Backpropagation

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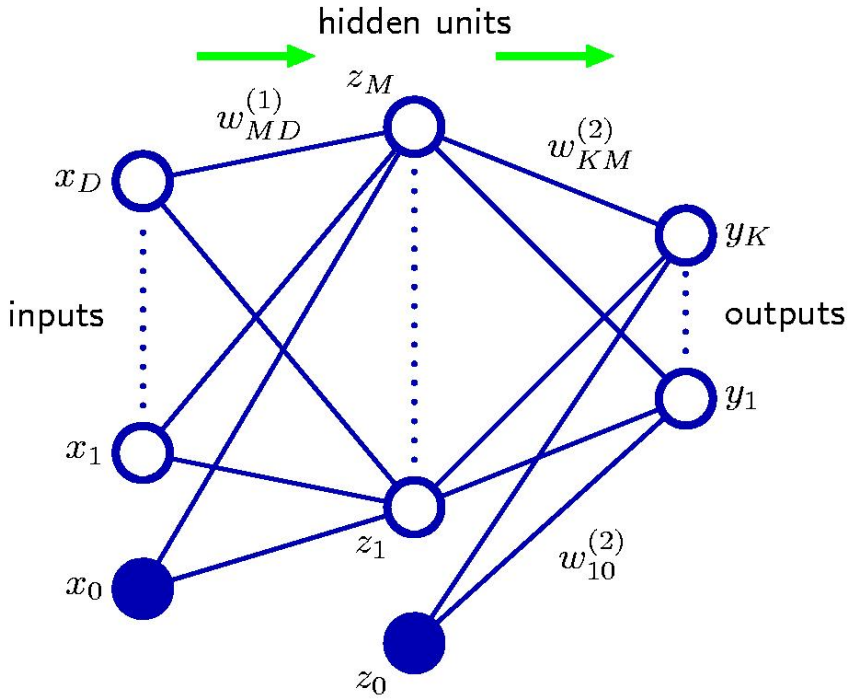
Topics in Backpropagation

1. Forward Propagation
2. Loss Function and Gradient Descent
3. Computing derivatives using chain rule
4. Computational graph for backpropagation
5. Backprop algorithm
6. The Jacobian matrix

A neural network with one hidden layer



Augmented network

No. of weights in $\boldsymbol{w}$:

$T=(D+1)M+(M+1)K$

$=M(D+K+1)+K$

D input variables $x_1,..,\ x_D$

M hidden unit activations

$$a_j = \sum_{i=1}^{D} w^{(1)}_{ji} x_i + w^{(1)}_{j0} \quad \text{where} \quad j = 1,..,M$$

Hidden unit activation functions

$$z_j = h(a_j)$$

K output activations

$$a_k = \sum_{i=1}^{M} w^{(2)}_{ki} x_i + w^{(2)}_{k0} \quad \text{where} \quad k = 1,..,K$$

Output activation functions

$$y_k = \sigma(a_k)$$

$$y_k(\boldsymbol{x},\boldsymbol{w}) = \sigma\left(\sum_{j=1}^{M} w^{(2)}_{kj} h\left(\sum_{i=1}^{D} w^{(1)}_{ji} x_i + w^{(1)}_{j0} \right) + w^{(2)}_{k0} \right)$$

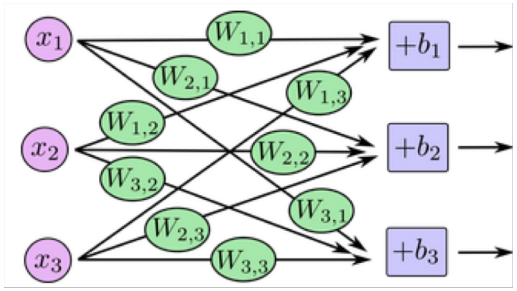
Matrix Multiplication: Forward Propagation

- Each layer is a function of layer that preceded it
  - First layer is given by $\boldsymbol{z} = h\left(\boldsymbol{W}^{(1)\mathrm{T}}\boldsymbol{x} + \boldsymbol{b}^{(1)}\right)$
  - Second layer is $\boldsymbol{y} = \sigma\left(\boldsymbol{W}^{(2)\mathrm{T}}\boldsymbol{x} + \boldsymbol{b}^{(2)}\right)$
  - Note that W is a matrix rather than a vector
    - Example with $D=3,\ M=3$

$$\boldsymbol{x} = [x_1, x_2, x_3]^{\mathrm{T}} \qquad \boldsymbol{w} = \begin{cases} W_1^{(1)} = \left[W_{11} W_{12} W_{13}\right]^T, W_2^{(1)} = \left[W_{21} W_{22} W_{23}\right]^T, W_3^{(1)} = \left[W_{31} W_{32} W_{33}\right]^T \\ W_1^{(2)} = \left[W_{11} W_{12} W_{13}\right]^T, W_2^{(2)} = \left[W_{21} W_{22} W_{23}\right]^T, W_3^{(2)} = \left[W_{31} W_{32} W_{33}\right]^T \end{cases}$$

  - Unaugmented network

First Network layer



Network layer output

$$\begin{pmatrix} W_{1,1}x_1 + W_{1,2}x_2 + W_{1,3}x_3 + b_1 \\ W_{2,1}x_1 + W_{2,2}x_2 + W_{2,3}x_3 + b_2 \\ W_{3,1}x_1 + W_{3,2}x_2 + W_{3,3}x_3 + b_3 \end{pmatrix}$$

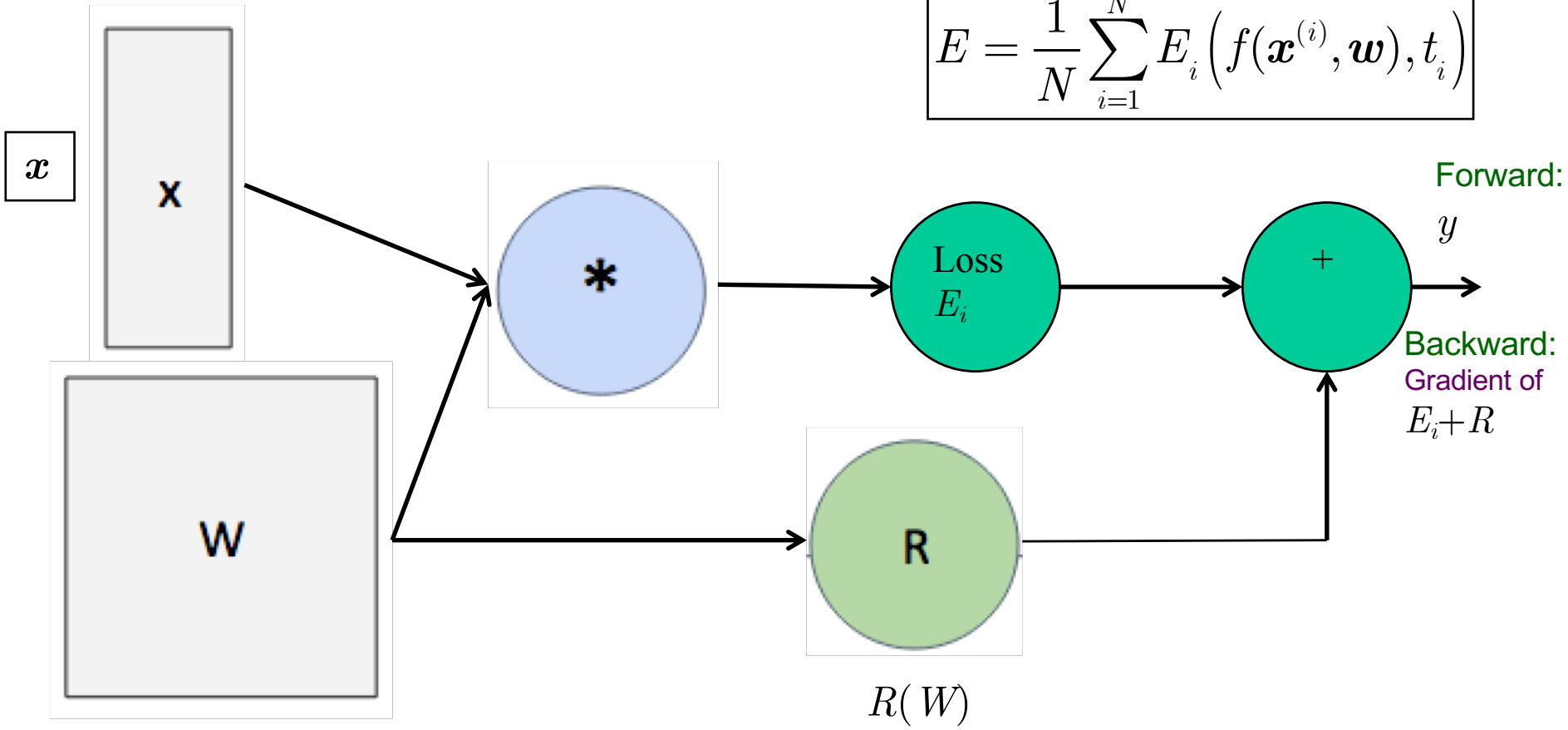
In matrix multiplication notation

$$\left(\begin{bmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

Loss and Regularization

$$y = f(\boldsymbol{x}, \boldsymbol{w})$$

$$E = \frac{1}{N}\sum_{i=1}^{N} E_i\left(f(\boldsymbol{x}^{(i)}, \boldsymbol{w}), t_i\right)$$



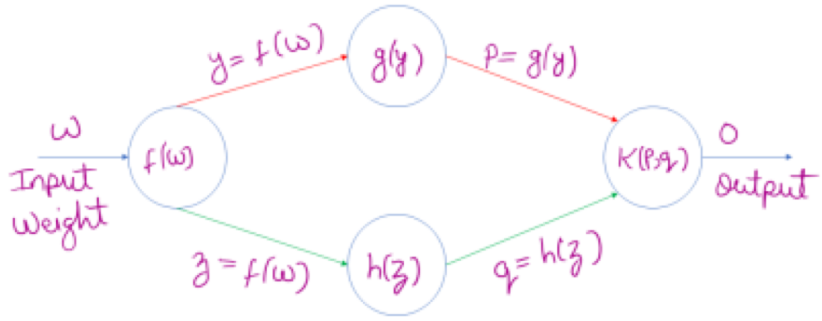
Gradient Descent

- Goal: determine weights $\boldsymbol{w}$ from labeled set of training samples
- Learning procedure has two stages
  1. Evaluate derivatives of loss $\nabla E(\boldsymbol{w})$ with respect to weights $w_1,..w_T$
  2. Use derivative vector to compute adjustments to weights

$$\boldsymbol{w}^{(\tau+1)} = \boldsymbol{w}^{(\tau)} - \eta \nabla E(\boldsymbol{w}^{(\tau)})$$

$$\nabla E(\boldsymbol{w}) = \begin{bmatrix} \frac{\partial E}{\partial w_0} \\ \frac{\partial E}{\partial w_1} \\ \\ \frac{\partial E}{\partial w_T} \end{bmatrix}$$

Computing derivatives using Chain Rule



$$o = K(p,q) = K(g(f(\omega)), h(f(\omega)))$$

Composition function

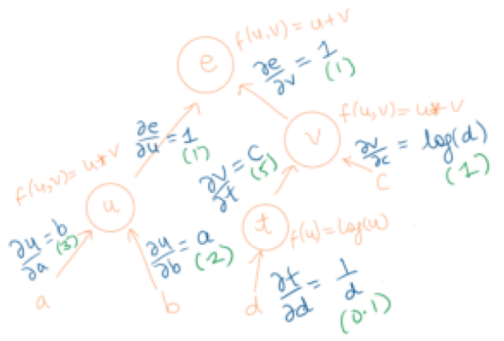
$$\frac{\partial o}{\partial \omega} = \frac{\partial o}{\partial p} \cdot \frac{\partial p}{\partial y} \cdot \frac{\partial y}{\partial \omega} + \frac{\partial o}{\partial q} \cdot \frac{\partial q}{\partial z} \cdot \frac{\partial z}{\partial \omega} \quad \text{[Chain Rule]}$$

$$= \frac{\partial K(p,q)}{\partial p} \cdot g'(y) \cdot f'(\omega) + \frac{\partial K(p,q)}{\partial q} \cdot h'(z) \cdot f'(\omega)$$

Path 1 Path 2

Back-propagation:

e.g. $a = 2, b = 3, c = 5, d = 10$



$e = a*b + c\log(d)$

$\frac{\partial e}{\partial a} = b(1) = b$

$\frac{\partial e}{\partial b} = a(1) = a$

$\frac{\partial e}{\partial c} = \log d \times 1 = \log d$

$\frac{\partial e}{\partial d} = \frac{1}{d} \times c * 1 = \frac{c}{d}$

Example of Derivative Computation

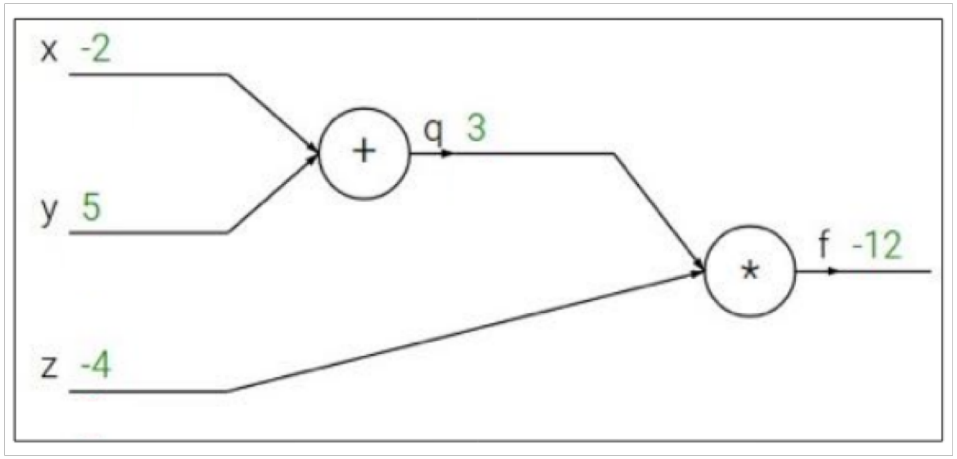
$$f(x,y,z) = (x+y)z$$

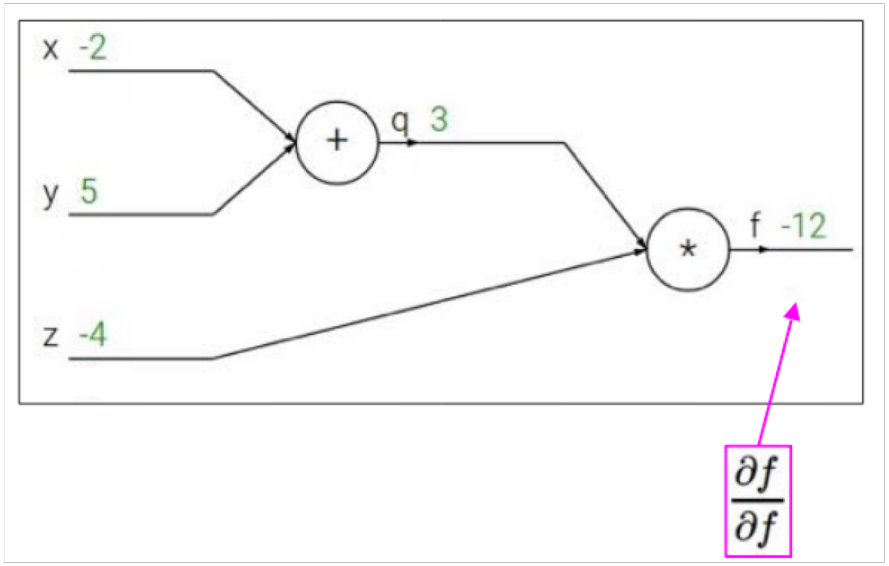
e.g. x = -2, y = 5, z = -4

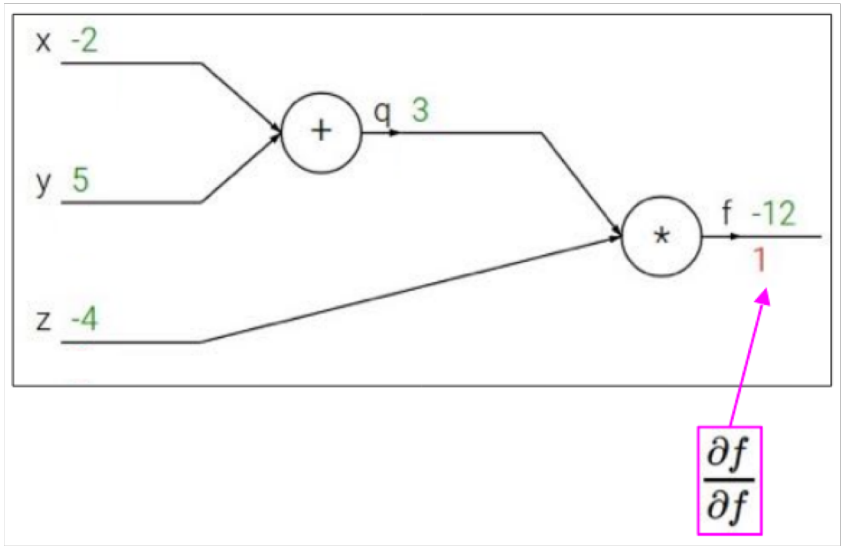
$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

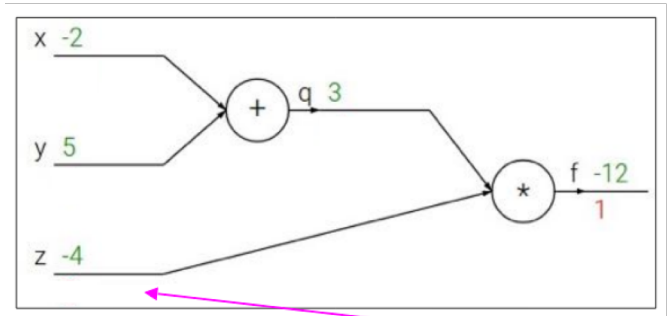
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



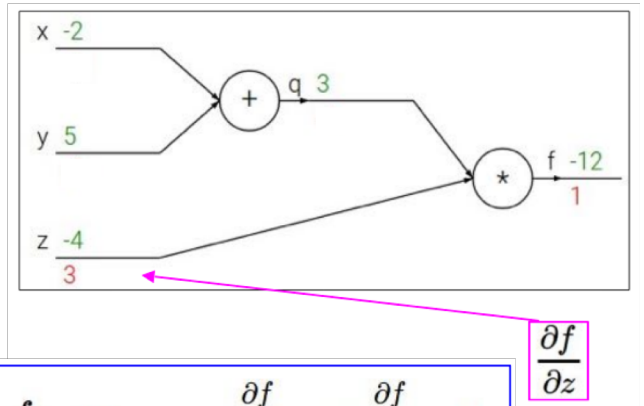




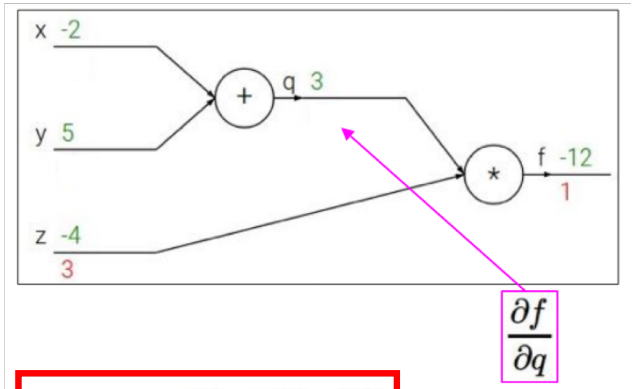
Computing derivatives of output wrt inputs



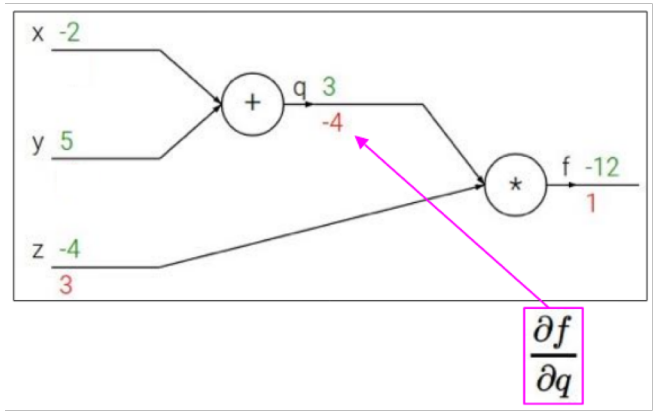
$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$

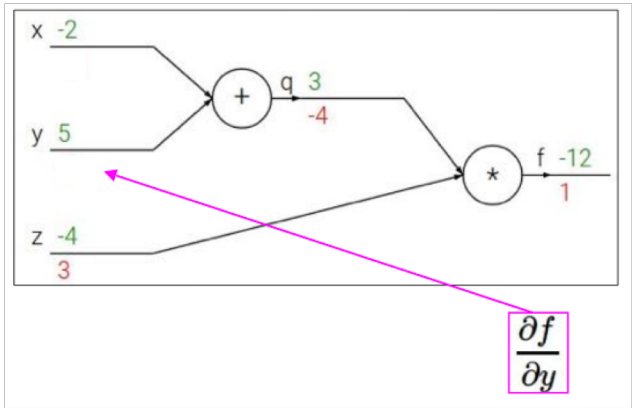


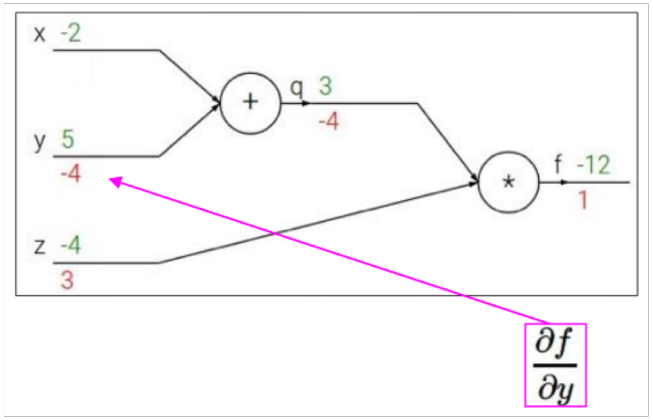
$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$

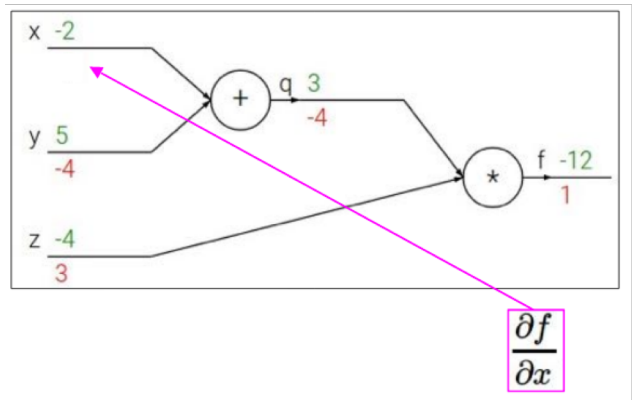


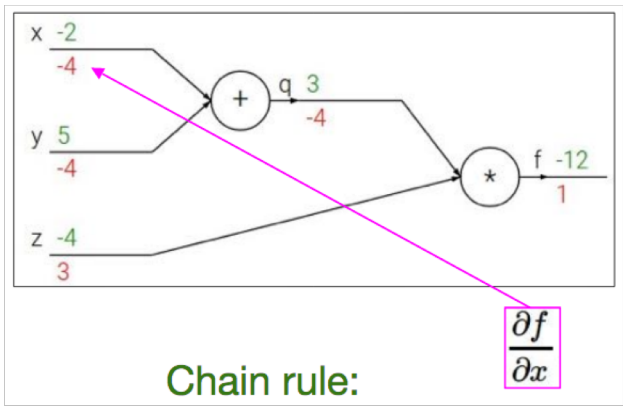
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$





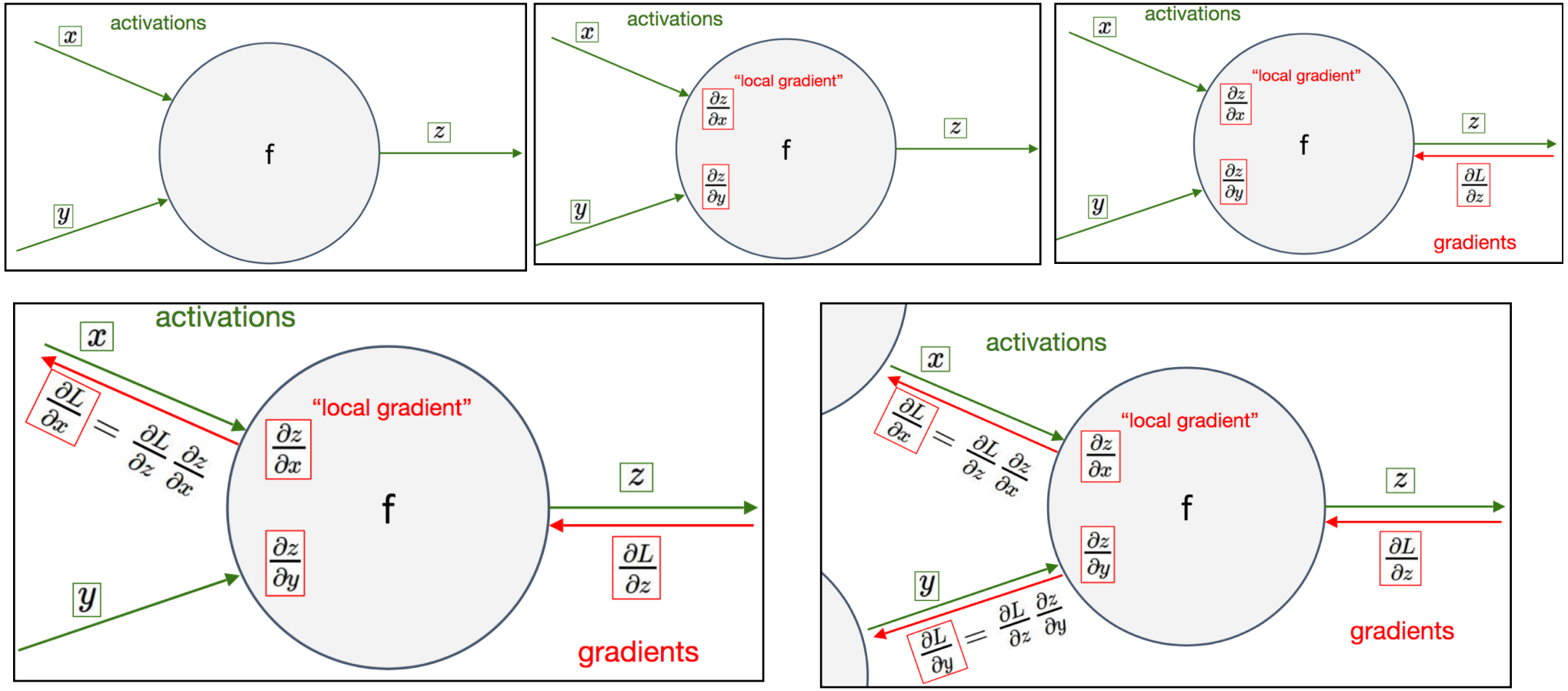






$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x}$$

Derivatives for a neuron: $z=f(x,y)$



Composite Function

- Consider a composite function $f\left(g\left(h\left(x\right)\right)\right)$
  - i.e., an outer function f, an inner function g and a final inner function $h(x)$
- Say $f(x) = e^{\sin(x^2)}$ we can decompose it as:

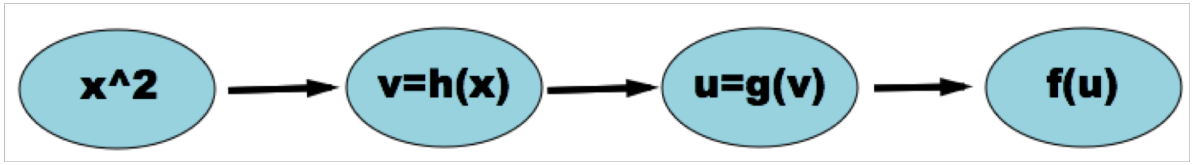
  $f\left(x\right)=e^{x}$

  $g(x)=sin\ x$ and

  $h(x)=x^2$ or

  $f\left(g(h(x))\right)=e^{\ g(h(x))}$

  - Its computational graph is



  - Every connection is an input, every node is a function or operation

Derivatives of Composite function

- To get derivatives of $f\left(g\left(h\left(x\right)\right)\right)= e^{g(h(x))}$ wrt x

1. We use the chain rule $\boxed{\frac{df}{dx}=\frac{df}{dg}\cdot\frac{dg}{dh}\cdot\frac{dh}{dx}}$ where

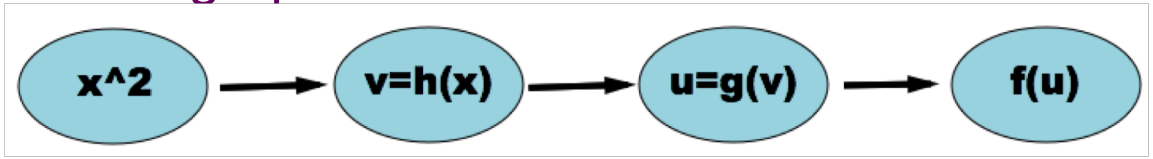
$\boxed{\frac{df}{dg}=e^{g(h(x))}}$ since $f\left(g(h(x))\right)=e^{g(h(x))}$ & derivative of e^x is e

$\boxed{\frac{dg}{dh}=\cos(h(x))}$ since $g(h(x))=sin\ h(x)$ & derivative $\sin$ is $\cos$

$\boxed{\frac{dh}{dx}=2x}$ because $h(x)=x^2$ & its derivative is $2x$

- Therefore $\boxed{\frac{df}{dx}=e^{g(h(x))}\cdot\cos\ h(x)\cdot 2x=e^{\sin x^{**}2}\cdot\cos x^2\cdot 2x}$
- In each of these cases we pretend that the inner function is a single variable and derive it as such

2. Another way to view it $f(x)=e^{\sin(x^2)}$
   - Create temp variables $u=\sin\ v$, $v=x^2$, then $f\left(u\right)=e^u$ with computational graph:



Derivative using Computational Graph

- All we need to do is get the derivative of each node wrt each of its inputs

With $u=\sin\ v$, $v=x^2$, $f\ (u)=e^u$

- We can get whichever derivative we want by multiplying the 'connection' derivatives

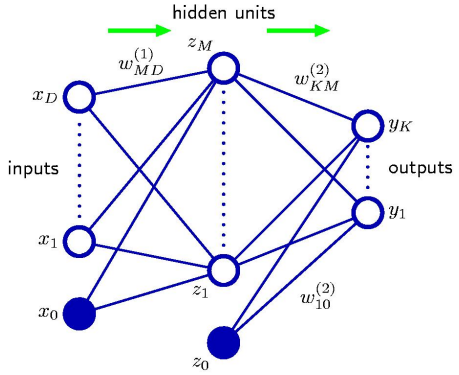
$$\boxed{\frac{dh}{dx}=2x} \qquad \boxed{\frac{dg}{dh}=\cos(h(x))} \qquad \boxed{\frac{df}{dg}=e^{g(h(x))}}$$

$$\boxed{\frac{df}{dx}=\frac{df}{dg}\cdot\frac{dg}{dh}\cdot\frac{dh}{dx}} \qquad \boxed{\begin{aligned}\frac{df}{dx}&=e^{g(h(x))}\cdot\cos\ \ h(x)\cdot 2x\\&=e^{\sin x^2}\cdot\cos x^2\cdot 2x\end{aligned}}$$

Since $f\ (x)=e^x,\ g(x)=sin\ x$ and $h(x)=x^2$

Evaluating the gradient

- Goal of this section:
  - Find an efficient technique for evaluating gradient of an error function $E(\boldsymbol{w})$ for a feed-forward neural network:



- Gradient evaluation can be performed using a local message passing scheme
  - In which information is alternately sent forwards and backwards through the network
  - Known as *error backpropagation* or simply as *backprop*

Back-propagation Terminology and Usage

- Backpropagation is term used in neural computing literature to mean a variety of different things
  - Term is used here for computing derivative of the error function wrt the weights
  - In a second separate stage the derivatives are used to compute the adjustments to be made to the weights
- Can be applied to error function other than sum of squared errors
- Used to evaluate other matrices such as Jacobian and Hessian matrices
- Second stage of weight adjustment using calculated derivatives can be tackled using variety of optimization schemes substantially more powerful than gradient descent

Overview of Backprop algorithm

- Choose *random* weights for the network
- Feed in an example and obtain a result
- Calculate the error for each node (starting from the last stage and propagating the error backwards)
- Update the weights
- *Repeat* with other examples until the network converges on the target output

- How to divide up the errors needs a little calculus

Evaluation of Error Function Derivatives

- Derivation of back-propagation algorithm for
  - Arbitrary feed-forward topology
  - Arbitrary differentiable nonlinear activation function
  - Broad class of error functions
- Error functions of practical interest are sums of errors associated with each training data point

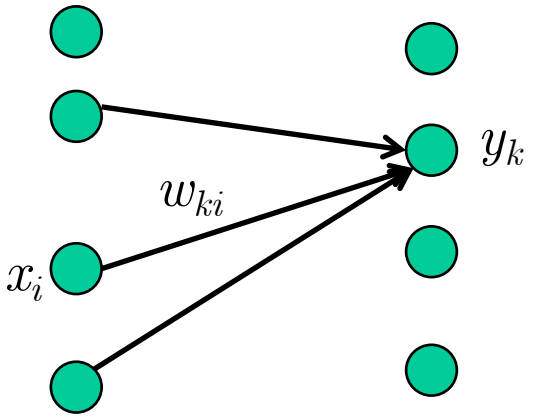
$$E(\boldsymbol{w}) = \sum_{n=1}^{N} E_n(\boldsymbol{w})$$

- We consider problem of evaluating $\nabla E_n(\boldsymbol{w})$
  - For the n^{th} term in the error function
  - Derivatives are wrt the weights $w_1,..w_T$
  - This can be used directly for sequential optimization or accumulated over training set (for batch)

Simple Model (Multiple Linear Regression)

- Outputs y_k are linear combinations of inputs x_i

$$y_k = \sum_i w_{ki} x_i$$



- Error function for a particular input $\boldsymbol{x}_n$ is

$$E_n = \frac{1}{2}\sum_k \left(y_{nk} - t_{nk}\right)^2$$

Where summation is over all K outputs

For a particular input x and weight w , squared error is:

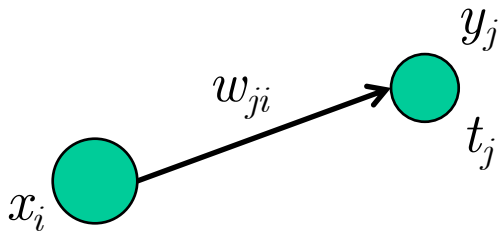
$$E = \frac{1}{2}\left(y(x,w) - t\right)^2$$

$$\frac{\partial E}{\partial w} = \left(y(x,w) - t\right)x = \delta \cdot x$$

  - where $y_{nk}=y_k(\boldsymbol{x}_n,\boldsymbol{w})$
  - Gradient of Error function wrt a weight w_{ji}:

$$\frac{\partial E_n}{\partial w_{ji}} = \left(y_{nj} - t_{nj}\right)x_{ni}$$

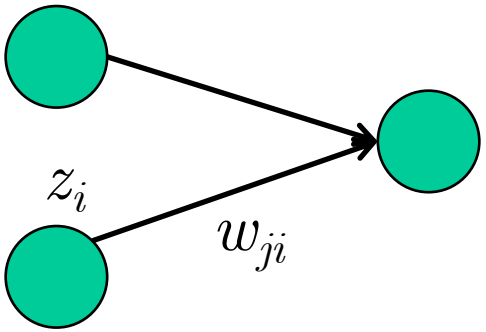
  - a local computation involving product of
    - error signal y_{nj}-t_{nj} associated with output end of link w_{ji}
    - variable x_{ni} associated with input end of link



$$\frac{\partial E}{\partial w_{ji}} = \left(y_j - t_j\right)x_i = \delta_j \cdot x_i$$

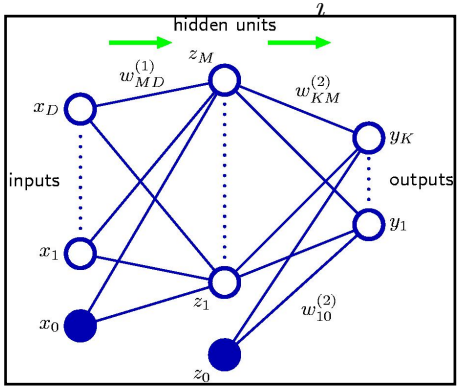
Extension to more complex multilayer Network

- Each unit computes a weighted sum of its inputs $a_j = \sum_i w_{ji} z_i$



$$a_j = \sum_i w_{ji} z_i$$

$$z_j = h(a_j)$$



  - z_i is activation of a unit (or input) that sends a connection to unit j and w_{ji} is the weight associated with the connection
- Output is transformed by a nonlinear activation function $z_j = h(a_j)$
  - The variable z_i can be an input and unit j could be an output
- For each input $\boldsymbol{x_n}$ in the training set, we calculate activations of all hidden and output units by applying above equations
  - This process is called forward propagation

Evaluation of Derivative E_n wrt a weight w_{ji}

- The outputs of the various units depend on particular input n
  - We shall omit the subscript n from network variables
  - Note that E_n depends on w_{ji} only via the summed input a_j to unit j.
  - We can therefore apply chain rule for partial derivatives to give

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j}\frac{\partial a_j}{\partial w_{ji}}$$

  - Derivative wrt weight is given by product of derivative wrt activity and derivative of activity wrt weight
  - We now introduce a useful notation $\delta_j \equiv \frac{\partial E_n}{\partial a_j}$
  - Where the δs are errors as we shall see
  - Using $a_j = \sum_i w_{ji} z_i$ we can write $\frac{\partial a_j}{\partial w_{ji}} = z_i$
- Substituting we get $\frac{\partial E_n}{\partial w_{ji}} = \delta_j z_i$
  - i.e., required derivative is obtained by multiplying the value of δ for the unit at the output end of the weight by the the value of z at the input end of the weight
  - This takes the same form as for the simple linear model

Summarizing evaluation of Derivative $\frac{\partial E_n}{\partial w_{ji}}$

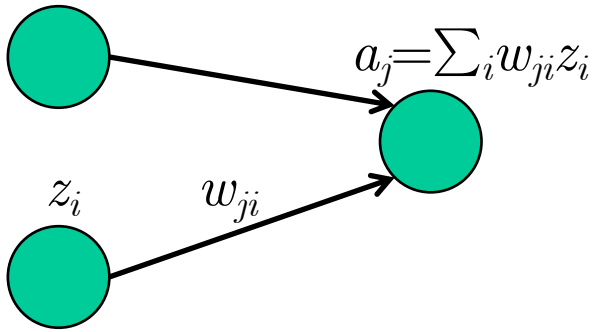
- By chain rule for partial derivatives

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j}\frac{\partial a_j}{\partial w_{ji}}$$

Define $\delta_j \equiv \frac{\partial E_n}{\partial a_j}$

$a_j = \sum_i w_{ji} z_i$

we have $\frac{\partial a_j}{\partial w_{ji}} = z_i$



- Substituting we get

$$\frac{\partial E_n}{\partial w_{ji}} = \delta_j z_i$$

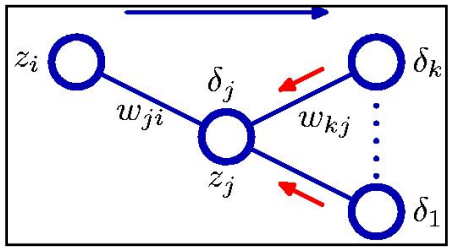
- Thus required derivative is obtained by multiplying
  1. Value of δ for the unit at output end of weight
  2. Value of z for unit at input end of weight
- Need to figure out how to calculate δ_j for each unit of network
  - For output units $\delta_j = y_j - t_j$

$$\text{If } E = \frac{1}{2}\sum_j (y_j - t_j)^2 \text{ and } y_j = a_j = \sum w_{ji} z_i \text{ then } \delta_j = \frac{\partial E}{\partial a_j} = y_j - t_j$$

For regression

  - For hidden units, we again need to make use of chain rule of derivatives to determine $\delta_j \equiv \frac{\partial E_n}{\partial a_j}$

Calculation of Error for hidden unit δ_j



Blue arrow for forward propagation
Red arrows indicate direction of information flow during error backpropagation

- For hidden unit j by chain rule

$$\delta_j \equiv \frac{\partial E_n}{\partial a_j} = \sum_k \frac{\partial E_n}{\partial a_k}\frac{\partial a_k}{\partial a_j}$$

Where sum is over all units k to which j sends connections

- Substituting $\delta_k \equiv \frac{\partial E_n}{\partial a_k}$

$$a_k = \sum_i w_{ki} z_i = \sum_i w_{ki} h(a_i)$$

$$\frac{\partial a_k}{\partial a_j} = \sum_k w_{kj} h'(a_j)$$

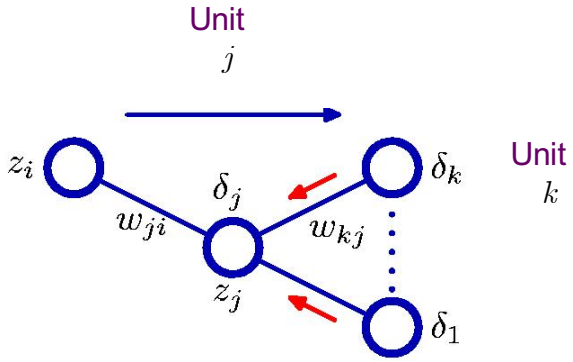
- We get the backpropagation formula for error derivatives at stage j

$$\delta_j = h'(a_j)\sum_k w_{kj}\delta_k$$

Input to activation from earlier units

error derivative at later unit k

Error Backpropagation Algorithm



- Backpropagation Formula

$$\delta_j = h'(a_j)\sum_k w_{kj}\delta_k$$

- Value of δ for a particular hidden unit can be obtained by propagating the δ's backward from units higher-up in the network

1. Apply input vector $\boldsymbol{x}_n$ to network and forward propagate through network using

$$a_j = \sum_i w_{ji} z_i \quad \text{and} \quad z_j = h(a_j)$$

2. Evaluate δ_k for all output units using

$$\delta_k = y_k - t_k$$

3. Backpropagate the δ's using

$$\delta_j = h'(a_j)\sum_k w_{kj}\delta_k$$

to obtain δ_j for each hidden unit

4. Use

$$\frac{\partial E_n}{\partial w_{ji}} = \delta_j z_i$$

to evaluate required derivatives

A Simple Example

- Two-layer network
- Sum-of-squared error
- Output units: *linear activation* functions, i.e., multiple regression

$$y_k = a_k$$

- Hidden units have *logistic sigmoid* activation function

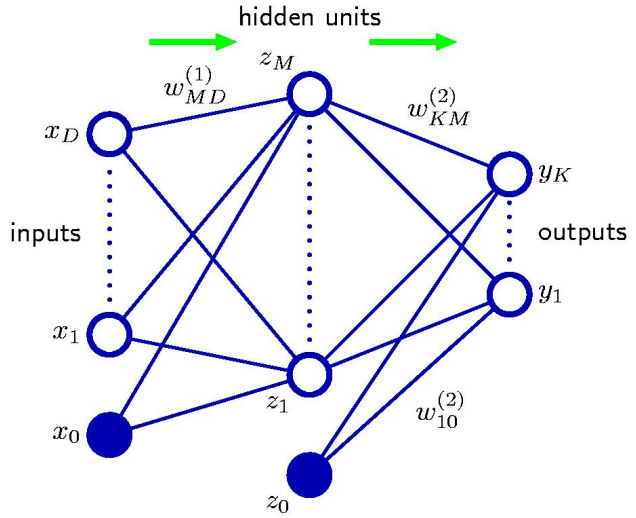
$$h(a) = \tanh(a)$$

where

$$\tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$$

simple form for derivative

$$h'(a) = 1 - h(a)^2$$



Standard Sum of Squared Error

$$E_n = \frac{1}{2}\sum_k \left(y_k - t_k\right)^2$$

y_k: activation of output unit k

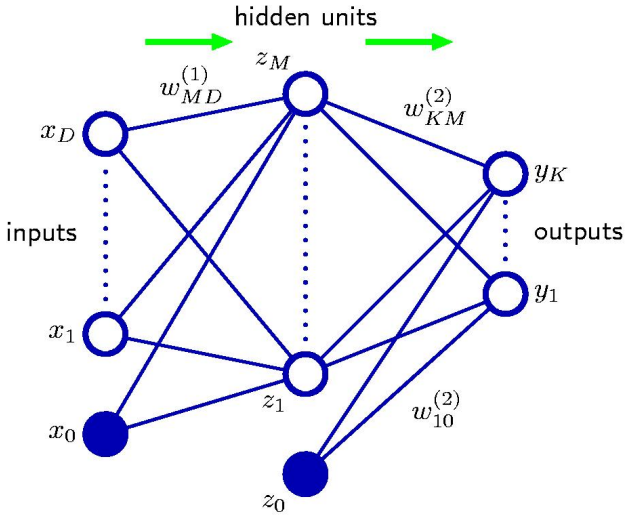
t_k : corresponding target for input x_k

Simple Example: Forward and Backward Prop

For each input in training set:

- Forward Propagation

$$a_j = \sum_{i=0}^{D} w_{ji}^{(1)} x_i$$
$$z_j = \tanh(a_j)$$
$$y_k = \sum_{j=0}^{M} w_{kj}^{(2)} z_j$$



- Output differences

$$\delta_k = y_k - t_k$$

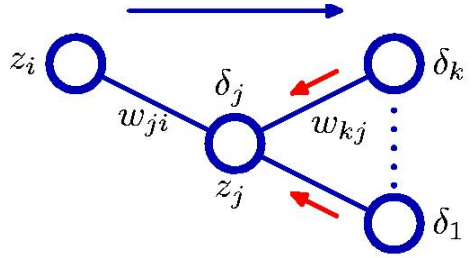
- Backward Propagation (δ s for hidden units)

$$\delta_j = (1 - z_j^2) \sum_{k=1}^{K} w_{kj} \delta_k$$

$$\delta_j = h'(a_j) \sum_k w_{kj} \delta_k$$
$$h'(a) = 1 - h(a)^2$$

- Derivatives wrt first layer and second layer weights

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \delta_j x_i \qquad \frac{\partial E_n}{\partial w_{kj}^{(2)}} = \delta_k z_j$$



- Batch method

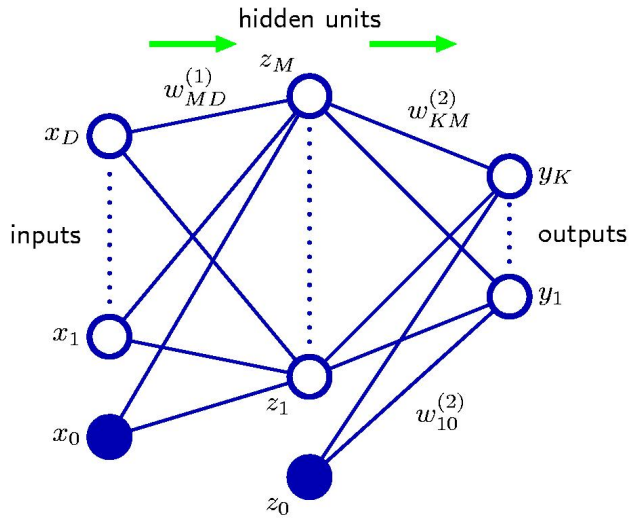
$$\frac{\partial E}{\partial w_{ji}} = \sum_n \frac{\partial E_n}{\partial w_{ji}}$$

Using derivatives to update weights

- Gradient descent
  - Update the weights using $\boldsymbol{w}^{(\tau+1)} = \boldsymbol{w}^{(\tau)} - \eta \nabla E\left(\boldsymbol{w}^{(\tau)}\right)$
  - Where the gradient vector $\nabla E\left(\boldsymbol{w}^{(\tau)}\right)$ consists of the vector of derivatives evaluated using back-propagation

$$\nabla E(\boldsymbol{w}) = \frac{d}{d\boldsymbol{w}} E(\boldsymbol{w}) = \begin{bmatrix} \frac{\partial E}{\partial w_{11}^{(1)}} \\ \cdot \\ \frac{\partial E}{\partial w_{MD}^{(1)}} \\ \frac{\partial E}{\partial w_{11}^{(2)}} \\ \cdot \\ \frac{\partial E}{\partial w_{KM}^{(2)}} \end{bmatrix}$$

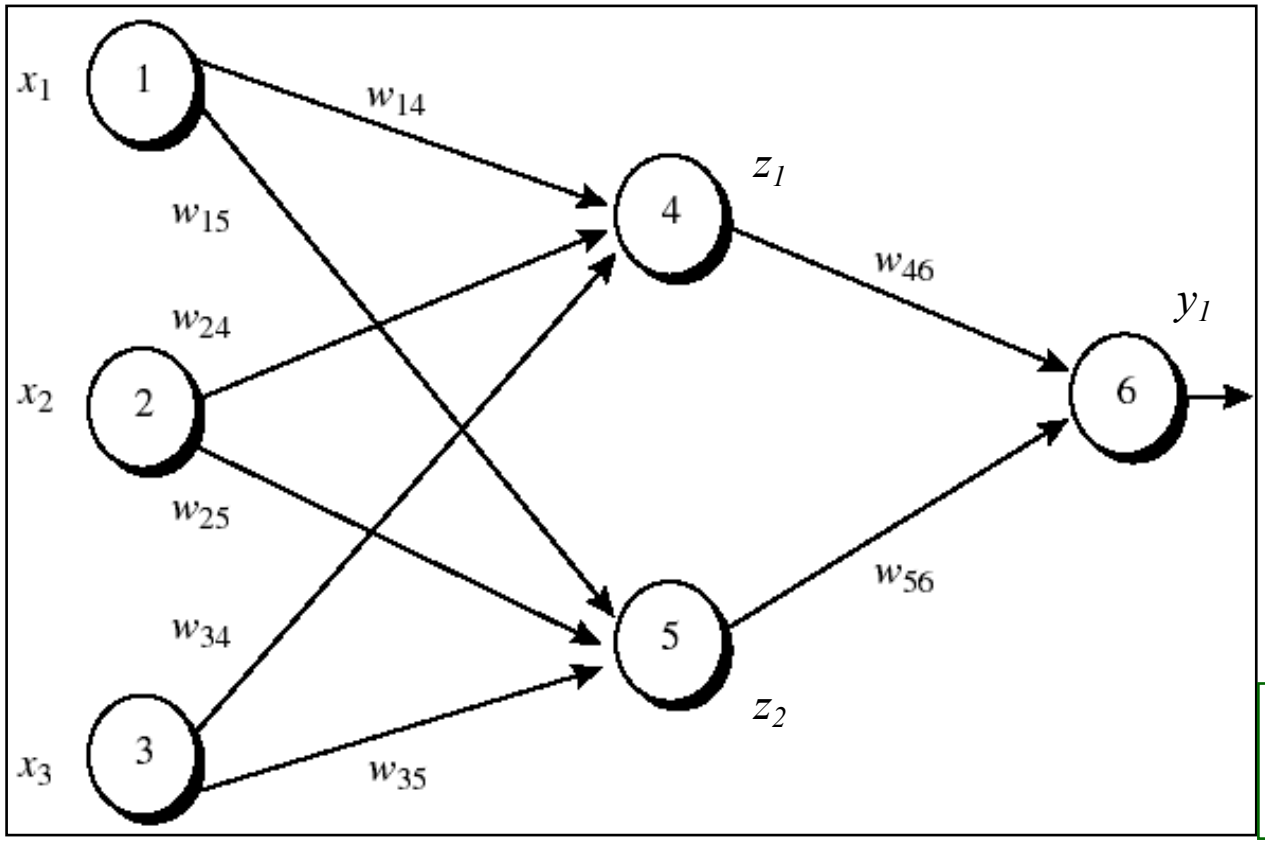
There are $W = M(D+1)+K(M+1)$ elements in the vector
Gradient $\nabla E\left(\boldsymbol{w}^{(\tau)}\right)$ is a W x 1 vector



Numerical example

(binary classification)

D=3
M=2
K=1
N=1



$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i$$

$$z_j = \sigma(a_j)$$

$$y_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j$$

Errors

$$\delta_j = \sigma'(a_j) \sum_k w_{kj} \delta_k$$

$$\delta_k = \sigma'(a_k)\left(y_k - t_k\right)$$

Error Derivatives

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \delta_j x_i \qquad \frac{\partial E_n}{\partial w_{kj}^{(2)}} = \delta_k z_j$$

- First training example, $\boldsymbol{x} = [1 \quad 0 \quad 1]^{\mathrm{T}}$ whose class label is $t = 1$
- The sigmoid activation function is applied to hidden layer and output layer
- Assume that the learning rate η is 0.9

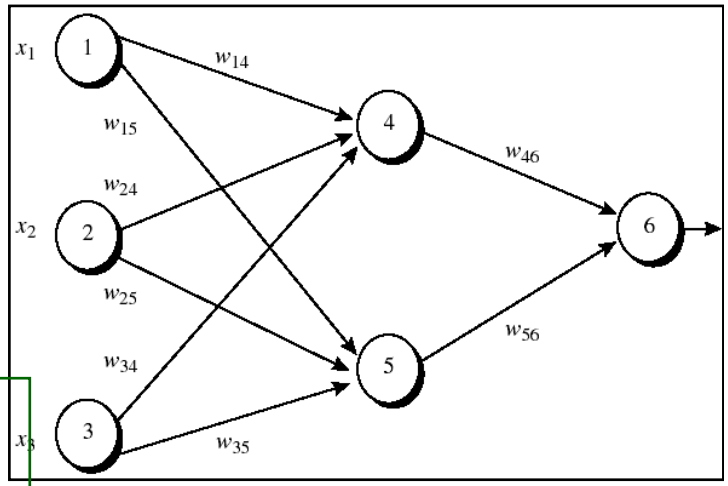
Outputs, Errors, Derivatives, Weight Update

$$\delta_k = \sigma'(a_k)(y_k - t_k) = [\sigma(a_k)(1-\sigma(a_k))](1-\sigma(a_k))$$

$$\delta_j = \sigma'(a_j)\sum_k w_{jk}\delta_k = \left[\sigma(a_j)(1-\sigma(a_j))\right]\sum_k w_{jk}\delta_k$$

Initial input and weight values

x_1	x_2	x_3	w_{14}	w_{15}	w_{24}	w_{25}	w_{34}	w_{35}	w_{46}	w_{56}	w_{04}	w_{05}	w_{06}
1	0	1	0.2	-0.3	0.4	0.1	-0.5	0.2	-0.3	-0.2	-0.4	0.2	0.1



Net input and output calculation

Unit	Net input a	Output $\sigma(a)$
4	0.2 + 0 -0.5 -0.4 = -0.7	$1/(1+e^{0.7})=0.332$
5	-0.3 +0+0.2 +0.2 =0.1	$1/(1+e^{0.1})=0.525$
6	(-0.3)(0.332)-(0.2)(0.525)+0.1 = -0.105	$1/(1+e^{0.105})=0.474$

Errors at each node

Unit	δ
6	(0.474)(1-0.474)(1-0.474)=0.1311
5	(0.525)(1-0.525)(0.1311)(-0.2)=-0.0065
4	(0.332)(1-0.332)(0.1311)(-0.3)=-0.0087

Weight Update*

Weight	New value
w_{46}	-03+(0.9)(0.1311)(0.332)= -0.261
w_{56}	-0.2+(0.9)(0.1311)(0.525)= -0.138
w_{14}	0.2 +(0.9)(-0.0087)(1) = 0.192
w_{15}	-0.3 +(0.9)(-0.0065)(1) = -0.306
w_{24}	0.4+ (0.9)(-0.0087)(0) = 0.4
w_{25}	0.1+ (0.9)(-0.0065)(0) = 0.1
w_{34}	-0.5+ (0.9)(-0.0087)(1) = -0.508
w_{35}	0.2 + (0.9)(-0.0065)(1) = 0.194
w_{06}	0.1 + (0.9)(0.1311) = 0.218
w_{05}	0.2 + (0.9)(-0.0065)=0.194
w_{04}	-0.4 +(0.9)(-0.0087) = -0.408

* Positive update since we used $(t_k - y_k)$

MATLAB Implementation (Pseudocode)

- Allows for multiple hidden layers
- Allows for training in batches
- Determines gradients using back-propagation using sum-of-squared error
- Determines misclassification probability

Initializations

```
% This pseudo-code illustrates implementing a
several layer neural %network. You need to fill in
the missing part to adapt the program to %your
own use. You may have to correct minor
mistakes in the program

%% prepare for the data

load data.mat

train_x = ..
test_x = ..


train_y = ..
test_y = ..

%% Some other preparations
%Number of hidden layers

numOfHiddenLayer = 4;
```

```
s{1} = size(train_x, 1);
s{2} = 100;
s{3} = 100;
s{4} = 100;
s{5} = 2;

%Initialize the parameters
%You may set them to zero or give them small
%random values. Since the neural network
%optimization is non-convex, your algorithm
%may get stuck in a local minimum which may
%be caused by the initial values you assigned.

for i = 1 : numOfHiddenLayers
   W{i} = ..
   b{i} = ..
end
```

x is the input to the neural network,
y is the output

Training epochs, Back-propagation

The training data is divided into several batches of size 100 for efficiency

```
losses = [];
train_errors = [];
test_wrongs = [];

%Here we perform mini-batch stochastic gradient descent
%If batchsize = 1, it would be stochastic gradient descent
%If batchsize = N, it would be basic gradient descent

batchsize = 100;

%Num of batches

numbatches = size(train_x, 2) / batchsize;

%% Training part
%Learning rate alpha
alpha = 0.01;

%Lambda is for regularization
lambda = 0.001;

%Num of iterations
numepochs = 20;
```

```
for j = 1 : numepochs
  %randomly rearrange the training data for each epoch
  %We keep the shuffled index in kk, so that the input and output could
   %be matched together
   kk = randperm(size(train_x, 2));

  for l = 1 : numbatches

    %Set the activation of the first layer to be the training data
    %while the target is training labels

    a{1} = train_x(:,    kk( (l-1)*batchsize+1 : l*batchsize )    );
    y = train_y(:,    kk( (l-1)*batchsize+1 : l*batchsize )    );

    %Forward propagation, layer by layer
   %Here we use sigmoid function as an example

    for i = 2 : numOfHiddenLayer + 1
       a{i} = sigm( bsxfun(@plus, W{i-1}*a{i-1}, b{i-1}) );
    end

    %Calculate the error and back-propagate error layer by layers
   d{numOfHiddenLayer + 1} =
   -(y - a{numOfHiddenLayer + 1}) .* a{numOfHiddenLayer + 1} .* (1-a{numOfHiddenLayer + 1}

    for i = numOfHiddenLayer : -1 : 2
       d{i} = W{i}' * d{i+1} .* a{i} .* (1-a{i});
    end

    %Calculate the gradients we need to update the parameters
    %L2 regularization is used for W

    for i = 1 : numOfHiddenLayer
       dW{i} = d{i+1} * a{i}';
       db{i} = sum(d{i+1}, 2);
       W{i} = W{i} - alpha * (dW{i} + lambda * W{i});
       b{i} = b{i} - alpha * db{i};
    end
  end
```

Performance Evaluation

```
% Do some predictions to know the performance
  a{1} = test_x;
 % forward propagation

  for i = 2 : numOfHiddenLayer + 1
      %This is essentially doing W{i-1}*a{i-1}+b{i-1}, but since they
      %have different dimensionalities, this addition is not allowed in
      %matlab. Another way to do it is to use repmat

     a{i} = sigm( bsxfun(@plus, W{i-1}*a{i-1}, b{i-1}) );
  end

%Here we calculate the sum-of-square error as loss function
  loss = sum(sum((test_y-a{numOfHiddenLayer + 1}).^2)) / size(test_x, 2);

  % Count no. of misclassifications so that we can compare it
  % with other classification methods
  % If we let max return two values, the first one represents the max
  % value and second one represents the corresponding index. Since we
  % care only about the class the model chooses, we drop the max value
  % (using ~ to take the place)  and keep the index.

  [~, ind_] = max(a{numOfHiddenLayer + 1}); [~, ind] = max(test_y);
  test_wrong = sum(  ind_ ~= ind  ) / size(test_x, 2) * 100;
```

```
  %Calculate training error
  %minibatch size
  bs = 2000;
  % no. of mini-batches
  nb = size(train_x, 2) / bs;

  train_error = 0;
  %Here we go through all the mini-batches
  for ll = 1 : nb
     %Use submatrix to pick out mini-batches
     a{1} = train_x(:,    (ll-1)*bs+1 : ll*bs    );
     yy = train_y(:,    (ll-1)*bs+1 : ll*bs    );

     for i = 2 : numOfHiddenLayer + 1
        a{i} = sigm( bsxfun(@plus, W{i-1}*a{i-1}, b{i-1}) );
     end
     train_error = train_error + sum(sum((yy-a{numOfHiddenLayer + 1}).^2));
  end
  train_error = train_error /  size(train_x, 2);

  losses = [losses loss];

  test_wrongs = [test_wrongs, test_wrong];
  train_errors = [train_errors train_error];

end
```

max calculation returns value and index

Efficiency of Backpropagation

- Computational Efficiency is main aspect of back-prop
- No of operations to compute derivatives of error function scales with total number W of weights and biases
- Single evaluation of error function for a single input requires $O(W)$ operations (for large W)
- This is in contrast to $O(W^2)$ for numerical differentiation
  - As seen next

Another Approach: Numerical Differentiation

- Compute derivatives using method of finite differences
  - Perturb each weight in turn and approximate derivatives by

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{E_n(w_{ji}+\varepsilon) - E_n(w_{ji})}{\varepsilon} + O(\varepsilon) \text{ where } \varepsilon << 1$$

  - Accuracy improved by making ε smaller until round-off problems arise
  - Accuracy can be improved by using central differences

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{E_n(w_{ji}+\varepsilon) - E_n(w_{ji}-\varepsilon)}{2\varepsilon} + O(\varepsilon^2)$$

  - This is $O(W^2)$
- Useful to check if software for backprop has been correctly implemented (for some test cases)

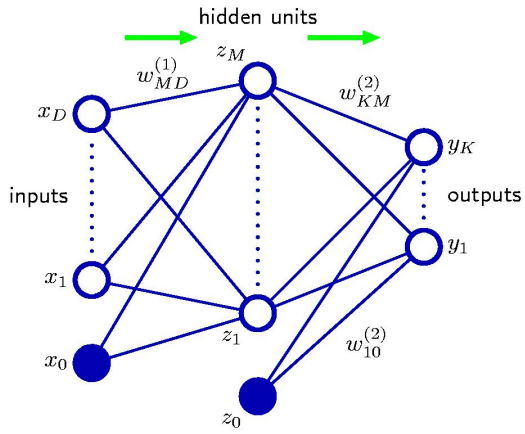
Summary of Backpropagation

- Derivatives of error function wrt weights are obtained by propagating errors backward
- It is more efficient than numerical differentiation
- It can also be used for other computations
  - As seen next for Jacobian

The Jacobian Matrix

- For a vector valued output $\boldsymbol{y}=\{y_1,..,y_m\}$ with vector input $\boldsymbol{x}=\{x_1,..x_n\}$,
- Jacobian matrix organizes all the partial derivatives into an m x n matrix

$$J = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix} \qquad J_{ki} = \frac{\partial y_k}{\partial x_i}$$



For a neural network we have a $D+1$ by K matrix

Determinant of Jacobian Matrix is referred to simply as the Jacobian

Jacobian Matrix Evaluation

- In backprop, derivatives of error function wrt weights are obtained by propagating errors backwards through the network

- The technique of backpropagation can also be used to calculate other derivatives
- Here we consider the Jacobian matrix
  - Whose elements are derivatives of network outputs wrt inputs

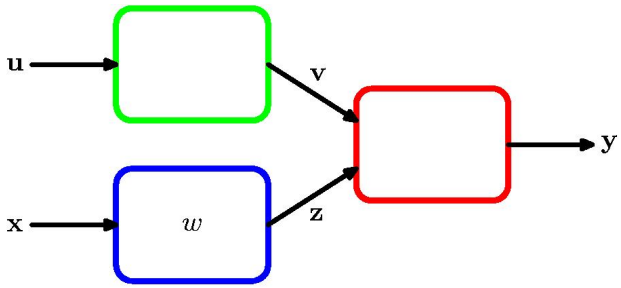
$$J_{ki} = \frac{\partial y_k}{\partial x_i}$$

  - Where each such derivative is evaluated with other inputs fixed

Use of Jacobian Matrix

- Jacobian plays useful role in systems built from several modules
  - Each module has to be differentiable
- Suppose we wish to minimize error E wrt parameter w in a modular classification system shown here:

$$\frac{\partial E}{\partial w} = \sum_{k,j} \frac{\partial E}{\partial y_k} \frac{\partial y_k}{\partial z_j} \frac{\partial z_j}{\partial w}$$



  - Jacobian matrix for red module appears in the middle term
- Jacobian matrix provides measure of local sensitivity of outputs to changes in each of the input variables

Summary of Jacobian Matrix Computation

- Apply input vector corresponding to point in input space where the $\mathrm{Jacobian\ matrix}$ is to be found
- Forward propagate to obtain activations of the hidden and output units in the network
- For each row k of $\mathrm{Jacobian\ matrix}$, corresponding to output unit k:
  - Backpropagate for all the hidden units in the network
  - Finally backpropagate to the inputs
- Implementation of such an algorithm can be checked using numerical differentiation in the form

$$\frac{\partial y_k}{\partial x_i} = \frac{y_k(x_i + \varepsilon) - y_k(x_i - \varepsilon)}{2\varepsilon} + O(\varepsilon^2)$$

Summary

- Neural network learning needs learning of weights from samples involves two steps:
  - Determine derivative of output of a unit wrt each input
  - Adjust weights using derivatives
- Backpropagation is a general term for computing derivatives
  - Evaluate δ_k for all output units
    - (using $\delta_k = y_k - t_k$ for regression)
  - Backpropagate the δ_k's to obtain δ_j for each hidden unit
  - Product of δ's with activations at the unit provide the derivatives for that weight
- Backpropagation is also useful to compute a Jacobian matrix with several inputs and outputs
  - Jacobian matrices are useful to determine the effects of different inputs