

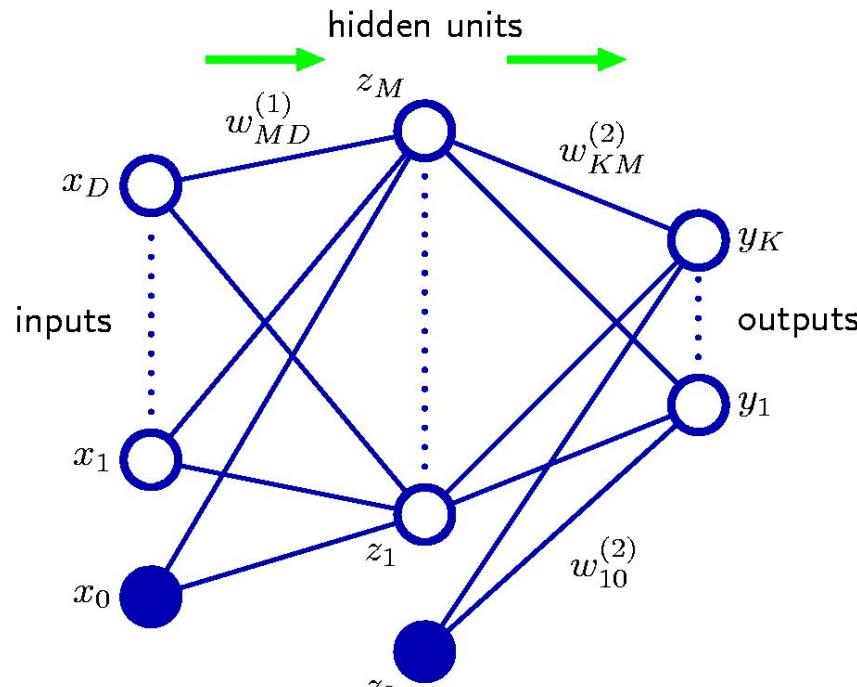
Backpropagation

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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 \mathbf{w} :
 $T = (D+1)M + (M+1)K$
 $= M(D+K+1) + K$

D input variables x_1, \dots, x_D
 M hidden unit activations

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

Hidden unit activation functions

$$z_j = h(a_j)$$

K output activations

$$a_k = \sum_{i=1}^M w_{ki}^{(2)} z_i + w_{k0}^{(2)} \quad \text{where } k = 1, \dots, K$$

Output activation functions

$$y_k = \sigma(a_k)$$

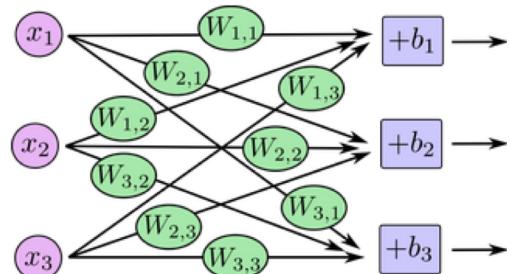
$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left(\sum_{j=1}^M w_{kj}^{(2)} h \left(\sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)} \right) + w_{k0}^{(2)} \right)$$

Matrix Multiplication: Forward Propagation

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

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

First Network layer



Network layer output

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

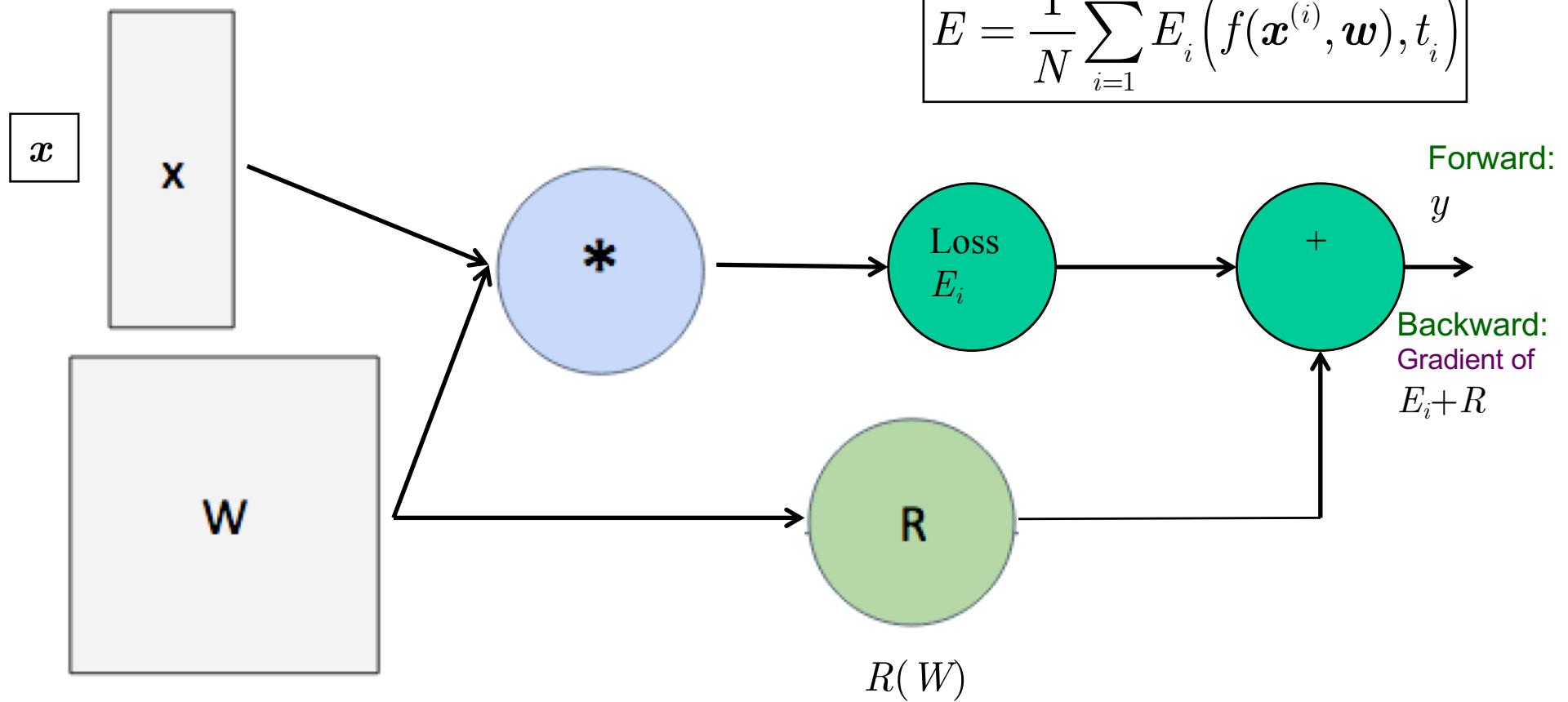
In matrix multiplication notation

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

Loss and Regularization

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

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

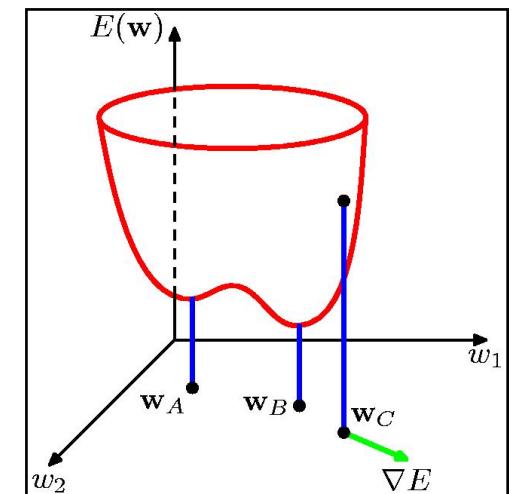


Gradient Descent

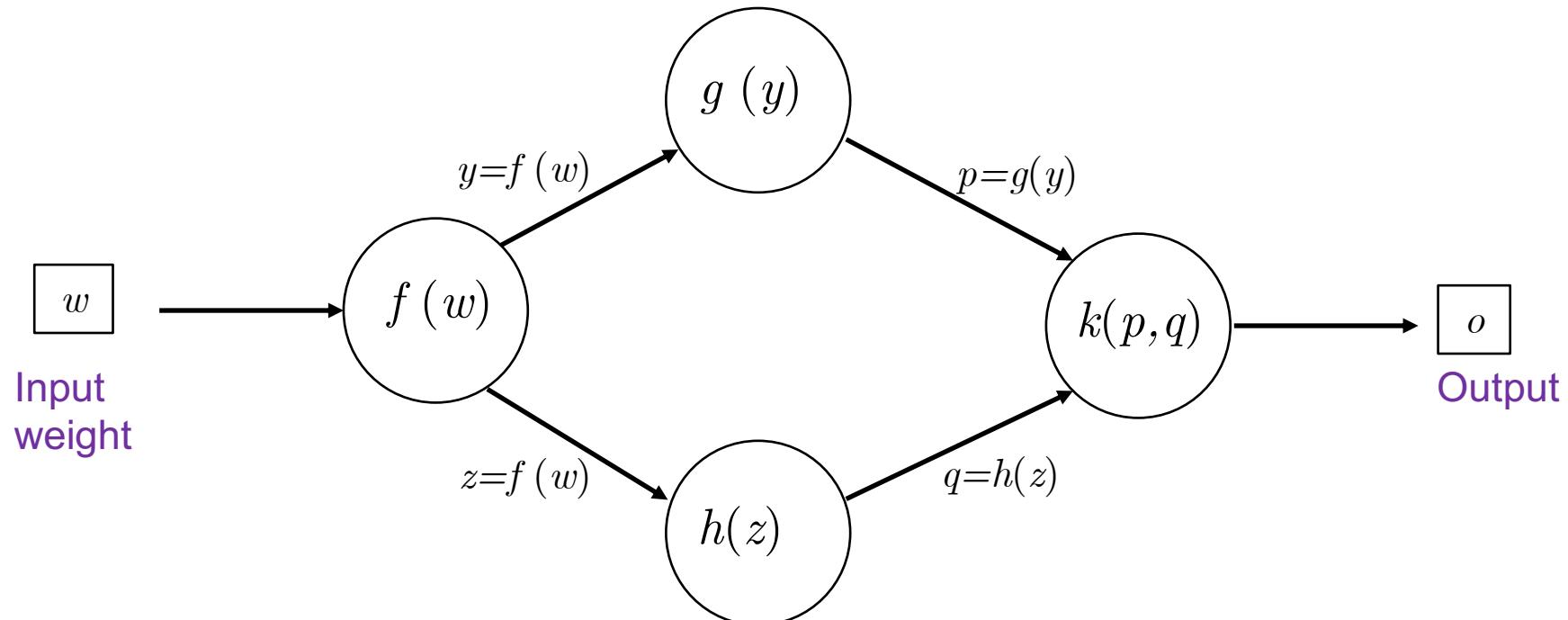
- Goal: determine weights w from labeled set of training samples
- Learning procedure has two stages
 1. Evaluate derivatives of loss $\nabla E(w)$ with respect to weights w_1, \dots, w_T
 2. Use derivative vector to compute adjustments to weights

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

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



Derivative of composite function with one weight



$$\frac{\partial o}{\partial w} = \frac{\partial o}{\partial p} \frac{\partial p}{\partial y} \frac{\partial y}{\partial w} + \frac{\partial o}{\partial q} \frac{\partial q}{\partial z} \frac{\partial z}{\partial w}$$

$$\frac{\partial o}{\partial w} = \frac{\partial k(p, q)}{\partial p} g'(y) f'(w) + \frac{\partial k(p, q)}{\partial q} h'(z) f'(w)$$

Path 1

Path 2

Derivative of a composite function with four inputs

$$E(a, b, c, d) = e = a \cdot b + c \log d$$

Derivatives by inspection:

$$\frac{\partial e}{\partial a} = b$$

$$\frac{\partial e}{\partial b} = a$$

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

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

Computational graph

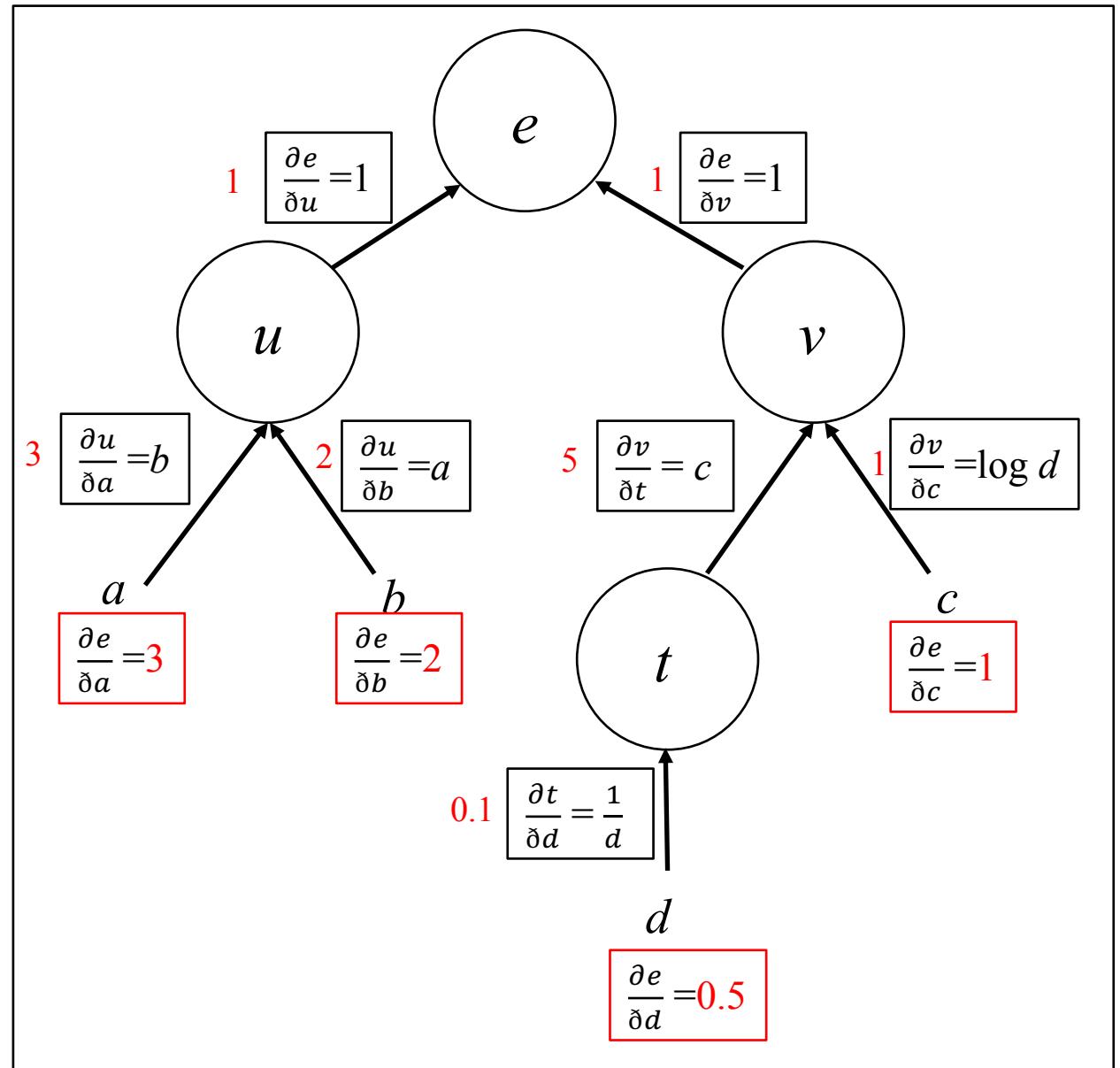
$$e = u + v, \quad u = a \cdot b, \quad v = c \cdot t, \quad t = \log d$$

We want to compute derivatives of output wrt the input values

$$a = 2, b = 3, c = 5, d = 10$$

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

$$\begin{bmatrix} 3 \\ 2 \\ 1 \\ 0.5 \end{bmatrix}$$



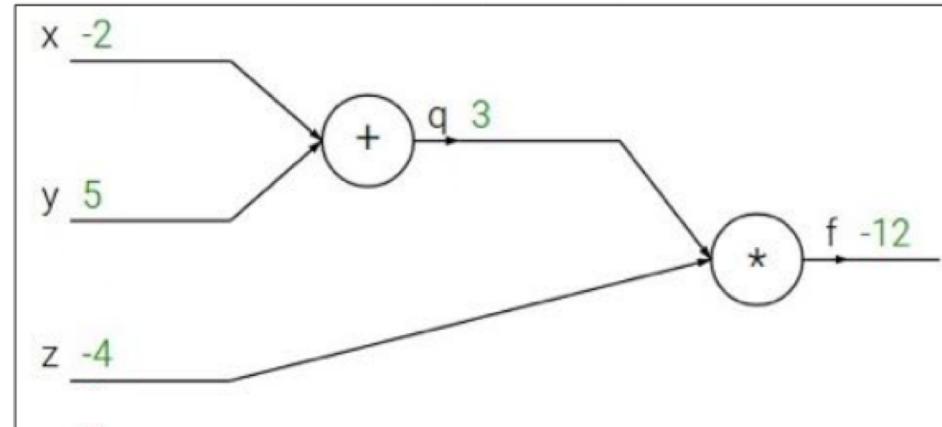
Example of Derivative Computation

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

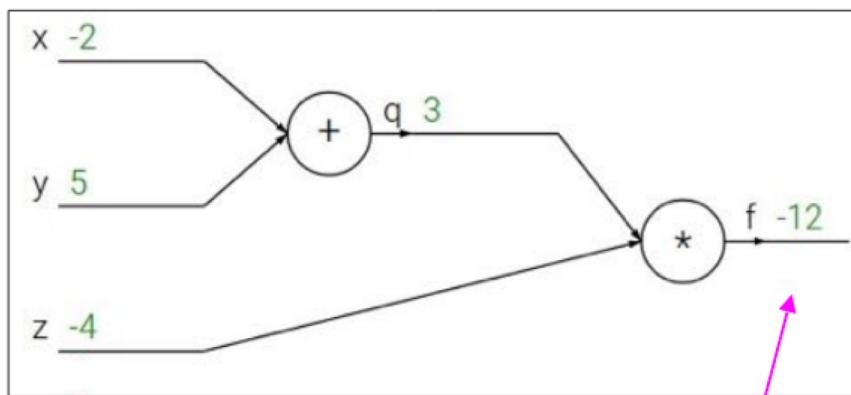
e.g. $x = -2, y = 5, z = -4$

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

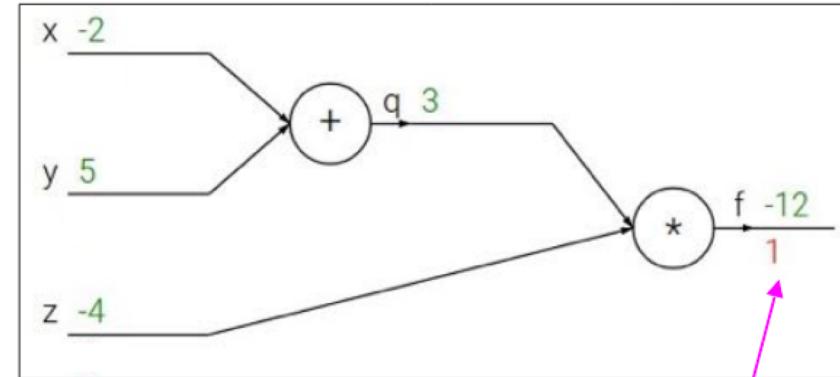
$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$



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

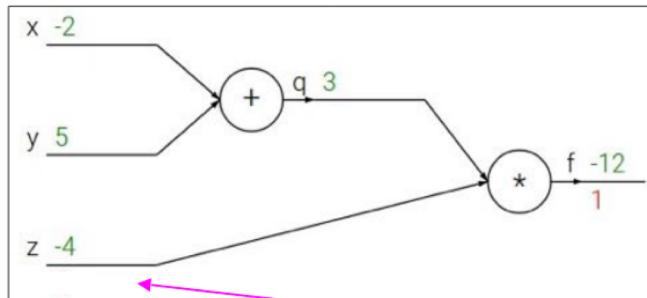


$$\frac{\partial f}{\partial f}$$

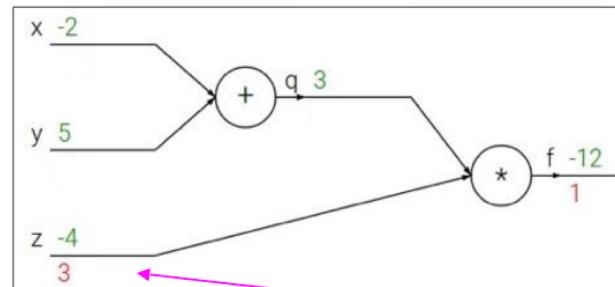


$$\frac{\partial f}{\partial f}$$

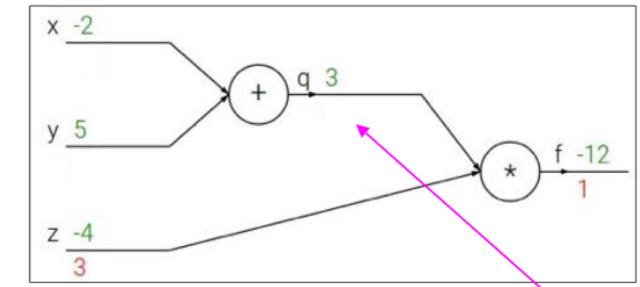
Derivatives of $f = (x+y)z$ wrt x, y, z



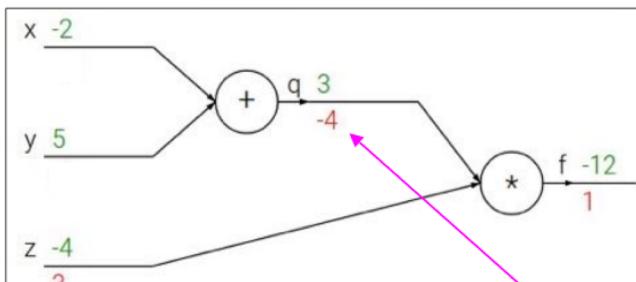
$$q = x + y \quad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1 \quad \frac{\partial f}{\partial q}$$



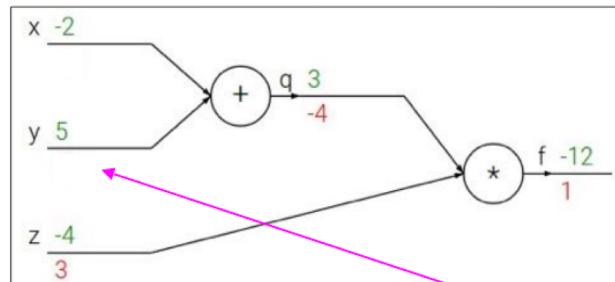
$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q \quad \frac{\partial f}{\partial z}$$



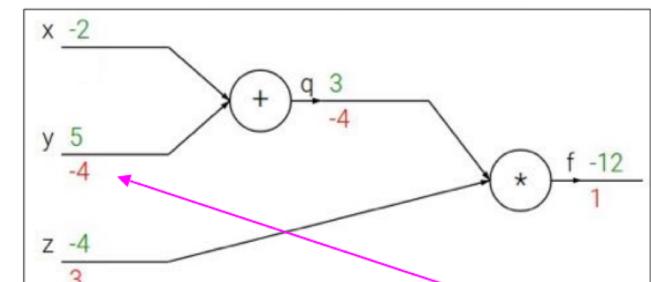
$$\text{Want: } \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \quad \frac{\partial f}{\partial q}$$



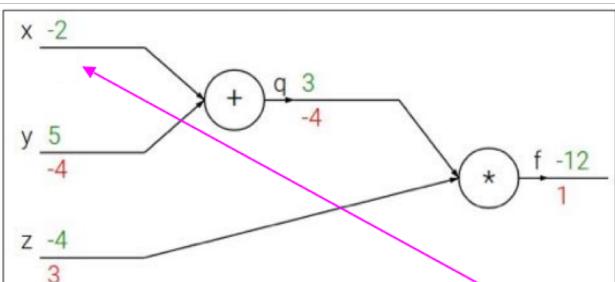
$$\frac{\partial f}{\partial q}$$



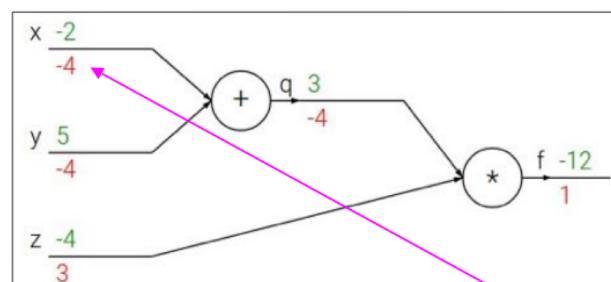
$$\frac{\partial f}{\partial y}$$



$$\frac{\partial f}{\partial y}$$



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

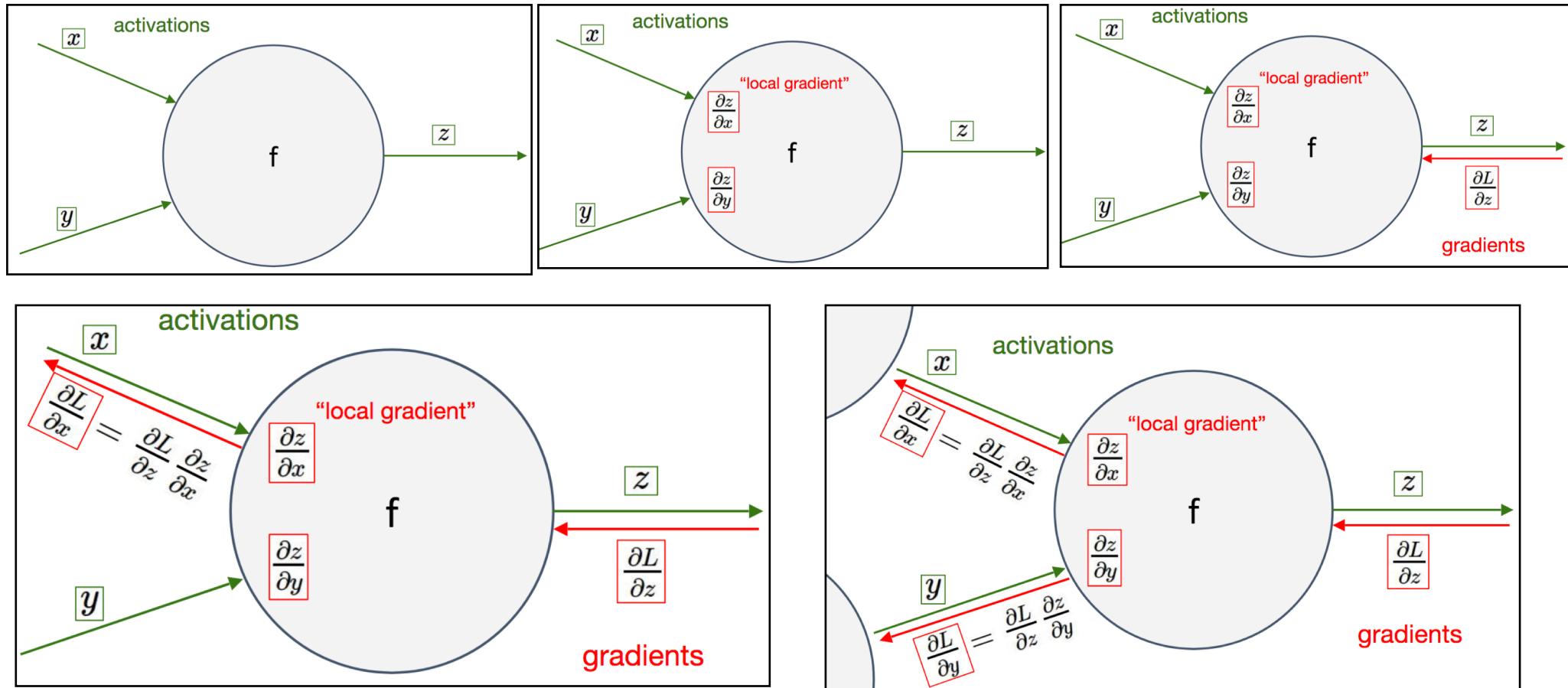


$$\frac{\partial f}{\partial x}$$

Chain rule:

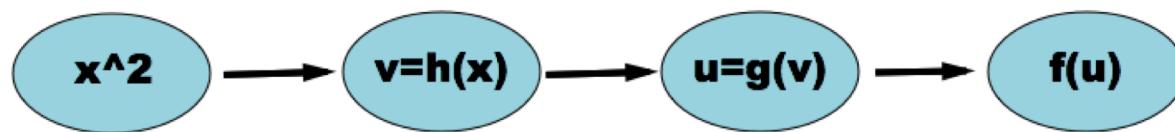
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

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



Composite Function

- Consider a composite function $f(g(h(x)))$
 - 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:
 - $f(x) = e^x$
 - $g(x) = \sin x$ and
 - $h(x) = x^2$ or
 - $f(g(h(x))) = e^{\sin(h(x))}$
- Its computational graph is



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

Derivatives of Composite function

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

- We use the chain rule

$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{dx} \quad \text{where}$$

$$\frac{df}{dg} = e^{g(h(x))}$$

since $f(g(h(x))) = e^{g(h(x))}$ & derivative of e^x is e

$$\frac{dg}{dh} = \cos(h(x))$$

since $g(h(x)) = \sin h(x)$ & derivative sin is cos

$$\frac{dh}{dx} = 2x$$

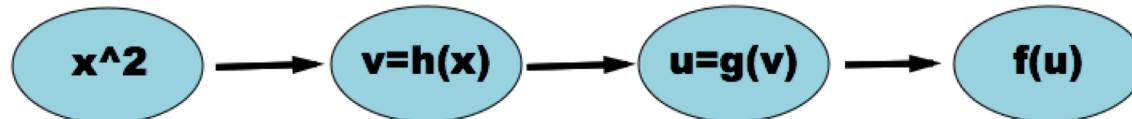
because $h(x) = x^2$ & its derivative is $2x$

$$\frac{df}{dx} = e^{g(h(x))} \cdot \cos h(x) \cdot 2x = e^{\sin x^2} \cdot \cos x^2 \cdot 2x$$

- Therefore
- In each of these cases we pretend that the inner function is a single variable and derive it as such

- Another way to view it $f(x) = e^{\sin(x^2)}$

- Create temp variables $u = \sin v$, $v = x^2$, then $f(u) = e^u$ with computational graph:



Derivative using Computational Graph

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



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

$$\frac{dh}{dx} = 2x$$

$$\frac{dg}{dh} = \cos(h(x))$$

$$\frac{df}{dg} = e^{g(h(x))}$$

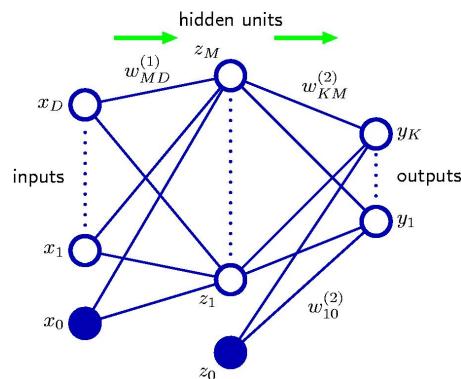
$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{dx}$$

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

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 $E(\mathbf{w})$ 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 means a variety of different things
 - Computing derivative of the error function wrt 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

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

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

Simple Model (Multiple Linear Regression)

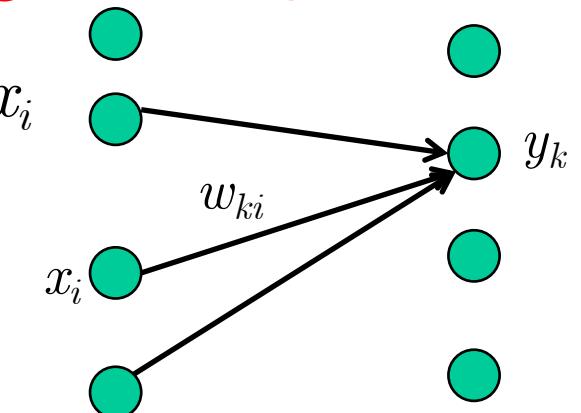
- Outputs y_k are linear combinations of inputs x_i

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

- Error function for a particular input x_n is

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

Where summation is over all K outputs



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

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

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

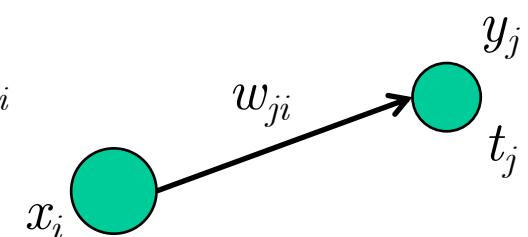
- where $y_{nk} = y_k(x_n, w)$

- Gradient of Error function wrt a weight w_{ji} :

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

- a local computation involving product of

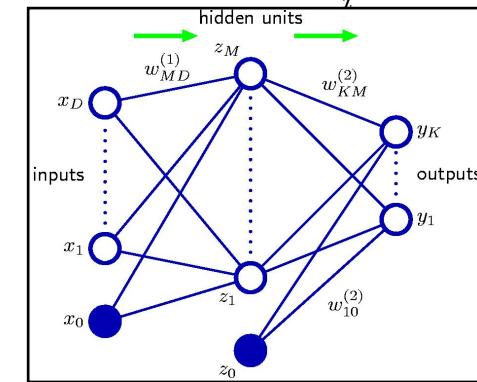
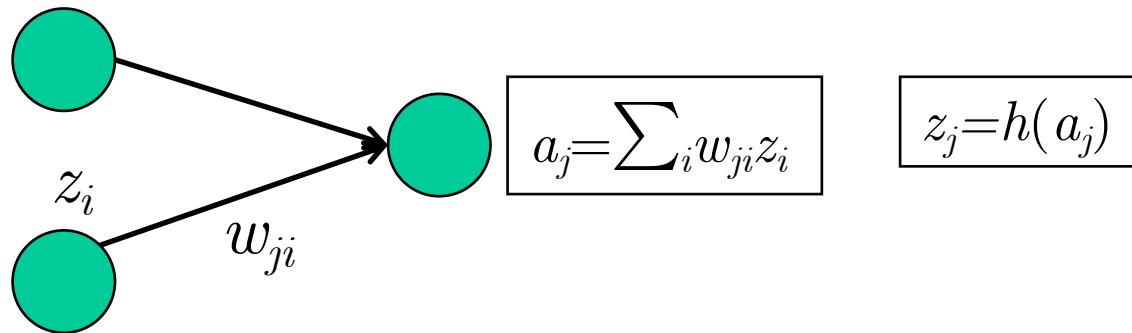
- error signal $y_{nj} - t_{nj}$ associated with output end of link w_{ji}
- variable x_{ni} associated with input end of link



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

Extension to more complex multilayer Network

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



- 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 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

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

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

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

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

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

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

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

- Substituting we get

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

- Thus required derivative is obtained by multiplying

- Value of δ for the unit at output end of weight
- 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 $\delta_j = y_j - t_j$

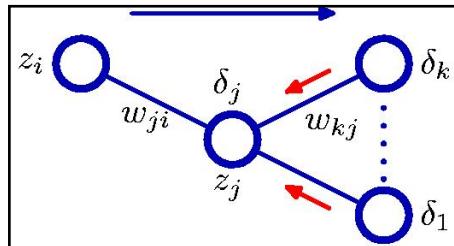
If $E = \frac{1}{2} \sum_j (y_j - t_j)^2$ and $y_j = a_j = \sum_i w_{ji} z_i$ then $\delta_j = \frac{\partial E}{\partial a_j} = y_j - t_j$

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

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

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

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

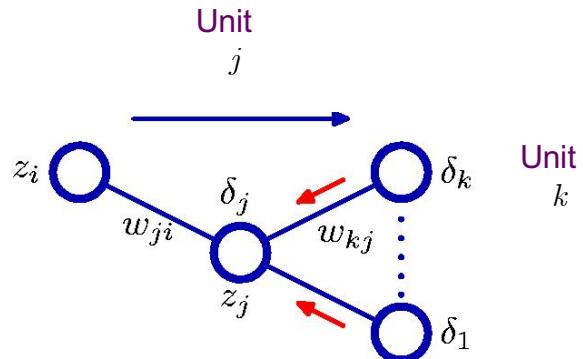
- We get the backpropagation formula for error derivatives at stage j

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

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 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

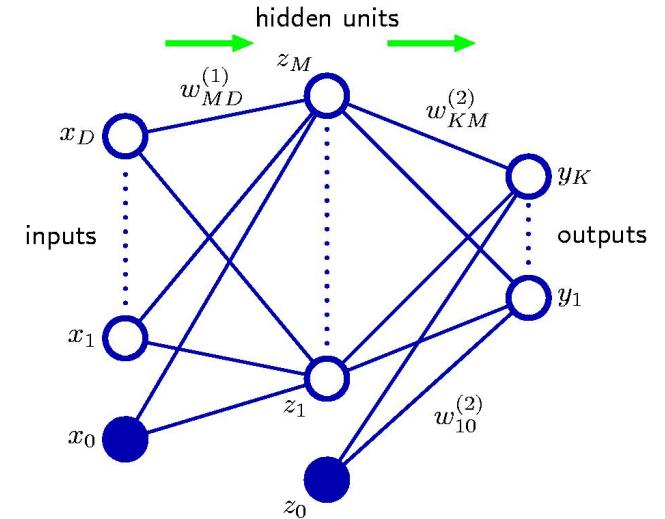
$$h(a) = \tanh(a)$$

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

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

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

$$\left\{ \begin{array}{l} a_j = \sum_{i=0}^D w_{ji}^{(1)} x_i \\ z_j = \tanh(a_j) \\ y_k = \sum_{j=0}^M w_{kj}^{(2)} z_j \end{array} \right.$$

- Output differences

$$\delta_k = y_k - t_k$$

- Backward Propagation (δ s for hidden units)

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

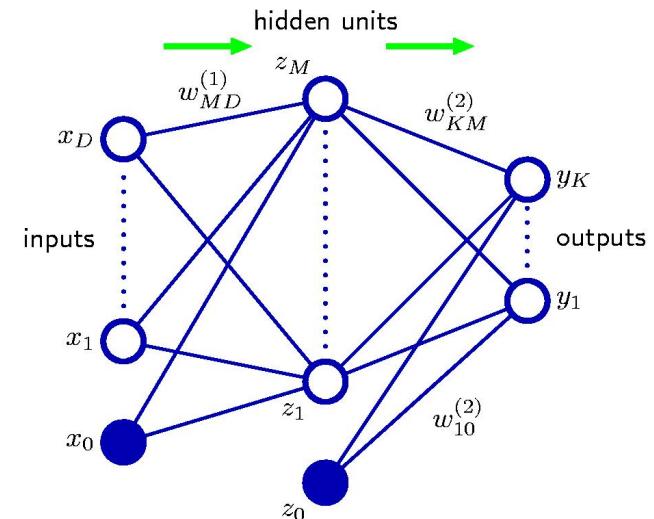
- Derivatives wrt first layer and second layer weights

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \delta_j x_i$$

$$\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \delta_k z_j$$

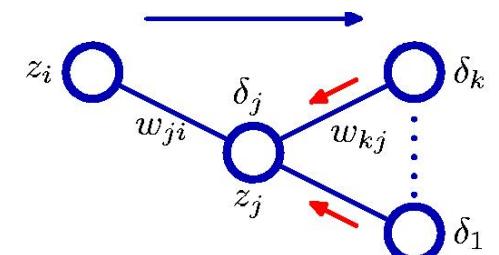
- Batch method

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



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

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



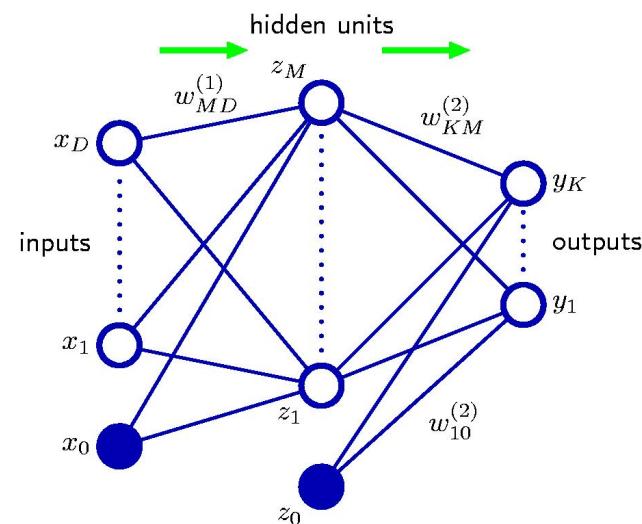
Using derivatives to update weights

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

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

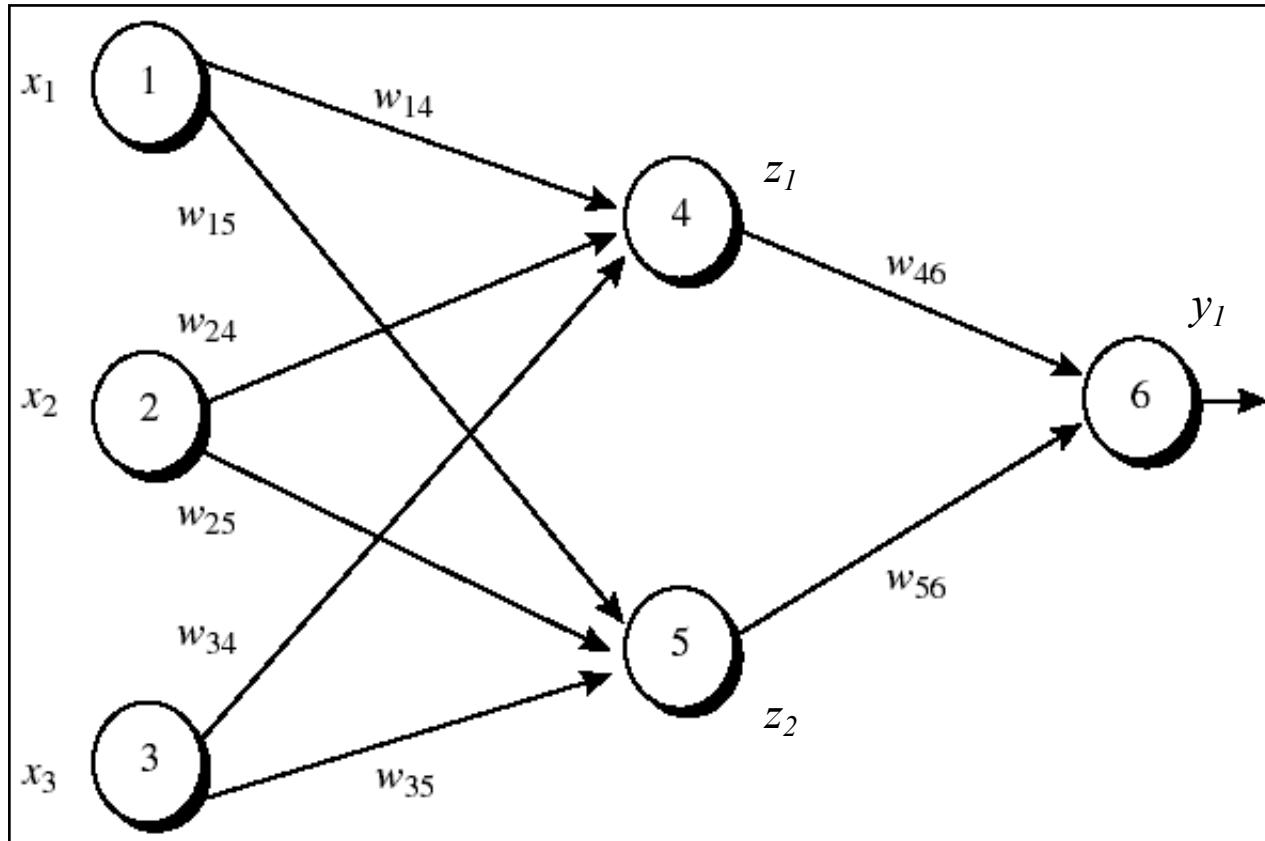
There are $W = M(D+1) + K(M+1)$ elements in the vector

Gradient $\nabla E (\mathbf{w}^{(\tau)})$ is a $W \times 1$ 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

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

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

Error Derivatives

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

- First training example, $x = [1 \ 0 \ 1]^T$ 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

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

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

Initial input and weight values

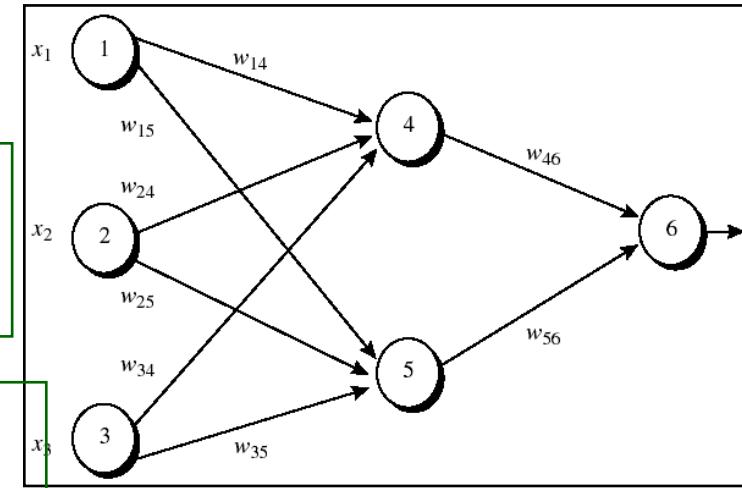
| x_1 | x_2 | x_3 | w_{14} | w_{15} | w_{24} | w_{25} | w_{34} | w_{35} | w_{46} | w_{56} | w_{04} | w_{05} | w_{06} |
|-------|-------|-------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1 | 0 | 1 | 0.2 | -0.3 | 0.4 | 0.1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

| Weight | New value |
|----------|--|
| w_{46} | $-0.3 + (0.9)(0.1311)(0.332) = -0.261$ |
| 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_wrong = [];

%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
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

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

- 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)

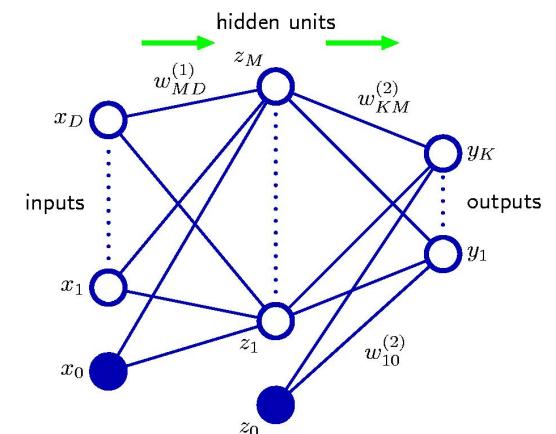
Summary of Backpropagation

- 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 $\mathbf{y} = \{y_1, \dots, y_m\}$ with vector input $\mathbf{x} = \{x_1, \dots, x_n\}$,
- Jacobian matrix organizes all the partial derivatives into an $m \times n$ matrix

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



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

Determinant of Jacobian Matrix is referred to simply as the Jacobian

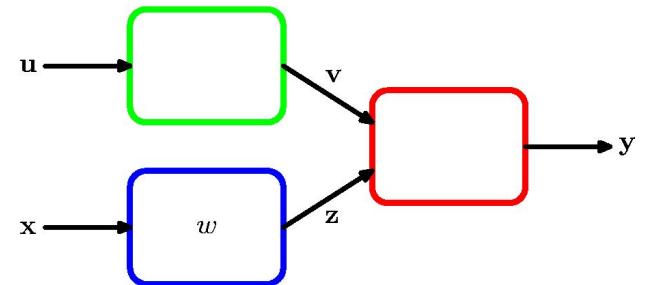
Jacobian Matrix Evaluation

- 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 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 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