Introduction to Deep Learning

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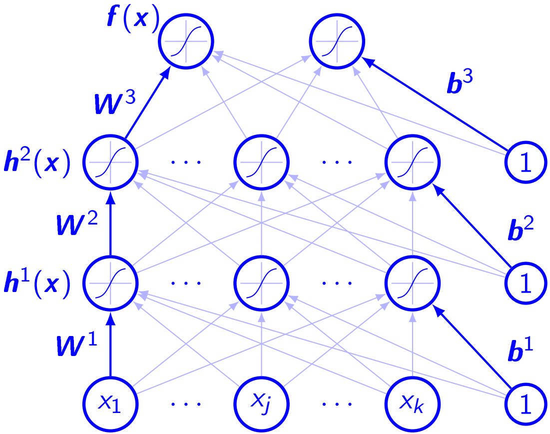
- Goal of NN is not to accurately model brain!

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

Overcome issues of linear FFN

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  - Manually design ϕ
    - Require domain knowledge
  - Strategy of deep learning is to learn ϕ

Goal of deep learning

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

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

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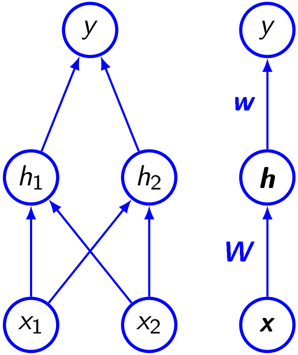
- Solving these, we get $\boldsymbol{w} = 0$ and $b = \frac{1}{2}$

Simple feedforward network with hidden layer

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



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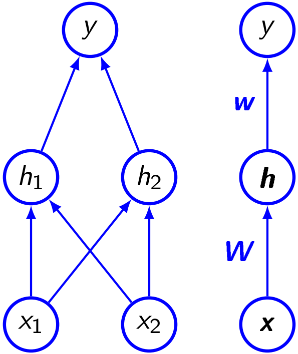

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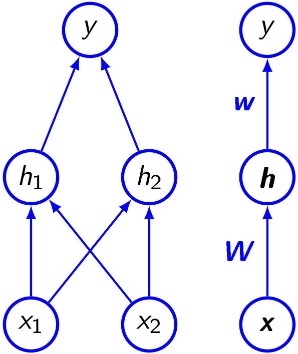

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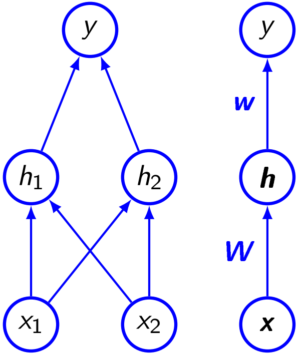

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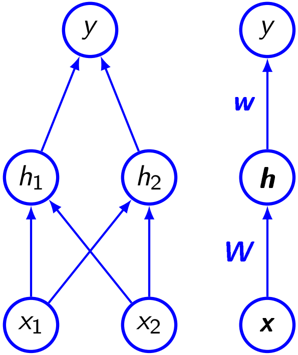

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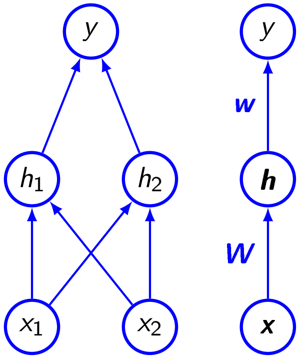
- We need to have nonlinear function to describe the features
- Usually NN have affine transformation of learned parameters followed by nonlinear activation function
- Let us use $\boldsymbol{h} = g(\boldsymbol{W}^T\boldsymbol{x} + \boldsymbol{c})$
- Let us use ReLU as activation function $g(z) = \max\{0,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



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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

- Suppose we have 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. $\frac{\partial}{\partial x_i} f(\boldsymbol{x})$
- Gradient vector is represented as $\nabla_{\boldsymbol{x}} f(\boldsymbol{x})$
- Gradient descent proposes a new point as $\boldsymbol{x}' = \boldsymbol{x} - \epsilon \nabla_{\boldsymbol{x}} f(x)$ where ϵ is the learning rate

Stochastic gradient descent

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

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

Cost function

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

Maximum likelihood estimation

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

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

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- Let $p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$ be a parametric family of probability distribution
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$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} p_{model}(\mathbb{X}; \boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{m} p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

- It can be written as $\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{m} \log p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$
- By dividing m we get $\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x} \sim \hat{p}_{data}} \log p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$
- We need to minimize $-\arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x} \sim \hat{p}_{data}} \log p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$

Conditional log-likelihood

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

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

Linear regression as maximum likelihood

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

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$$\sum_{i=1}^{m} \log p(\boldsymbol{y}^{(i)}|\boldsymbol{x}^{(i)}; \boldsymbol{\theta}) = -m \log \sigma - \frac{m}{2} \log(2\pi) - \sum_{i=1}^{m} \frac{\|\hat{y}^{(i)} - y^{(i)}\|^2}{2\sigma^2}$$

Learning conditional distributions with max likelihood

- 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 $J(\boldsymbol{\theta}) = -\mathbb{E}_{\mathbf{X},\mathbf{Y}\sim\hat{p}_{data}} \log p_{model}(\mathbf{y}|\mathbf{x})$
- 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 $p(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\theta})$, we want to learn one conditional statistics of $\boldsymbol{y}$ given $\boldsymbol{x}$
  - For a predicting function $f(\boldsymbol{x};\boldsymbol{\theta})$, we would like to predict the mean of $\boldsymbol{y}$

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  - Mean of $\boldsymbol{y}$ for each value of $\boldsymbol{x}$
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Calculus of variation

- Now we have

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

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- Now we have

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

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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 $A[y] = \int_{x_1}^{x_2} \sqrt{1 + [y'(x)]^2}\, dx$
  - $y'(x) = \frac{dy}{dx}\,, \quad y_1 = f(x_1)\,, \quad y_2 = f(x_2)$

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- Now we have, $\dfrac{d}{dx}\dfrac{f'(x)}{\sqrt{1 + [f'(x)]^2}} = 0$

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- Taking derivative we get $\frac{d^2 f}{dx^2} \cdot \frac{1}{\left[\sqrt{1+[f'(x)]^2}\right]^3} = 0$

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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 $b = \frac{x_2 y_1 - x_1 y_2}{x_2 - x_1}$

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 $\boldsymbol{h}$, linear output unit produces $\hat{\boldsymbol{y}} = \boldsymbol{W}^T\boldsymbol{h} + \boldsymbol{b}$
- This can be treated as conditional probability $p(\boldsymbol{y}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{y}; \hat{\boldsymbol{y}}, \boldsymbol{I})$
- 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 $p(y = 1|\boldsymbol{x})$
  - If linear unit has been chosen, $p(y = 1|\boldsymbol{x}) = \max\left\{0, \min\{1, \boldsymbol{W}^T\boldsymbol{h} + \boldsymbol{b}\}\right\}$
  - Gradient?
- Model should have strong gradient whenever the answer is wrong
- Let us assume unnormalized log probability is linear with $z = \boldsymbol{W}^T\boldsymbol{h} + \boldsymbol{b}$
- Therefore, $\log \tilde{P}(y) = yz \Rightarrow \tilde{P}(y) = \exp(yz) \Rightarrow P(y) = \dfrac{\exp(yz)}{\sum_{y' \in \{0,1\}} \exp(y'z)}$
  - It can be written as $P(y) = \sigma((2y-1)z))$
- The loss function for maximum likelihood is
  $J(\boldsymbol{\theta}) = -\log P(y|\boldsymbol{x}) = -\log \sigma((2y-1)z) = \zeta((1-2y)z)$

Softmax unit

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

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, $h_i = g(\boldsymbol{z}, \boldsymbol{\alpha})_i = \max(0, z_i) + \alpha_i \min(0, z_i)$
  - 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 $g(\boldsymbol{z})_i = \max_{j \in \mathbb{G}^{(i)}} z_j$
  - 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 $h = \cos(\boldsymbol{Wx} + \boldsymbol{b})$ performs well for MNIST data set
- Sometimes no activation function helps in reducing the number of parameters
- Radial Basis Function - $\phi(\boldsymbol{x}, \boldsymbol{c}) = \phi(\|\boldsymbol{x} - \boldsymbol{c}\|)$
  - Gaussian - $\exp(-(\varepsilon r)^2)$
- 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

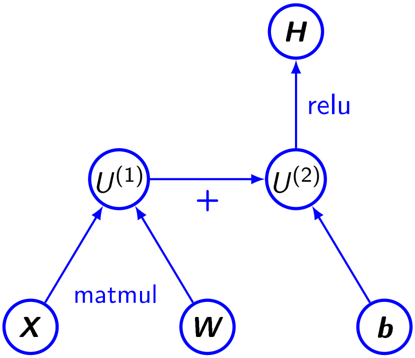
Architecture design

- 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 $\boldsymbol{x}$ is read and produces an output $\hat{\boldsymbol{y}}$
  - This is forward propagation
- During training forward propagation continues until it produces cost $J(\boldsymbol{\theta})$
- 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. $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

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 $\boldsymbol{x} \in \mathbb{R}^m$, $\boldsymbol{y} \in \mathbb{R}^n$, $g : \mathbb{R}^m \rightarrow \mathbb{R}^n$ and $f : \mathbb{R} \rightarrow \mathbb{R}$ and $\boldsymbol{y} = g(\boldsymbol{x})$ and $z = f(\boldsymbol{y})$

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j}\frac{\partial y_j}{\partial x_i}$$

- In vector notation it will be where $\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$ is the $n \times m$ Jacobian matrix of g

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

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 $i = 1, 2, \ldots, n_i$
- 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. $u^{(i)} = f(\mathbb{A}^{(i)})$

Algorithm for forward pass

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

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

end for

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

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

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

end for

return $u^{(n)}$

Algorithm for backward pass

$\texttt{grad\_table}[u^{(i)}] \leftarrow 1$

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

$$\texttt{grad\_table}[u^{(j)}] \leftarrow \sum_{i:j \in Pa(u^{(i)})} \texttt{grad\_table}[u^{(i)}] \frac{\partial u^{(i)}}{\partial u^{(j)}}$$

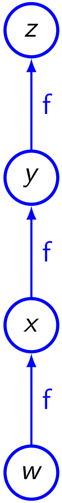
end for

return grad_table

Computational graph & subexpression

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

$$
\begin{aligned}
\frac{\partial z}{\partial w} \\
&= \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}\frac{\partial x}{\partial w} \\
&= f'(y)f'(x)f'(w) \\
&= f'(f(f(w)))f'(f(w))f'(w)
\end{aligned}
$$



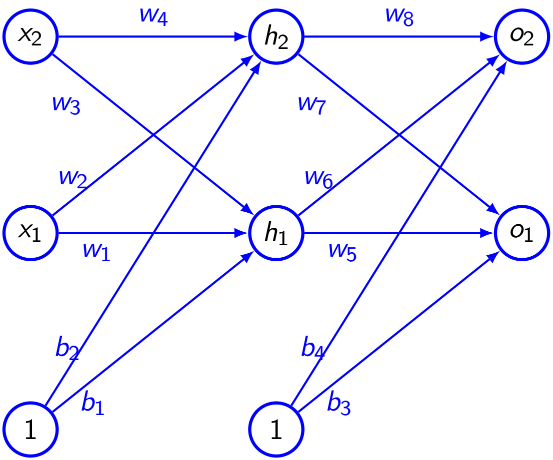
Forward propagation in MLP

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

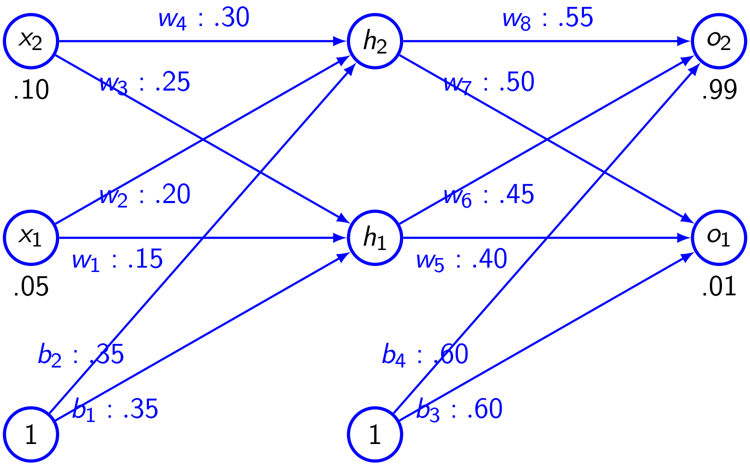
Backward computation in MLP

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

Example



Example



w_4 : .30
w_8 : .55
x_2
h_2
o_2
.10
w_3 : .25
w_7 : .50
.99
w_2 : .20
w_6 : .45
x_1
h_1
o_1
w_1 : .15
w_5 : .40
.05
.01
b_2 : .35
b_4 : .60
b_1 : .35
b_3 : .60
1
1