(\theta x + b_\theta) \qquad \hat{y} = \sigma(\lambda a + b_\lambda)$$

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$



Feed-forward networks



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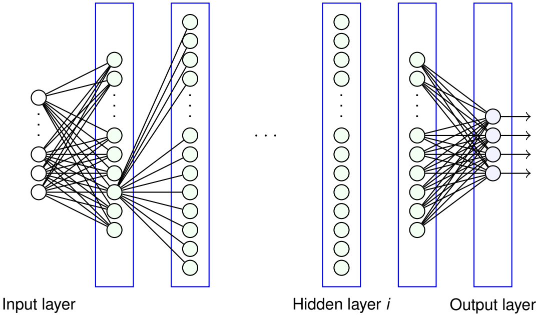


For hidden layer 1:
$$z_1 = \theta_1 x$$
$$a_1 = g_1(z_1)$$

For hidden layer i:
$$z_i = \theta_i a_{i-1}$$
$$a_i = g_i(z_i)$$

For the output layer:
$$z_n = \theta_n a_{n-1}$$
$$\hat{y} = g_n(z_n)$$

where each g_i is some non-linear function.

Feed-forward networks

- The network computes a non-linear function of the input: $\hat{y} = f(x)$
- Each layer computes a linear and a non-linear transformation of the input
- The network thus computes a composition of functions

$$f = f_1 \circ f_2 \circ \ldots \circ f_n$$

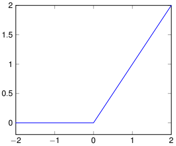
where each function f_i is parametrized by θ_i.

Activation functions

The activation function is a non-linear function.
Most commonly used are:

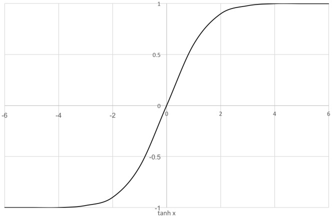
[Rectified Linear Unit (RELU)

$z = \max(0, x)$

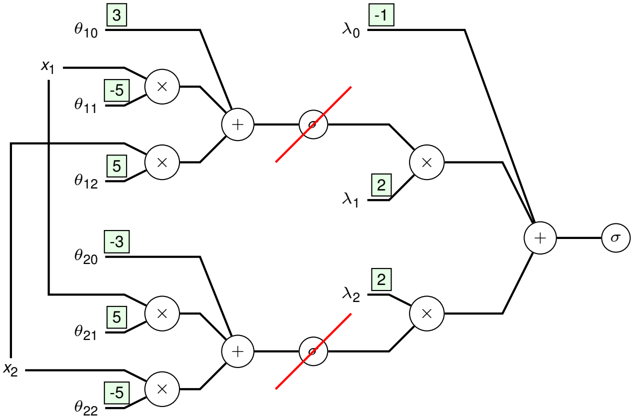


Hyperbolic tangent (tanh)

$z = \frac{e^x - e^{-x}}{e^x + e^{-x}}$



Are non-linearities essential?



Are non-linearities essential?

Yes.

Otherwise, we would have in each layer

$$a_i = \theta_i a_{i-1}$$

and thus

$$\hat{y} = \theta_n(\theta_{n-1}(\dots\theta_1 x\dots))$$

But then we could simply multiply the matrices:

$$\theta = \theta_n \theta_{n-1} \dots \theta_1$$

and let $\hat{y} = \theta x$.

That is, a multi-layer network without non-linear transformations is equivalent to a single neuron!

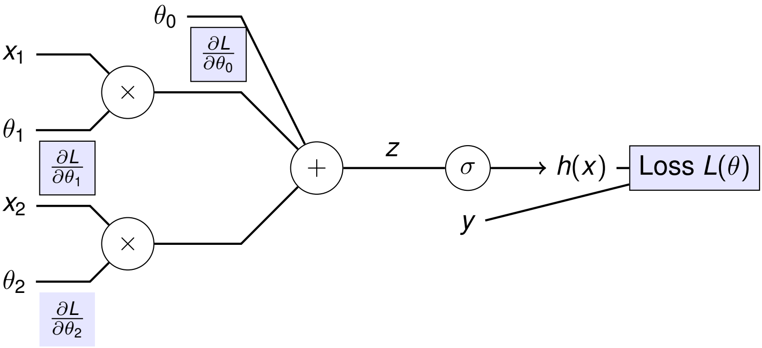
DD2418: Language Engineering
7b: Training neural networks

Johan Boye, KTH

Learning in logistic regression

To do gradient descent, we need to...

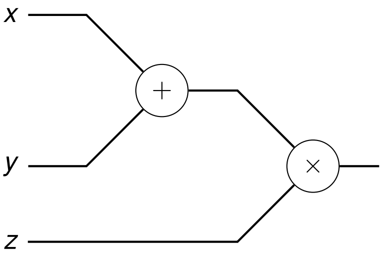
- ... do a *forward pass* to compute the predicted value,
- ... followed by a *backward pass* where we compute the gradient of the loss function



Backward differentiation (backpropagation)

Consider a simpler example (borrowed from A. Karpathy):

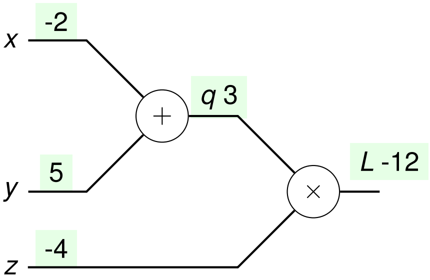
$$L(x, y, z) = (x + y)z$$



Backward differentiation (backpropagation)

$L(x, y, z) = (x + y)z$

$x = -2, y = 5, z = -4$

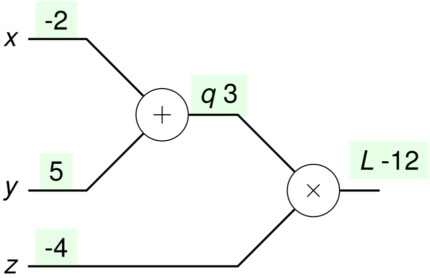


Backward differentiation (backpropagation)

$L(x, y, z) = (x + y)z$

$$\boxed{q = x + y,\ \frac{\partial q}{\partial x} = 1,\ \frac{\partial q}{\partial y} = 1}$$

$x = -2, y = 5, z = -4$



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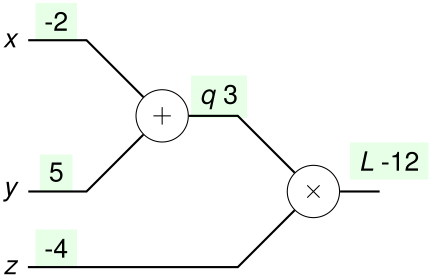
$$\boxed{L = qz,\ \frac{\partial L}{\partial q} = z,\ \frac{\partial L}{\partial z} = q}$$



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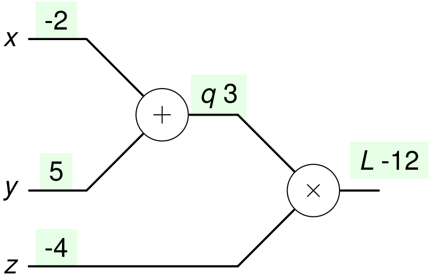
We seek $\frac{\partial L}{\partial x}, \frac{\partial L}{\partial y}, \frac{\partial L}{\partial z}$



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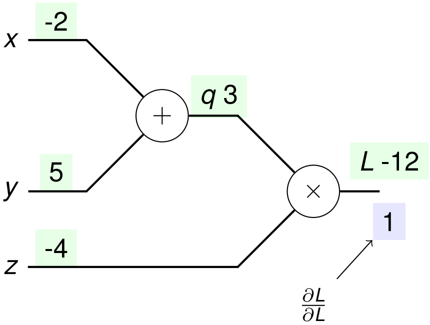

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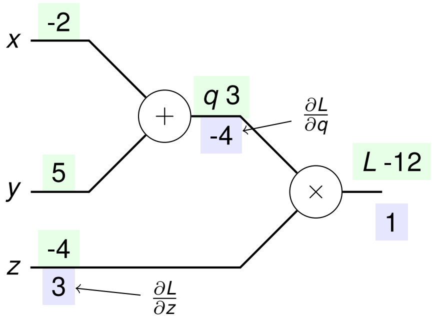

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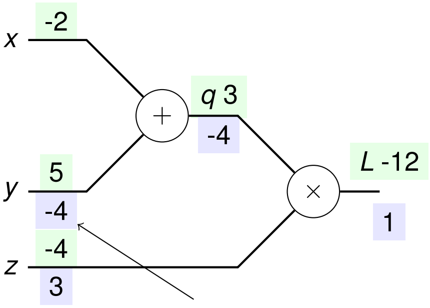

$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial q}\frac{\partial q}{\partial y}$$

Backward differentiation (backpropagation)

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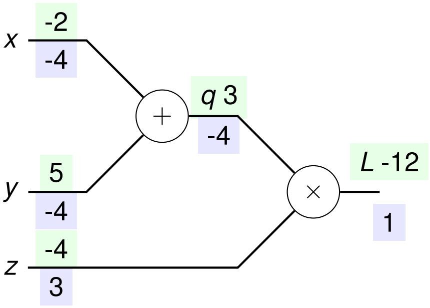
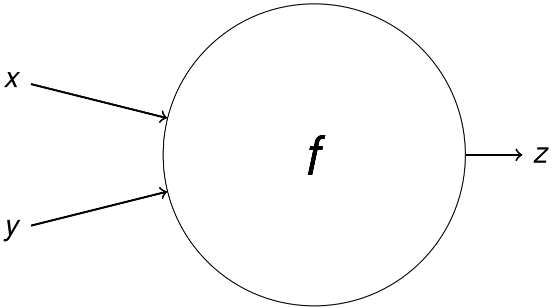


Backward differentiation (backpropagation)



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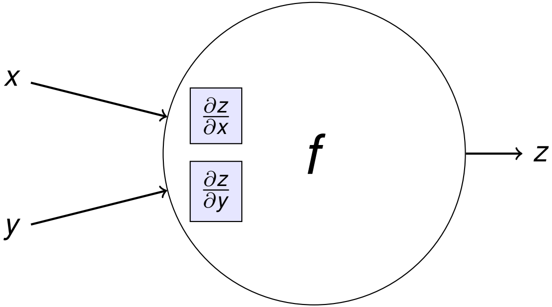

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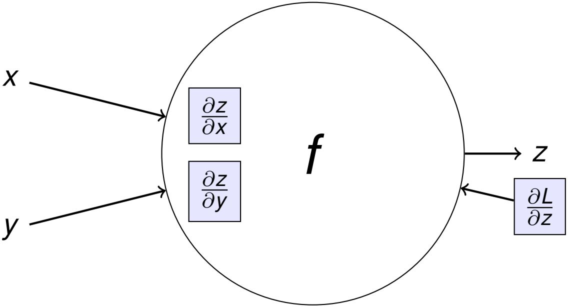

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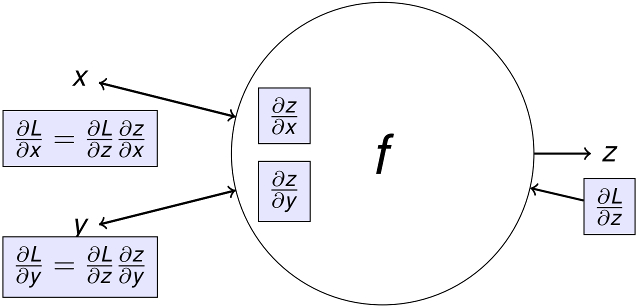
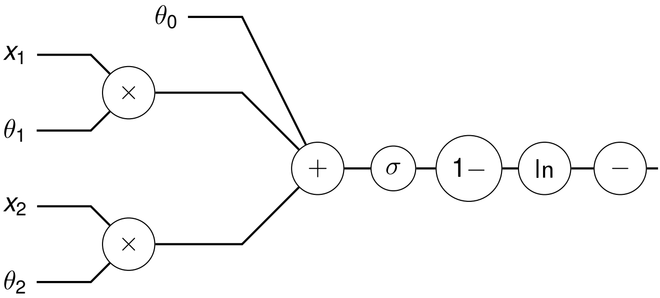


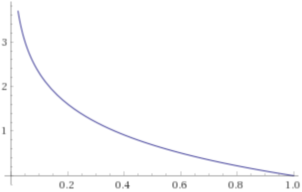
Backpropagation again

Suppose $x = (1, 1)$ and $y = 0$.
Then the loss is $-\ln(1 - \sigma(\theta^T x))$.

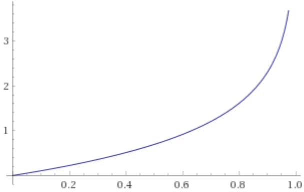


Cross-entropy loss function

$$\ell(x^{(i)}, y^{(i)}) = \begin{cases} -\log(\sigma(\theta^T x^{(i)})) & \text{if } y^{(i)} = 1 \\ -\log(1 - \sigma(\theta^T x^{(i)})) & \text{if } y^{(i)} = 0 \end{cases}$$



$$-\log(\sigma(\theta^T x^{(i)}))$$



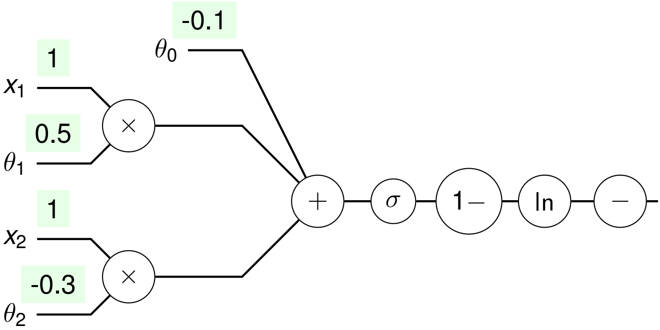
$$-\log(1 - \sigma(\theta^T x^{(i)}))$$

Since either $y^{(i)} = 1$ or $y^{(i)} = 0$:

$$\ell(\theta) = \frac{1}{m} \sum_{i=0}^{m} [-y^{(i)} \log(\sigma(\theta^T x^{(i)})) - (1 - y^{(i)}) \log(1 - (\sigma(\theta^T x^{(i)})))]$$

Backpropagation again

Suppose $\theta = (-0.1, 0.5, -0.3)$. First we do the forward pass.



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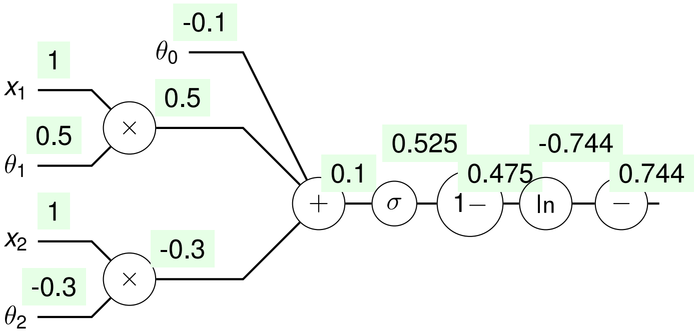
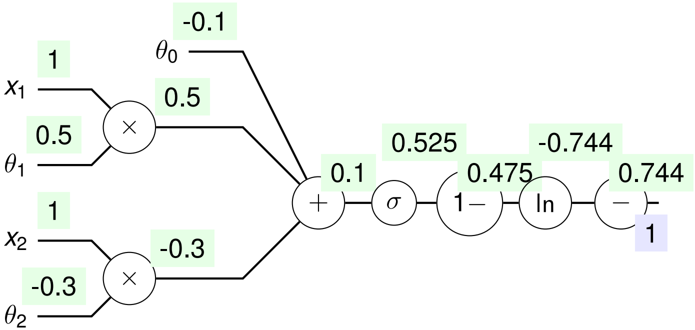


Backpropagation again

Now do the backward pass.



Backpropagation again

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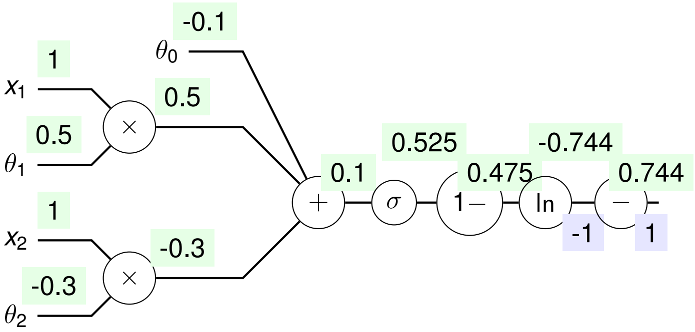

Backpropagation again

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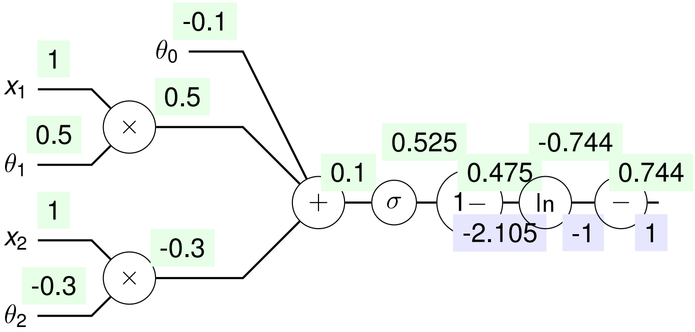

Backpropagation again

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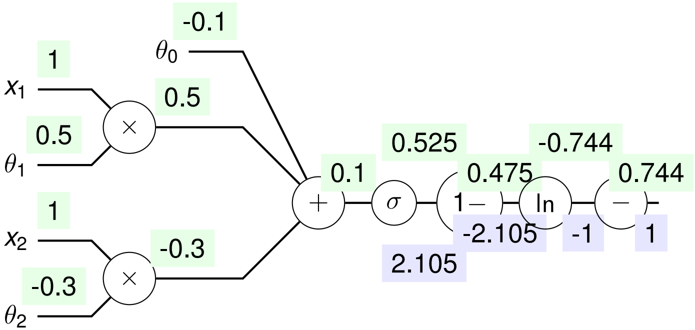

Backpropagation again

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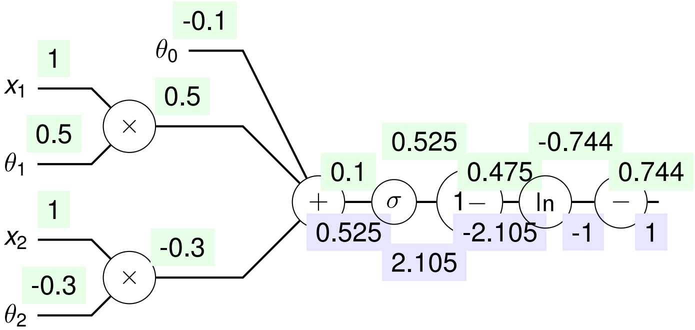
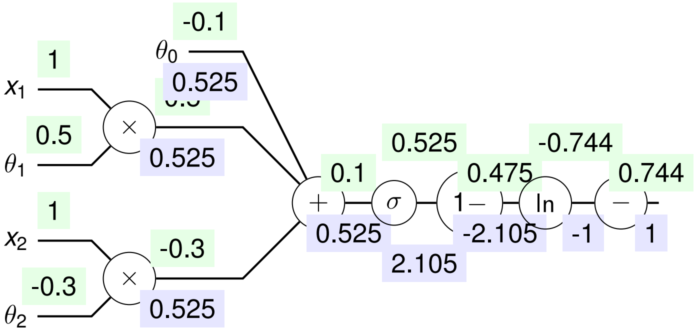


$$0.525 = \sigma(0.1)(1 - \sigma(0.1))(2.105)$$

Backpropagation again

Now do the backward pass.



Backpropagation again

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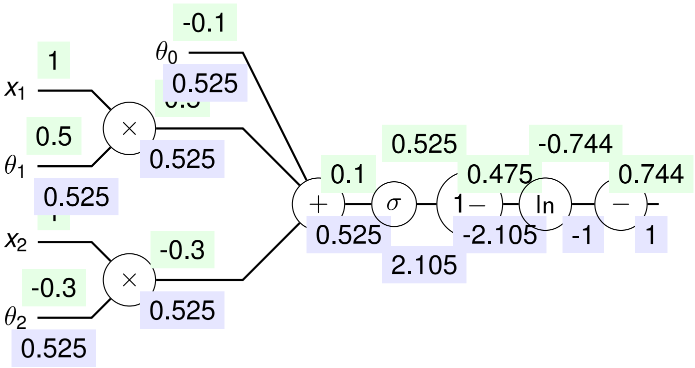
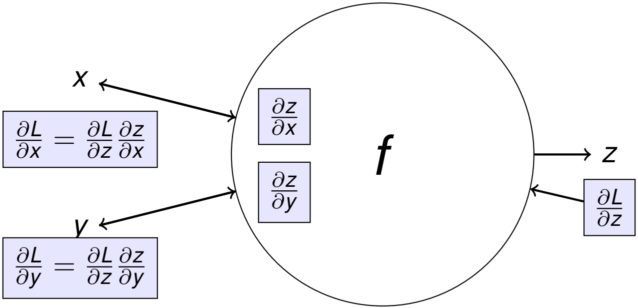
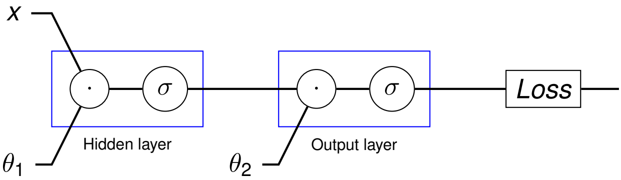


Backward differentiation (backpropagation)

x, y, z are vectors. $\frac{\partial z}{\partial x}$ is now a (Jacobian) matrix: the derivative of every element of z w.r.t. every element of x.



Backpropagation with a hidden layer



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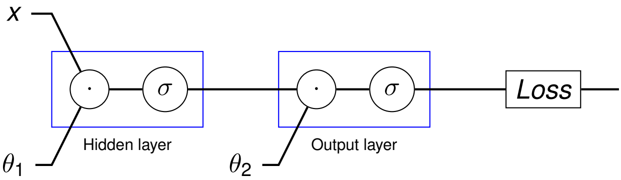
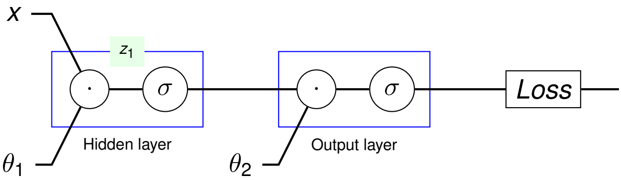


$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \quad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix}$$

Backpropagation with a hidden layer



$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix}$$

$$z_1 = \begin{pmatrix} 0.5 \\ 0.36 \end{pmatrix}$$

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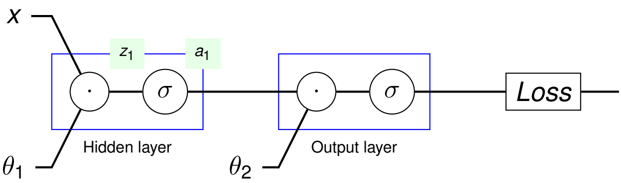


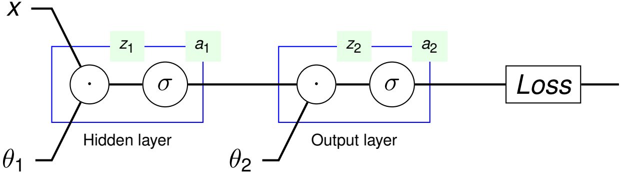
$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix}$$

$$z_1 = \begin{pmatrix} 0.5 \\ 0.36 \end{pmatrix}$$

$$a_1 = \begin{pmatrix} 0.62 \\ 0.59 \end{pmatrix}$$

Backpropagation with a hidden layer



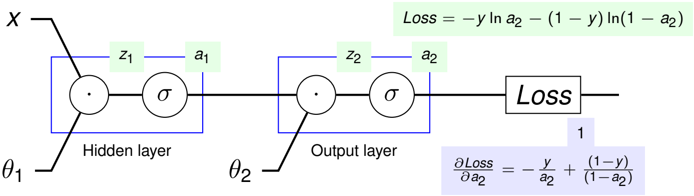
$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix}$$

$$z_1 = \begin{pmatrix} 0.5 \\ 0.36 \end{pmatrix} \qquad z2 = 0.48$$

$$a_1 = \begin{pmatrix} 0.62 \\ 0.59 \end{pmatrix} \qquad a2 = 0.62$$

Backpropagation with a hidden layer



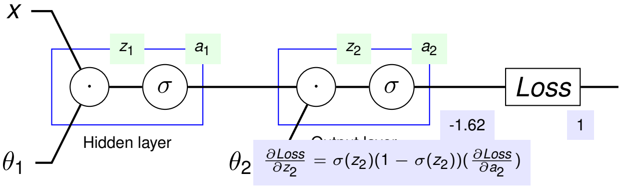
$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix} \qquad \frac{\partial Loss}{\partial a_2} = -1.62$$

$$z_1 = \begin{pmatrix} 0.5 \\ 0.36 \end{pmatrix} \qquad z2 = 0.48$$

$$a_1 = \begin{pmatrix} 0.62 \\ 0.59 \end{pmatrix} \qquad a2 = 0.62$$

Backpropagation with a hidden layer



$$\frac{\partial Loss}{\partial z_2} = \sigma(z_2)(1-\sigma(z_2))(\frac{\partial Loss}{\partial a_2})$$

$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

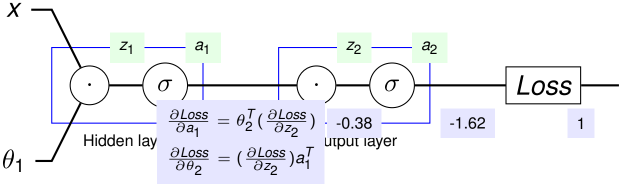
$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix} \qquad \frac{\partial Loss}{\partial a_2} = -1.62$$

$$z_1 = \begin{pmatrix} 0.5 \\ 0.36 \end{pmatrix} \qquad z2 = 0.48$$

$$a_1 = \begin{pmatrix} 0.62 \\ 0.59 \end{pmatrix} \qquad a2 = 0.62$$

$$\frac{\partial Loss}{\partial z_2} = -0.38$$

Backpropagation with a hidden layer



$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix} \qquad \frac{\partial Loss}{\partial a_2} = -1.62$$

$$z_1 = \begin{pmatrix} 0.5 \\ 0.36 \end{pmatrix} \qquad z2 = 0.48$$

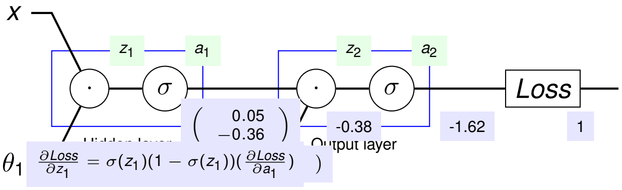
$$a_1 = \begin{pmatrix} 0.62 \\ 0.59 \end{pmatrix} \qquad a2 = 0.62$$

$$\frac{\partial Loss}{\partial z_2} = -0.38$$

$$\frac{\partial Loss}{\partial \theta_2} = \begin{pmatrix} -0.24 & -0.22 \end{pmatrix}$$

$$\frac{\partial Loss}{\partial a_1} = \begin{pmatrix} 0.05 \\ -0.36 \end{pmatrix}$$

Backpropagation with a hidden layer



$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix} \qquad \frac{\partial Loss}{\partial a_2} = -1.62$$

$$z_1 = \begin{pmatrix} 0.5 \\ 0.36 \end{pmatrix} \qquad z2 = 0.48$$

$$a_1 = \begin{pmatrix} 0.62 \\ 0.59 \end{pmatrix} \qquad a2 = 0.62$$

$$\frac{\partial Loss}{\partial z_1} = \begin{pmatrix} 0.01 \\ -0.09 \end{pmatrix} \qquad \frac{\partial Loss}{\partial z_2} = -0.38$$

$$\frac{\partial Loss}{\partial \theta_2} = \begin{pmatrix} -0.24 & -0.22 \end{pmatrix}$$

$$\frac{\partial Loss}{\partial a_1} = \begin{pmatrix} 0.05 \\ -0.36 \end{pmatrix}$$

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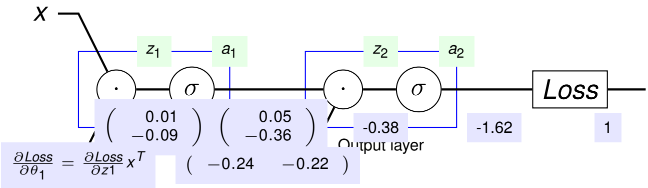

$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

$$\theta_1 = \begin{pmatrix} 0.45 & 0.05 \\ -0.38 & 0.74 \end{pmatrix} \qquad \theta_2 = \begin{pmatrix} -0.13 & 0.95 \end{pmatrix} \qquad \frac{\partial Loss}{\partial a_2} = -1.62$$

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$$\frac{\partial Loss}{\partial \theta_1} = \begin{pmatrix} 0.01 & 0.01 \\ -0.09 & -0.09 \end{pmatrix} \qquad \frac{\partial Loss}{\partial \theta_2} = \begin{pmatrix} -0.24 & -0.22 \end{pmatrix}$$

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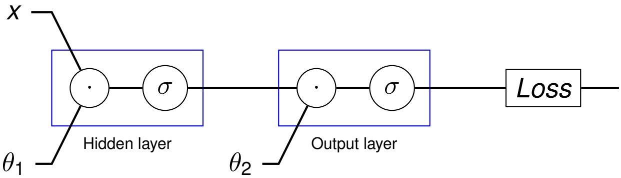

$$x = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad y = 1$$

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