

Introduction to Deep Learning



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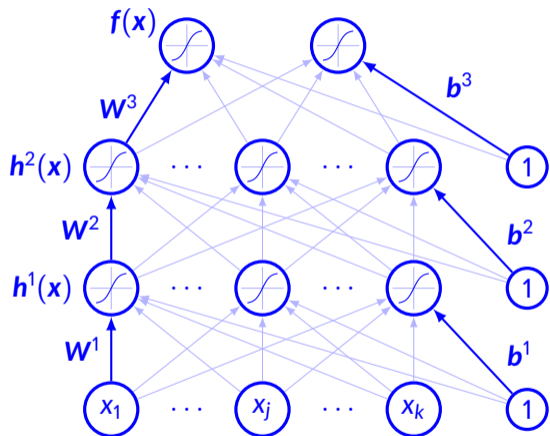
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 - Three functions $f^{(1)}, f^{(2)}, f^{(3)}$ are connected in chain
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- Goal of NN is not to model brain accurately!

Multilayer neural network



Issues with linear FFN

- Fit well for linear and logistic regression
- Convex optimization technique may be used
- Capacity of such function is limited
- Model cannot understand interaction between any two variables

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 - Strategy of deep learning is to learn ϕ

Goal of deep learning

- We have a model $y = f(\mathbf{x}; \boldsymbol{\theta}, \mathbf{w}) = \phi(\mathbf{x}; \boldsymbol{\theta})^T \mathbf{w}$
- We use $\boldsymbol{\theta}$ to learn ϕ
- \mathbf{w} and ϕ determines the output. ϕ defines the hidden layer
- It loses the convexity of the training problem but benefits a lot
- Representation is parameterized as $\phi(\mathbf{x}, \boldsymbol{\theta})$
 - $\boldsymbol{\theta}$ can be determined by solving optimization problem
- Advantages
 - ϕ can be very generic
 - Human practitioner can encode their knowledge to designing $\phi(\mathbf{x}; \boldsymbol{\theta})$

Design issues of feedforward network

- Choice of optimizer
- Cost function
- The form of output unit
- Choice of activation function
- Design of architecture - number of layers, number of units in each layer
- Computation of gradients

Example

- Let us choose XOR function
- Target function is $y = f^*(\mathbf{x})$ and our model provides $y = f(\mathbf{x}; \theta)$
- Learning algorithm will choose the parameters θ to make f close to f^*

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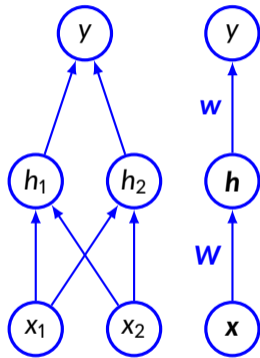
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- Target is to fit output for $\mathbf{X} = \{[0, 0]^T, [0, 1]^T, [1, 0]^T, [1, 1]^T\}$
- This can be treated as regression problem and MSE error can be chosen as loss function $(J(\theta) = \frac{1}{4} \sum_{\mathbf{x} \in \mathbf{X}} (f^*(\mathbf{x}) - f(\mathbf{x}; \theta))^2)$
- We need to choose $f(\mathbf{x}; \theta)$ where θ depends on \mathbf{w} and b
- Let us consider a linear model $f(\mathbf{x}; \mathbf{w}, b) = \mathbf{x}^T \mathbf{w} + b$

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- Solving these, we get $\mathbf{w} = 0$ and $b = \frac{1}{2}$

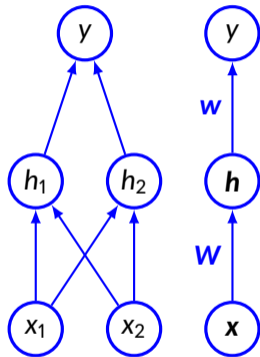
Simple FFN with hidden layer

- Let us assume that the hidden unit h computes $f^{(1)}(\mathbf{x}; \mathbf{W}, \mathbf{c})$



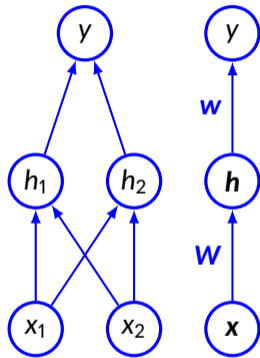
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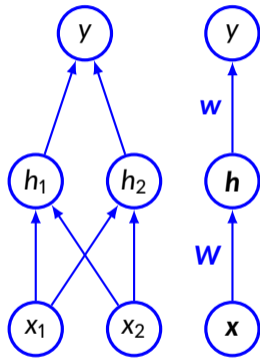
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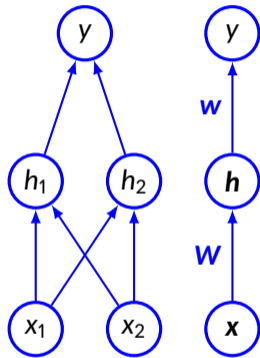
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- Suppose $f^{(1)}(\mathbf{x}) = \mathbf{W}^T \mathbf{x}$ and $f^{(2)}(\mathbf{h}) = \mathbf{h}^T \mathbf{w}$



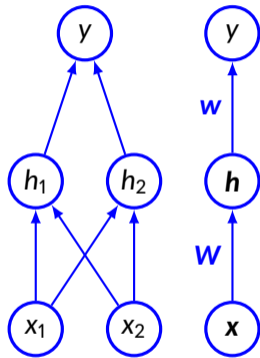
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- Suppose $f^{(1)}(\mathbf{x}) = \mathbf{W}^T \mathbf{x}$ and $f^{(2)}(\mathbf{h}) = \mathbf{h}^T \mathbf{w}$ then $f(\mathbf{x}) = \mathbf{w}^T \mathbf{W}^T \mathbf{x}$



Simple FFN with hidden layer (contd.)

- We need to have nonlinear function to describe the features
- Usually NN have affine transformation of learned parameters followed by nonlinear activation function
- Let us use $\mathbf{h} = g(\mathbf{W}^T \mathbf{x} + \mathbf{c})$
- Let us use ReLU as activation function $g(z) = \max\{0, z\}$
- g is chosen element wise $h_i = g(\mathbf{x}^T \mathbf{W}_{:,i} + c_i)$



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 - $\mathbf{W} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, $\mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$, $\mathbf{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$, $b = 0$

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Gradient based learning

- Similar to machine learning tasks, gradient descent based learning is used
 - Need to specify optimization procedure, cost function and model family
- For NN, model is nonlinear and function becomes nonconvex
 - Usually trained by iterative, gradient based optimizer
- Solved by using gradient descent or stochastic gradient descent (SGD)

Gradient descent

- For a function $y = f(x)$, derivative (slope at point x) of it is $f'(x) = \frac{dy}{dx}$
- A small change in the input can cause output to move to a value given by $f(x + \epsilon) \approx f(x) + \epsilon f'(x)$
- We need to take a jump so that y reduces (assuming minimization problem)
- We can say that $f(x - \epsilon \text{sign}(f'(x)))$ is less than $f(x)$
- For multiple inputs partial derivatives are used ie. $\frac{\partial}{\partial x_i} f(\mathbf{x})$
- Gradient vector is represented as $\nabla_{\mathbf{x}} f(\mathbf{x})$
- Gradient descent proposes a new point as $\mathbf{x}' = \mathbf{x} - \epsilon \nabla_{\mathbf{x}} f(\mathbf{x})$ where ϵ is the learning rate

Stochastic gradient descent

- Large training set are necessary for good generalization
- Cost function used for optimization is $J(\theta) = \frac{1}{m} \sum_{i=1}^m L(\mathbf{x}^{(i)}, y^{(i)}, \theta)$
- Gradient descent requires $\nabla_{\theta} J(\theta) = \frac{1}{m} \sum_{i=1}^m \nabla_{\theta} L(\mathbf{x}^{(i)}, y^{(i)}, \theta)$

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 - Computation cost is $O(m)$
- For SGD, gradient is an expectation estimated from a small sample known as minibatch ($\mathbb{B} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m')}\}$)
- Estimated gradient is $\mathbf{g} = \frac{1}{m'} \sum_{i=1}^{m'} \nabla_{\theta} L(\mathbf{x}^{(i)}, y^{(i)}, \theta)$
- New point will be $\theta = \theta - \epsilon \mathbf{g}$

Cost function

- Similar to other parametric model like linear models
- Parametric model defines distribution $p(\mathbf{y}|\mathbf{x}; \theta)$
- Principle of maximum likelihood is used (cross entropy between training data and model prediction)
- Instead of predicting the whole distribution of \mathbf{y} , some statistic of \mathbf{y} conditioned on \mathbf{x} is predicted
- It can also contain regularization term

Maximum likelihood estimation

- Consider a set of m examples $\mathbb{X} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ drawn independently from the true but unknown data generating distribution $p_{data}(\mathbf{x})$
- Let $p_{model}(\mathbf{x}; \theta)$ be a parametric family of probability distribution

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- By dividing m we get $\theta_{ML} = \arg \max_{\theta} \mathbb{E}_{\mathbf{x} \sim p_{data}} \log p_{model}(\mathbf{x}; \theta)$

Maximum likelihood estimation (cont.)

- Minimizing dissimilarity between the empirical \hat{p}_{data} and model distribution p_{model} and it is measured by KL divergence

$$D_{KL}(\hat{p}_{data} || p_{model}) = \arg \min_{\theta} \mathbb{E}_{\mathbf{x} \sim \hat{p}_{data}} [\log \hat{p}_{data}(\mathbf{x}) - \log p_{model}(\mathbf{x}; \theta)]$$

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- We need to minimize $-\arg \min_{\theta} \mathbb{E}_{\mathbf{x} \sim \hat{p}_{data}} \log p_{model}(\mathbf{x}; \theta)$

Conditional log-likelihood

- In most of the supervised learning we estimate $P(\mathbf{y}|\mathbf{x}; \theta)$
- If \mathbf{X} be the all inputs and \mathbf{Y} be observed targets then conditional maximum likelihood estimator is $\theta_{ML} = \arg \max_{\theta} P(\mathbf{Y}|\mathbf{X}; \theta)$
- If the examples are assumed to be i.i.d then we can say

$$\theta_{ML} = \arg \max_{\theta} \sum_{i=1}^m \log P(\mathbf{y}^{(i)}|\mathbf{x}^{(i)}; \theta)$$

Linear regression as maximum likelihood

- Instead of producing single prediction \hat{y} for a given \mathbf{x} , we assume the model produces conditional distribution $p(y|\mathbf{x})$
- For infinitely large training set, we can observe multiple examples having the same \mathbf{x} but different values of y
- Goal is to fit the distribution $p(y|\mathbf{x})$

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- Let us assume, $p(y|\mathbf{x}) = \mathcal{N}(y; \hat{y}(\mathbf{x}; \mathbf{w}), \sigma^2)$

Linear regression as maximum likelihood

- Instead of producing single prediction \hat{y} for a given \mathbf{x} , we assume the model produces conditional distribution $p(y|\mathbf{x})$
- For infinitely large training set, we can observe multiple examples having the same \mathbf{x} but different values of y
- Goal is to fit the distribution $p(y|\mathbf{x})$
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$$\sum_{i=1}^m \log p(\mathbf{y}^{(i)}|\mathbf{x}^{(i)}; \theta) = -m \log \sigma - \frac{m}{2} \log(2\pi) - \sum_{i=1}^m \frac{\|\hat{\mathbf{y}}^{(i)} - \mathbf{y}^{(i)}\|^2}{2\sigma^2}$$

Learning conditional distributions

- Usually neural networks are trained using maximum likelihood. Therefore the cost function is negative log-likelihood. Also known as cross entropy between training data and model distribution
- Cost function $J(\theta) = -\mathbb{E}_{\mathbf{x}, \mathbf{y} \sim \hat{p}_{data}} \log p_{model}(\mathbf{y}|\mathbf{x}, \theta)$
- Uniform across different models
- Gradient of cost function is very much crucial
 - Large and predictable gradient can serve good guide for learning process
 - Function that saturates will have small gradient
 - Activation function usually produces values in a bounded zone (saturates)
 - Negative log-likelihood can overcome some of the problems
 - Output unit having exp function can saturate for high negative value
 - Log-likelihood cost function undoes the exp of some output functions

Learning conditional statistics

- Instead of learning the whole distribution $p(\mathbf{y}|\mathbf{x}; \theta)$, we want to learn one conditional statistics of \mathbf{y} given \mathbf{x}
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- Need to solve the optimization problem

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Calculus of variations (contd.)

- Now we have

$$\int_{x_1}^{x_2} \left. \frac{dL}{d\varepsilon} \right|_{\varepsilon=0} dx = \int_{x_1}^{x_2} \left(\frac{\partial L}{\partial f} \eta + \frac{\partial L}{\partial f'} \eta' \right) dx$$

Calculus of variations (contd.)

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- Euler-Lagrange equation $\frac{\partial L}{\partial f} - \frac{d}{dx} \frac{\partial L}{\partial f'} = 0$

Example

- Let us consider distance between two points $A[y] =$

$$\int_{x_1}^{x_2} \sqrt{1 + [y'(x)]^2} dx$$

- $y'(x) = \frac{dy}{dx}$, $y_1 = f(x_1)$, $y_2 = f(x_2)$

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- Therefore we have, $\frac{d^2f}{dx^2} = 0$
- Hence we have $f(x) = mx + b$ with $m = \frac{y_2 - y_1}{x_2 - x_1}$ and $b = \frac{x_2y_1 - x_1y_2}{x_2 - x_1}$

Output units

- **Choice of cost function is directly related with the choice of output function**
- **In most cases cost function is determined by cross entropy between data and model distribution**
- **Any kind of output unit can be used as hidden unit**

Linear units

- Suited for Gaussian output distribution
- Given features \mathbf{h} , linear output unit produces $\hat{\mathbf{y}} = \mathbf{W}^T \mathbf{h} + \mathbf{b}$
- This can be treated as conditional probability $p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}; \hat{\mathbf{y}}, I)$
- Maximizing log-likelihood is equivalent to minimizing mean square error

Sigmoid unit

- Mostly suited for binary classification problem that is Bernoulli output distribution
- The neural networks need to predict $p(y = 1|\mathbf{x})$
 - If linear unit has been chosen, $p(y = 1|\mathbf{x}) = \max\{0, \min\{1, \mathbf{W}^T \mathbf{h} + \mathbf{b}\}\}$
 - Gradient?
- Model should have strong gradient whenever the answer is wrong
- Let us assume unnormalized log probability is linear with $z = \mathbf{W}^T \mathbf{h} + \mathbf{b}$
- Therefore, $\log \tilde{P}(y) = yz \Rightarrow \tilde{P}(y) = \exp(yz) \Rightarrow P(y) = \frac{\exp(yz)}{\sum_{y' \in \{0,1\}} \exp(y'z)}$
 - It can be written as $P(y) = \sigma((2y - 1)z)$
- The loss function for maximum likelihood is
$$J(\theta) = -\log P(y|\mathbf{x}) = -\log \sigma((2y - 1)z) = \zeta((1 - 2y)z)$$

Softmax unit

- Similar to sigmoid. Mostly suited for multinoulli distribution
- We need to predict a vector \hat{y} such that $\hat{y}_i = P(Y = i|\mathbf{x})$
- A linear layer predicts unnormalized probabilities $\mathbf{z} = \mathbf{W}^T \mathbf{h} + \mathbf{b}$ that is $z_i = \log \tilde{P}(y = i|\mathbf{x})$
- Formally, $\text{softmax}(\mathbf{z})_i = \frac{\exp z_i}{\sum_j \exp(z_j)}$
- Log in log-likelihood can undo exp $\log \text{softmax}(\mathbf{z})_i = z_i - \log \sum_j \exp(z_j)$
 - Does it saturate?
 - What about incorrect prediction?
- Invariant to addition of some scalar to all input variables ie. $\text{softmax}(\mathbf{z}) = \text{softmax}(\mathbf{z} + \mathbf{c})$

Hidden units

- Active area of research and does not have good guiding theoretical principle
- Usually rectified linear unit (ReLU) is chosen in most of the cases
- Design process consists of trial and error, then the suitable one is chosen
- Some of the activation functions are not differentiable (eg. ReLU)
 - Still gradient descent performs well
 - Neural network does not converge to local minima but reduces the value of cost function to a very small value

Generalization of ReLU

- ReLU is defined as $g(z) = \max\{0, z\}$
- Using non-zero slope, $h_i = g(\mathbf{z}, \alpha)_i = \max(0, z_i) + \alpha_i \min(0, z_i)$
 - Absolute value rectification will make $\alpha_i = -1$ and $g(z) = |z|$
- Leaky ReLU assumes very small values for α_i
- Parametric ReLU tries to learn α_i parameters
- Maxout unit $g(\mathbf{z})_i = \max_{j \in G^{(i)}} z_j$
 - Suitable for learning piecewise linear function

Logistic sigmoid & hyperbolic tangent

- Logistic sigmoid $g(z) = \sigma(z)$
- Hyperbolic tangent $g(z) = \tanh(z)$
 - $\tanh(z) = 2\sigma(2z) - 1$
- Widespread saturation of sigmoidal unit is an issue for gradient based learning
 - Usually discouraged to use as hidden units
- Usually, hyperbolic tangent function performs better where sigmoidal function must be used
 - Behaves linearly at 0
 - Sigmoidal activation function are more common in settings other than feedforward network

Other hidden units

- Differentiable functions are usually preferred
- Activation function $h = \cos(\mathbf{W}\mathbf{x} + \mathbf{b})$ performs well for MNIST data set
- Sometimes no activation function helps in reducing the number of parameters
- Radial Basis Function - $\phi(\mathbf{x}, \mathbf{c}) = \phi(\|\mathbf{x} - \mathbf{c}\|)$
 - Gaussian - $\exp(-(\epsilon r)^2)$
- Softplus - $g(x) = \zeta(x) = \log(1 + \exp(x))$
- Hard tanh - $g(x) = \max(-1, \min(1, x))$
- Hidden unit design is an active area of research

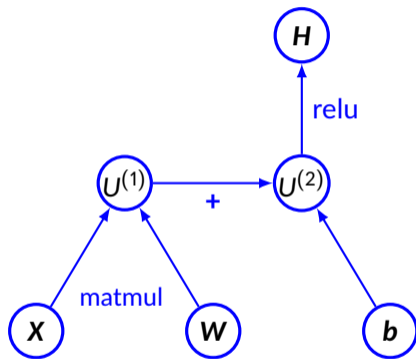
Architecture design

- **Structure of neural network (chain based architecture)**
 - Number of layers
 - Number of units in each layer
 - Connectivity of those units
- **Single hidden layer is sufficient to fit the training data**
- **Often deeper networks are preferred**
 - Fewer number of units
 - Fewer number of parameters
 - Difficult to optimize

Back propagation

- In a feedforward network, an input x is read and produces an output \hat{y}
 - This is forward propagation
- During training forward propagation continues until it produces cost $J(\theta)$
- Back-propagation algorithm allows the information to flow backward in the network to compute the gradient
- Computation of analytical expression for gradient is easy
- We need to find out gradient of the cost function with respect to the parameters ie. $\nabla_{\theta}J(\theta)$

Computational graph



Chain rule of calculus

- Back-propagation algorithm heavily depends on it
- Let x be a real number and $y = g(x)$ and $z = f(g(x)) = f(y)$
- Chain rule says $\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$
- This can be generalized: Let $\mathbf{x} \in \mathbb{R}^m$, $\mathbf{y} \in \mathbb{R}^n$, $g : \mathbb{R}^m \rightarrow \mathbb{R}^n$ and $f : \mathbb{R} \rightarrow \mathbb{R}$ and $\mathbf{y} = g(\mathbf{x})$ and $z = f(\mathbf{y})$ then $\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$
- In vector notation it will be where $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$ is the $n \times m$ Jacobian matrix of g

$$\nabla_{\mathbf{x}} z = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right)^T \nabla_{\mathbf{y}} z$$

Application of chain rule

- Let us consider $u^{(n)}$ be the loss quantity. Need to find out the gradient for this.
- Let $u^{(1)}$ to $u^{(n_i)}$ are the inputs
- Therefore, we wish to compute $\frac{\partial u^{(n)}}{\partial u^{(i)}}$ where $i = 1, 2, \dots, n_i$
- Let us assume the nodes are ordered so that we can compute one after another
- Each $u^{(i)}$ is associated with an operation $f^{(i)}$ ie. $u^{(i)} = f(\Delta^{(i)})$

Algorithm for forward pass

for $i = 1, \dots, n_i$ **do**

$u^{(i)} \leftarrow x_i$

end for

for $i = n_i + 1, \dots, n$ **do**

$\mathbb{A}^{(i)} \leftarrow \{u^{(j)} \mid j \in Pa(u^{(i)})\}$

$u^{(i)} \leftarrow f^{(i)}(\mathbb{A}^{(i)})$

end for

return $u^{(n)}$

Algorithm for backward pass

`grad_table`[$u^{(n)}$] \leftarrow 1

for $j = n - 1$ **down to** 1 **do**

$$\text{grad_table}[u^{(j)}] \leftarrow \sum_{i: j \in \text{Pa}(u^{(i)})} \text{grad_table}[u^{(i)}] \frac{\partial u^{(i)}}{\partial u^{(j)}}$$

end for

return `grad_table`

Computational graph & subexpression

- We have $x = f(w)$, $y = f(x)$, $z = f(y)$

$$\frac{\partial z}{\partial w}$$

$$= \frac{\partial z}{\partial y} \frac{\partial y}{\partial x} \frac{\partial x}{\partial w}$$

$$= f'(y)f'(x)f'(w)$$

$$= f'(f(f(w)))f'(f(w))f'(w)$$



Forward propagation in MLP

- **Input**
 - $\mathbf{h}^{(0)} = \mathbf{x}$
- **Computation for each layer $k = 1, \dots, l$**
 - $\mathbf{a}^{(k)} = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}$
 - $\mathbf{h}^{(k)} = f(\mathbf{a}^{(k)})$
- **Computation of output and loss function**
 - $\hat{\mathbf{y}} = \mathbf{h}^{(l)}$
 - $J = L(\hat{\mathbf{y}}, \mathbf{y}) + \lambda\Omega(\theta)$

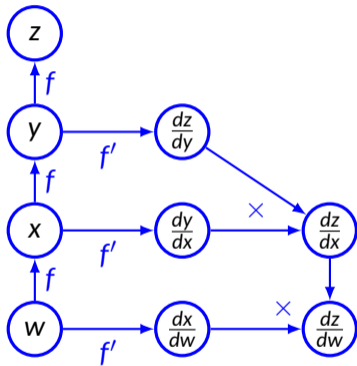
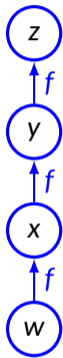
Backward computation in MLP

- Compute gradient at the output
 - $\mathbf{g} \leftarrow \nabla_{\hat{\mathbf{y}}} J = \nabla_{\hat{\mathbf{y}}} L(\hat{\mathbf{y}}, \mathbf{y})$
- Convert the gradient at output layer into gradient of pre-activation
 - $\mathbf{g} \leftarrow \nabla_{\mathbf{a}^{(k)}} J = \mathbf{g} \odot f'(\mathbf{a}^{(k)})$
- Compute gradient on weights and biases
 - $\nabla_{\mathbf{b}^{(k)}} J = \mathbf{g} + \lambda \nabla_{\mathbf{b}^{(k)}} \Omega(\theta)$
 - $\nabla_{\mathbf{W}^{(k)}} J = \mathbf{g} \mathbf{h}^{(k-1)T} + \lambda \nabla_{\mathbf{W}^{(k)}} \Omega(\theta)$
- Propagate the gradients wrt the next lower level activation
 - $\mathbf{g} \leftarrow \nabla_{\mathbf{h}^{(k-1)}} J = \mathbf{W}^{(k)T} \mathbf{g}$

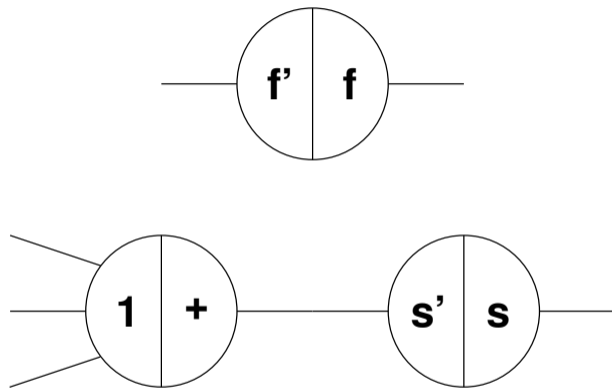
Computation of derivatives

- Takes a computational graph and a set of numerical values for the inputs, then return a set of numerical values
 - Symbol-to-number differentiation
 - Torch, Caffe
- Takes computational graph and add additional nodes to the graph that provide symbolic description of derivative
 - Symbol-to-symbol derivative
 - Theano, TensorFlow

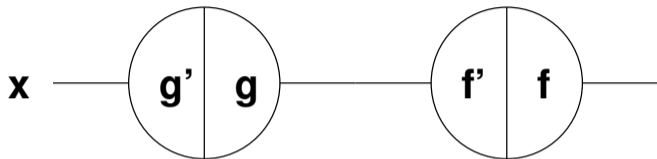
Example



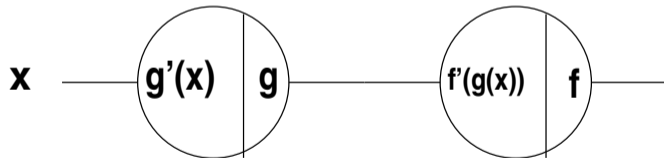
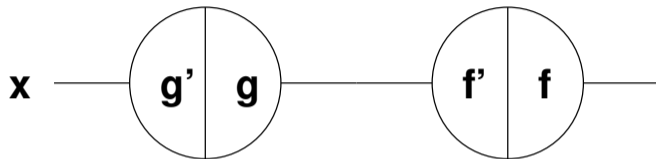
Back propagation



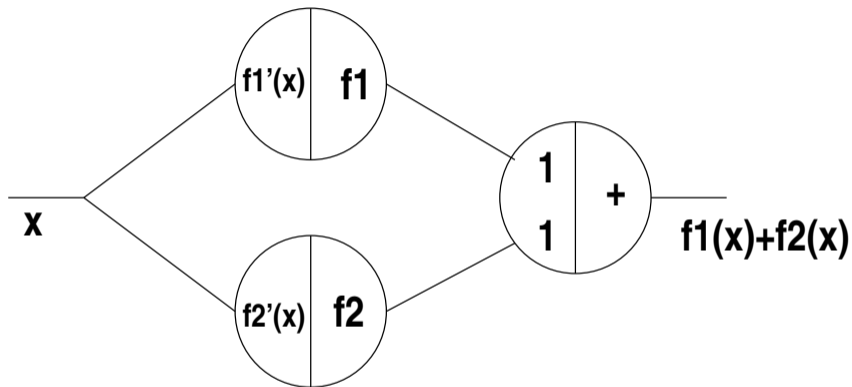
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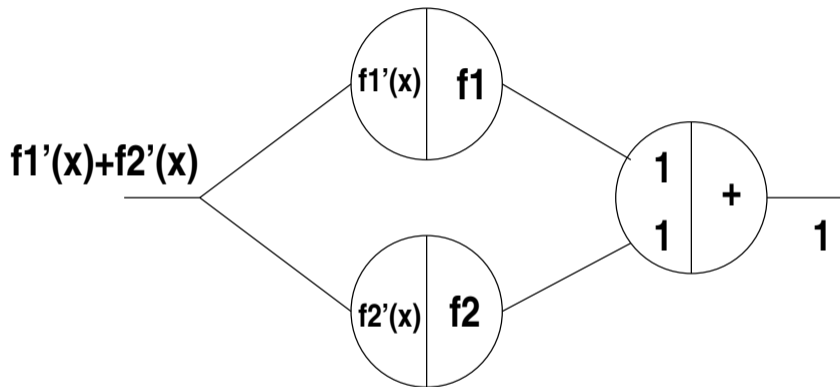
Back propagation



Back propagation



Back propagation

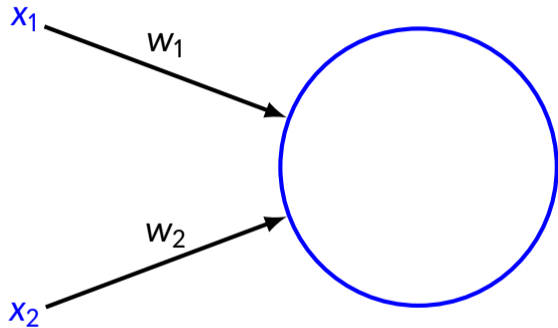


Backpropagation

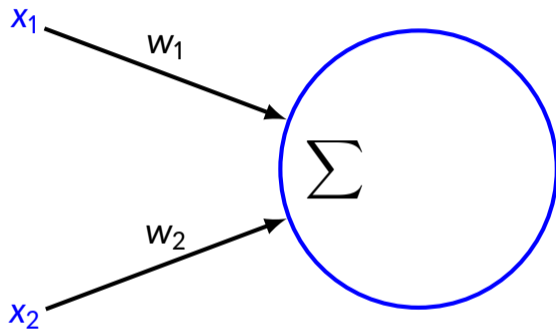
x_1

x_2

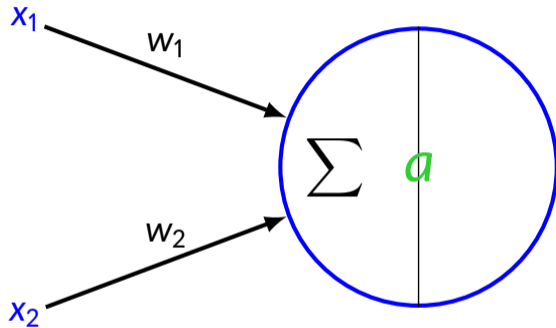
Backpropagation



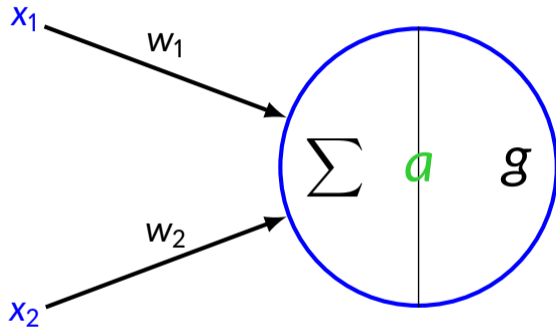
Backpropagation



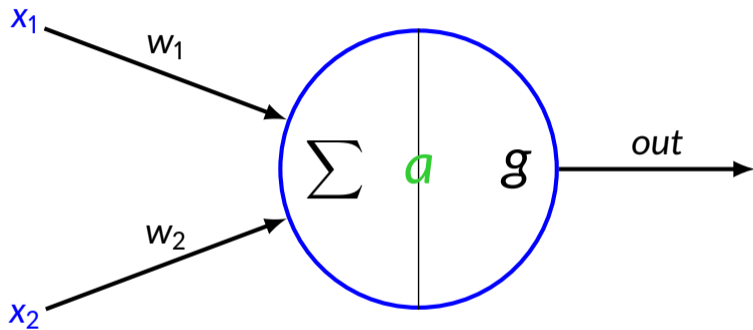
Backpropagation



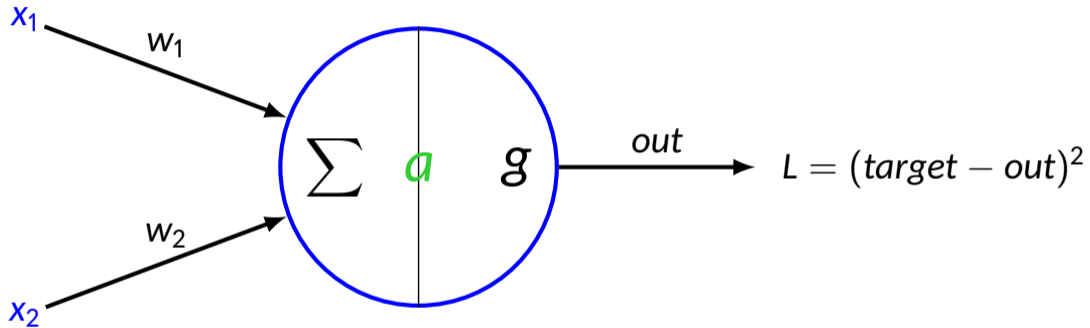
Backpropagation



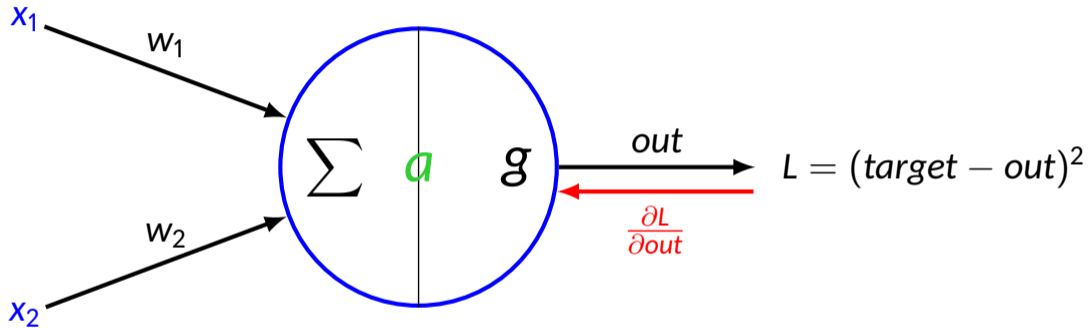
Backpropagation



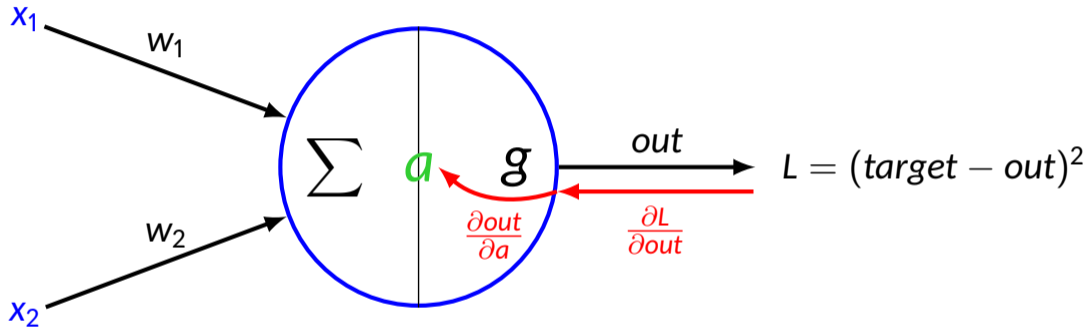
Backpropagation



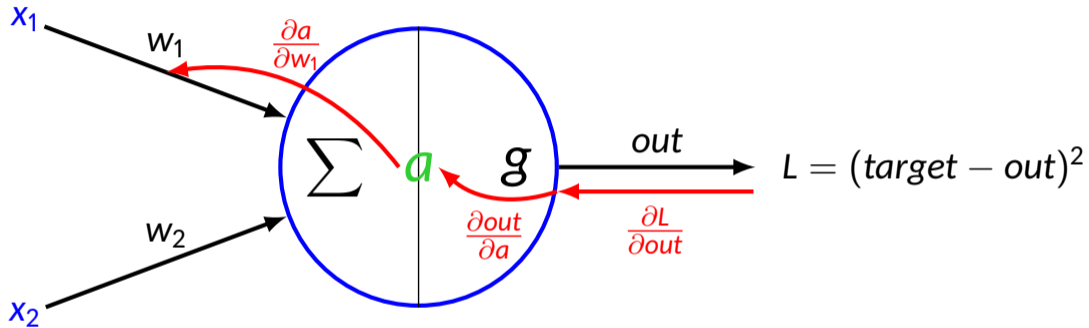
Backpropagation



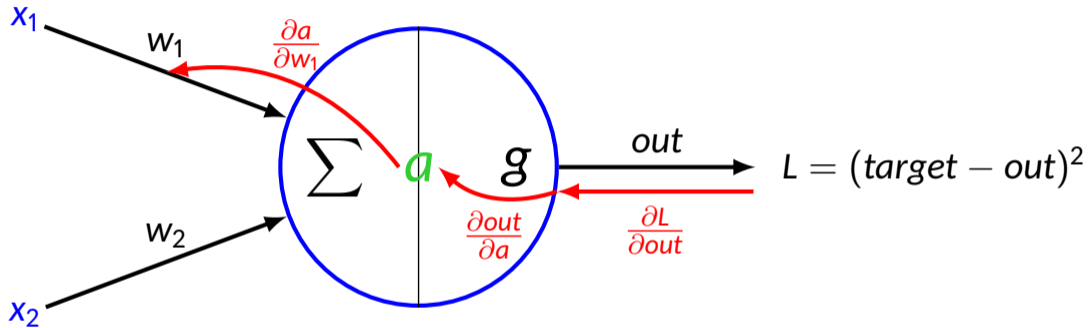
Backpropagation



Backpropagation



Backpropagation

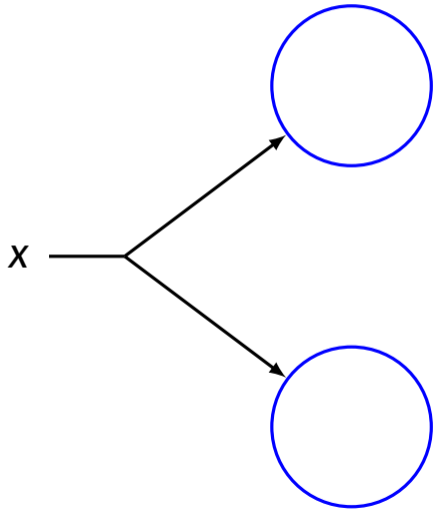


$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial out} \frac{\partial out}{\partial a} \frac{\partial a}{\partial w_1}$$

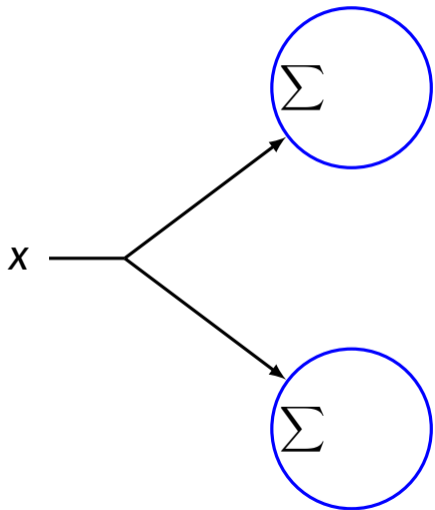
Backpropagation

x —

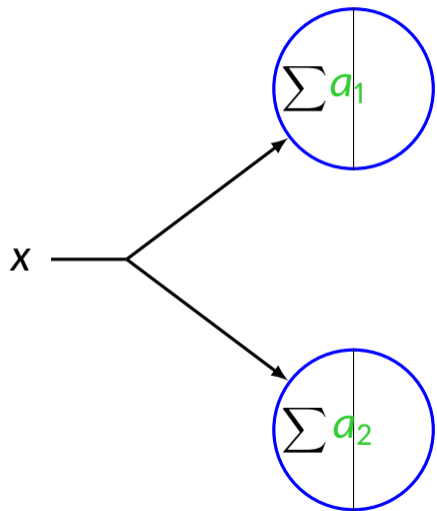
Backpropagation



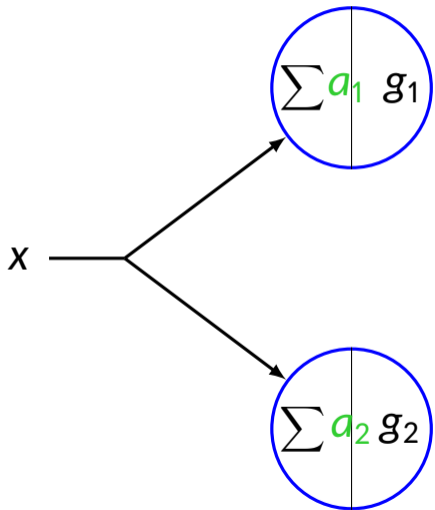
Backpropagation



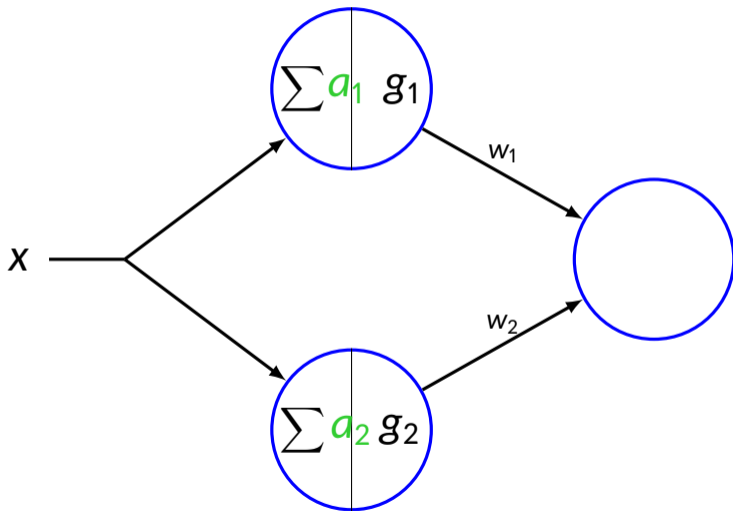
Backpropagation



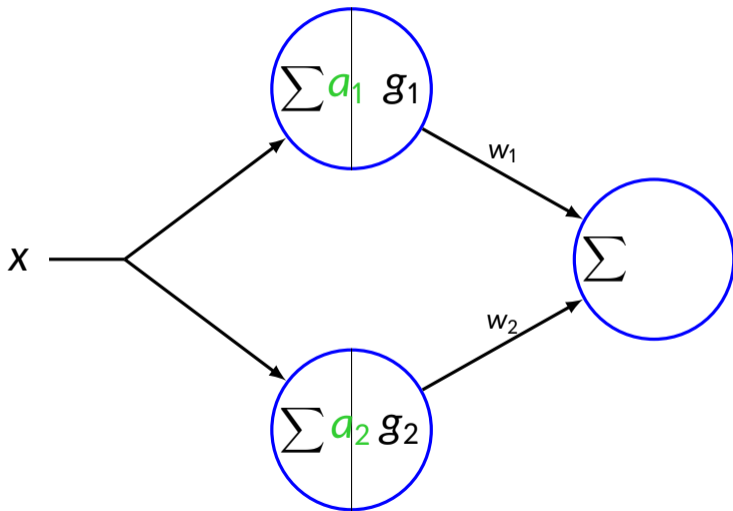
Backpropagation



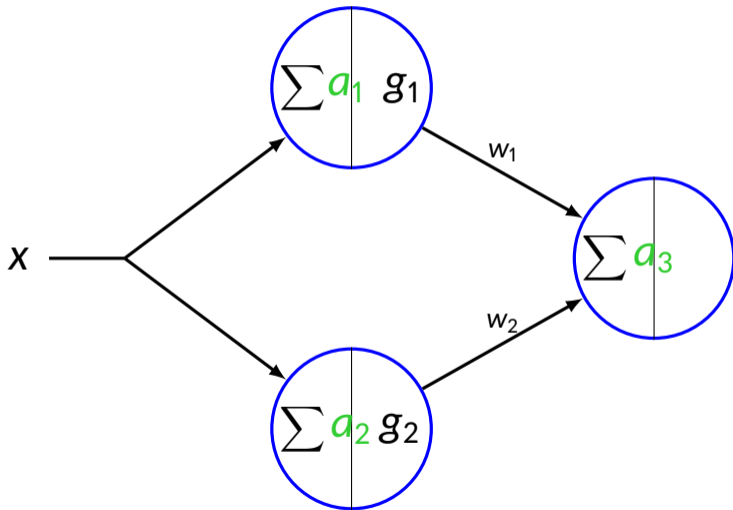
Backpropagation



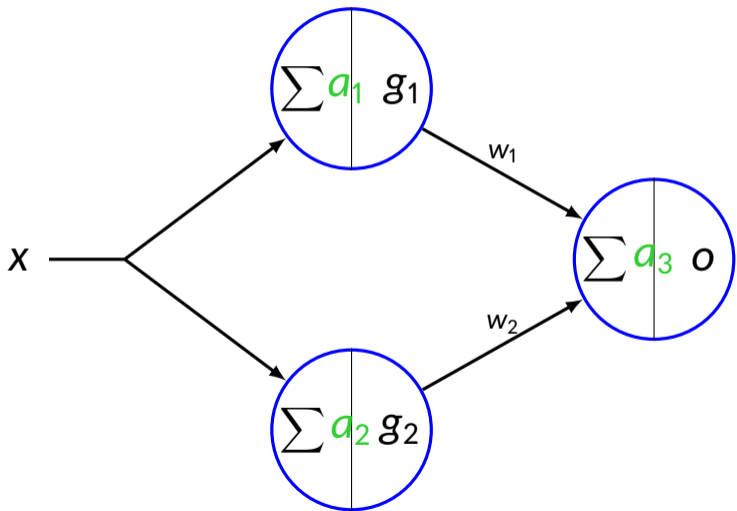
Backpropagation



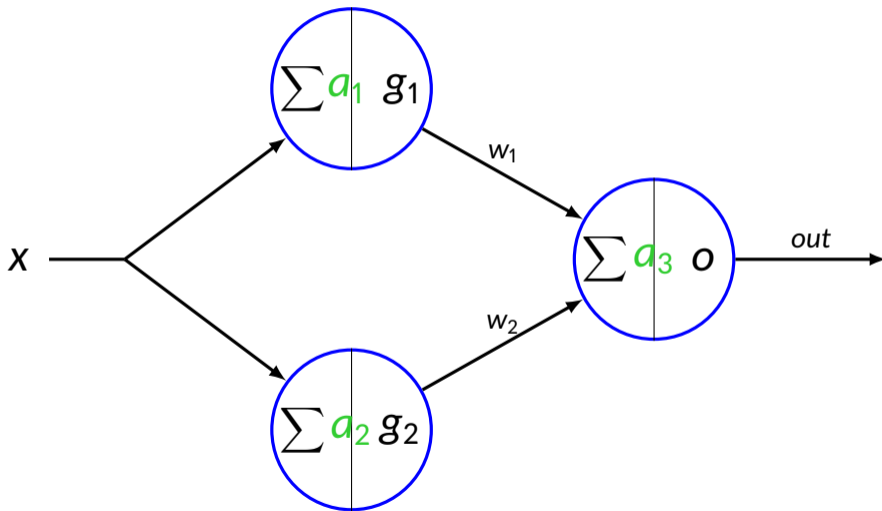
Backpropagation



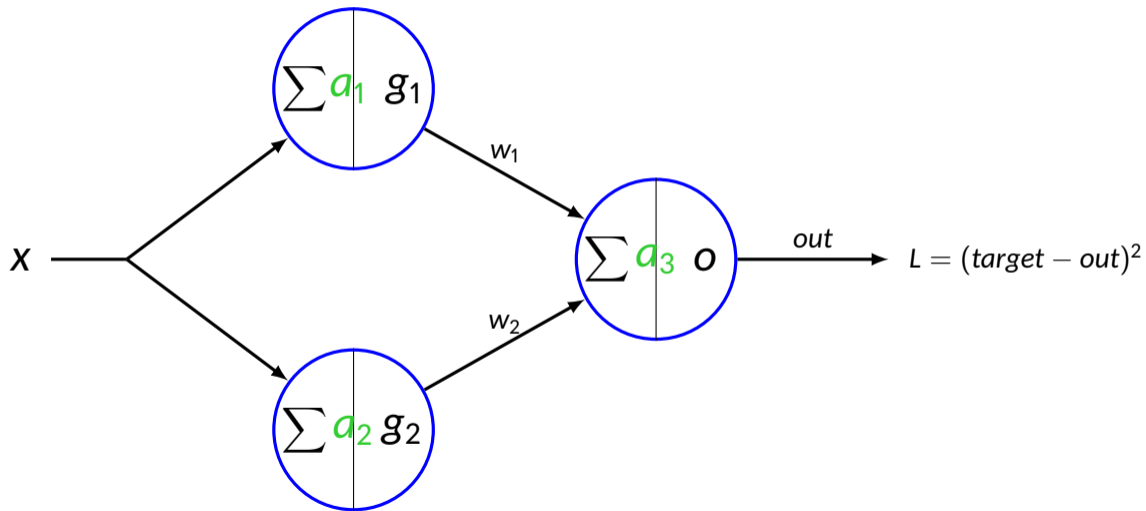
Backpropagation



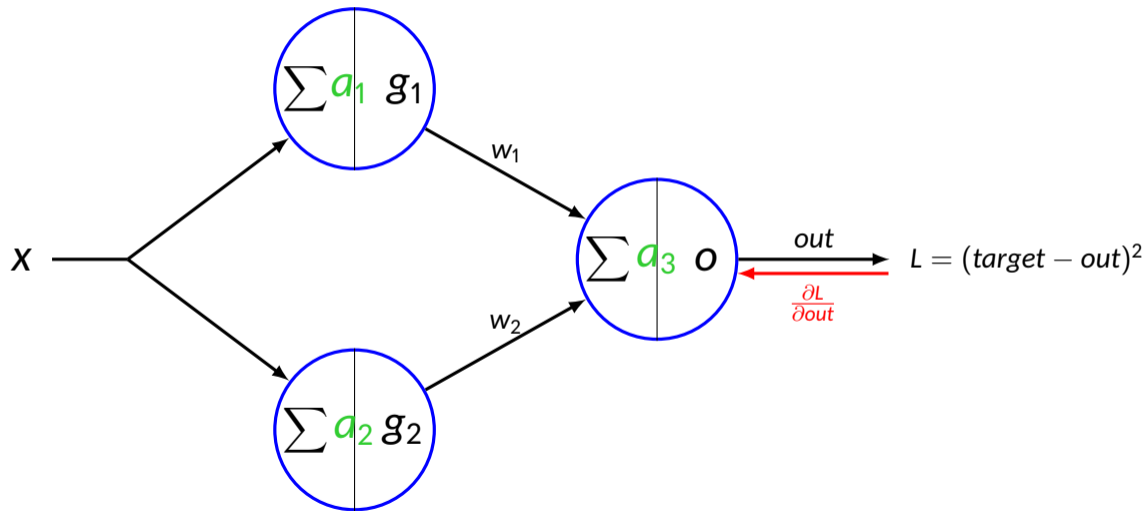
Backpropagation



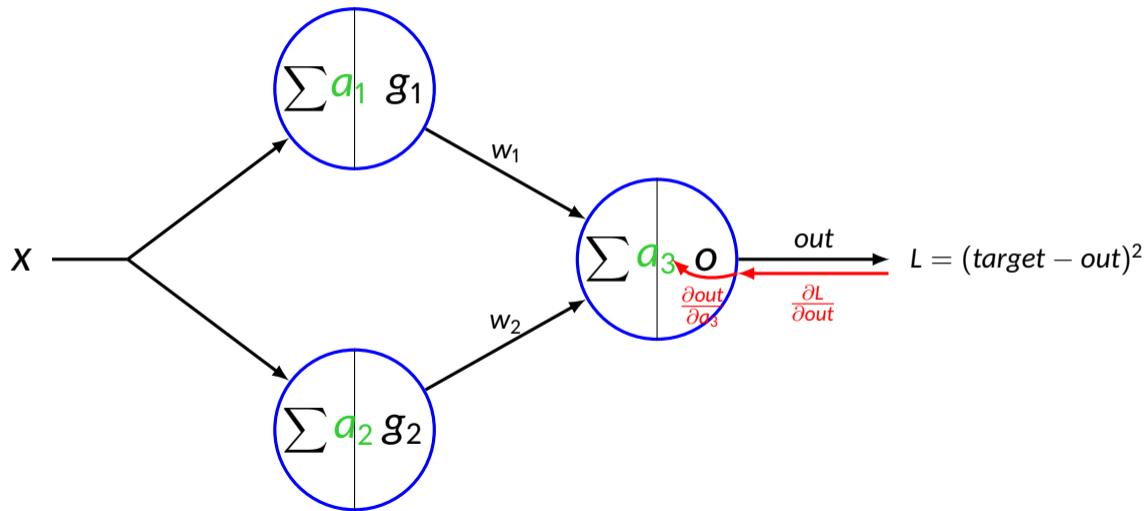
Backpropagation



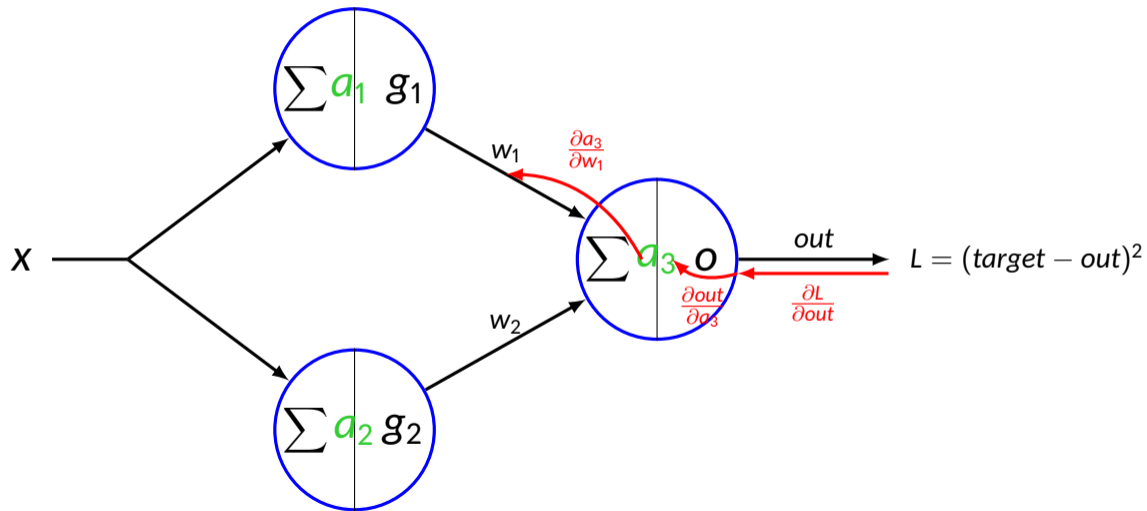
Backpropagation



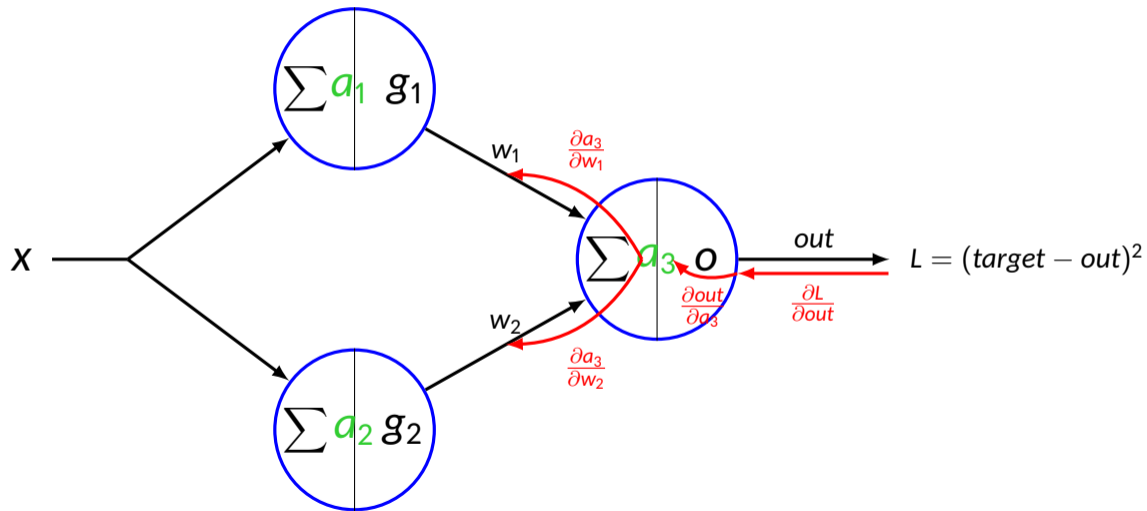
Backpropagation



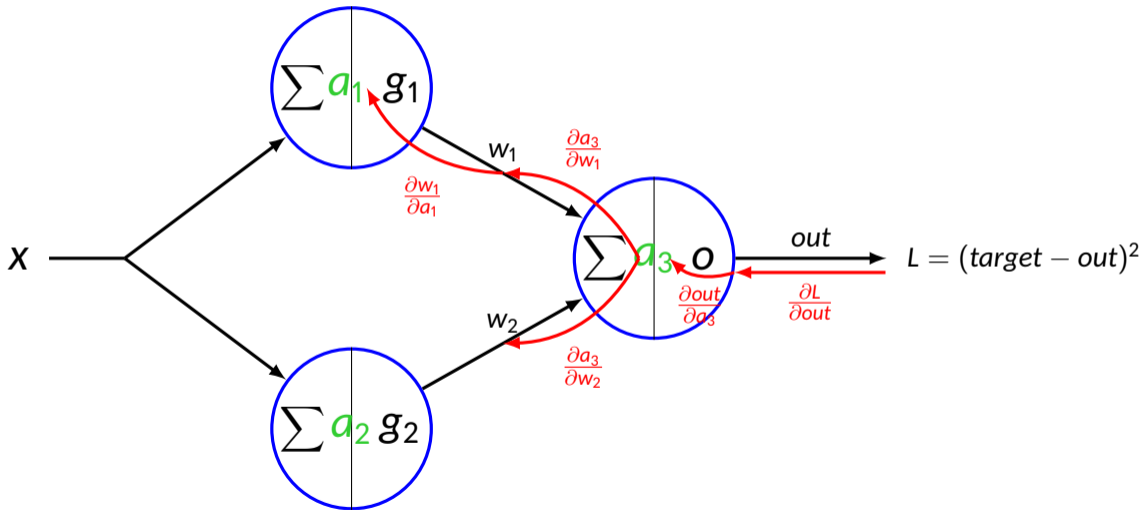
Backpropagation



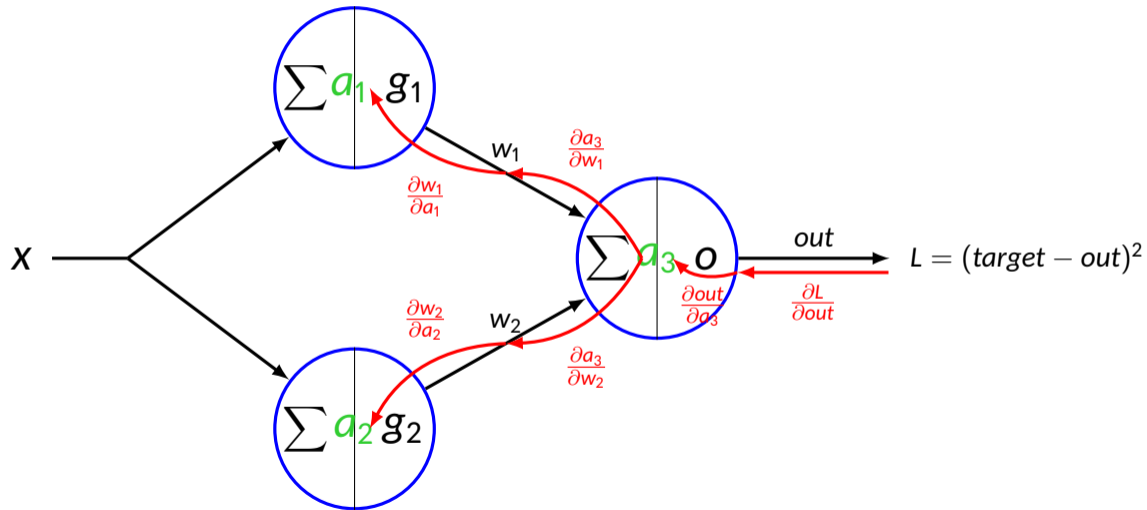
Backpropagation



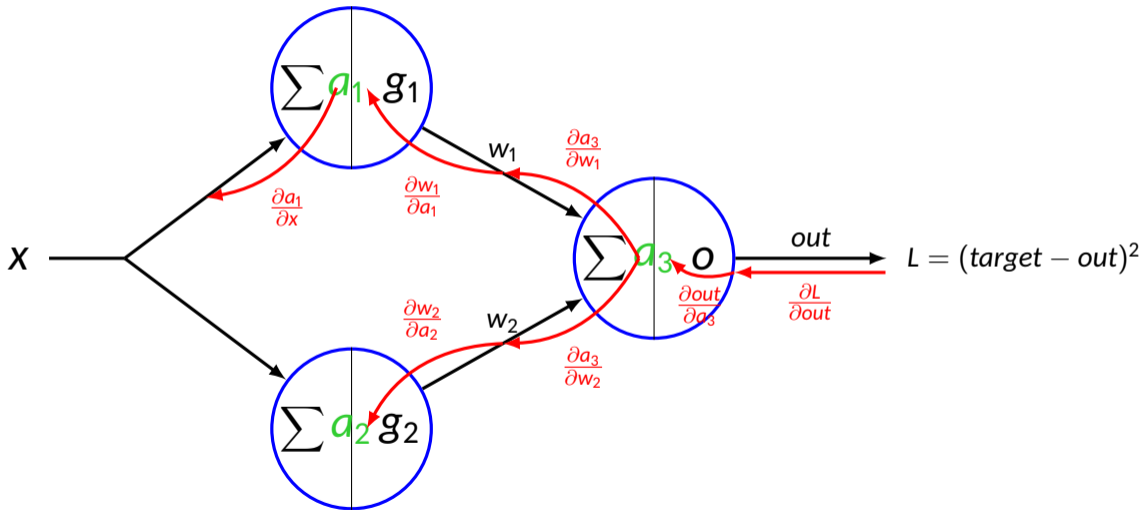
Backpropagation



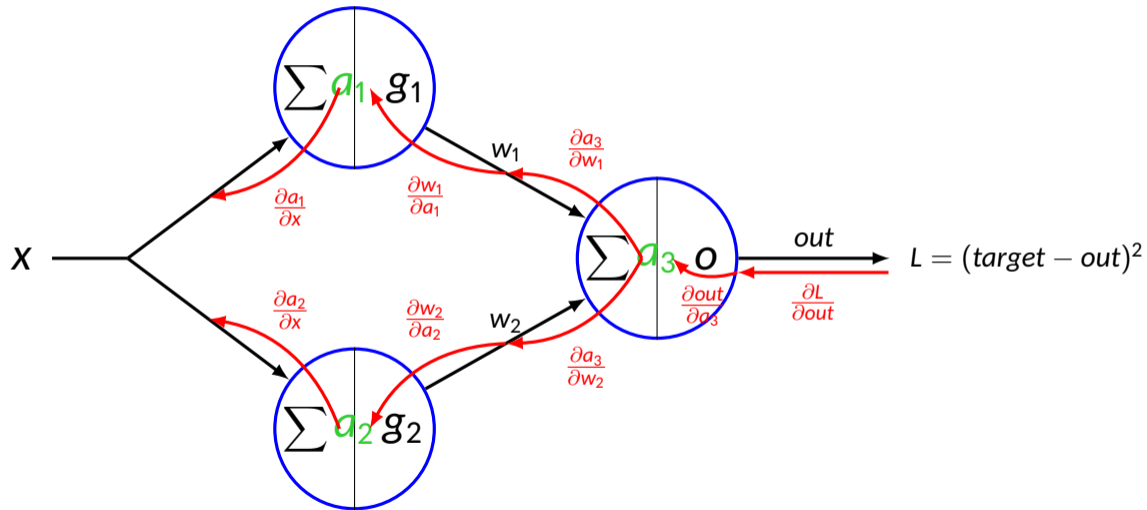
Backpropagation



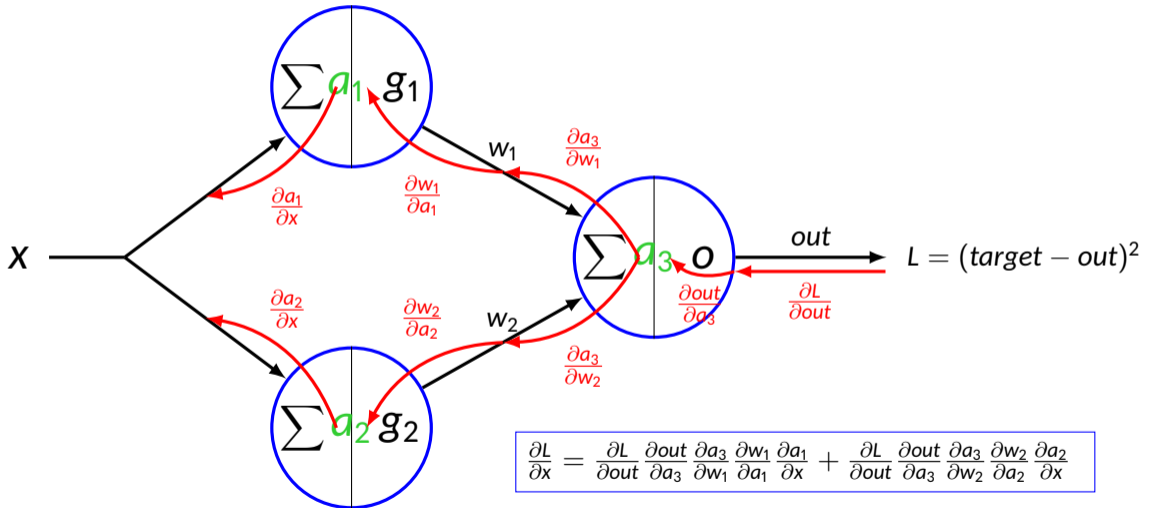
Backpropagation



Backpropagation

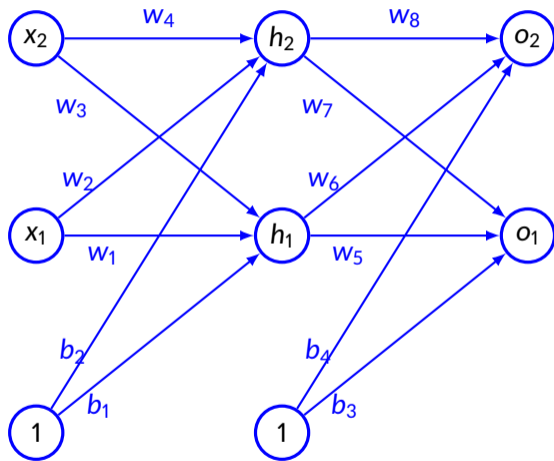


Backpropagation



$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial out} \frac{\partial out}{\partial a_3} \frac{\partial a_3}{\partial W_1} \frac{\partial W_1}{\partial a_1} \frac{\partial a_1}{\partial x} + \frac{\partial L}{\partial out} \frac{\partial out}{\partial a_3} \frac{\partial a_3}{\partial W_2} \frac{\partial W_2}{\partial a_2} \frac{\partial a_2}{\partial x}$$

Example



Example

