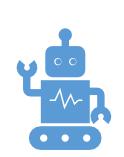
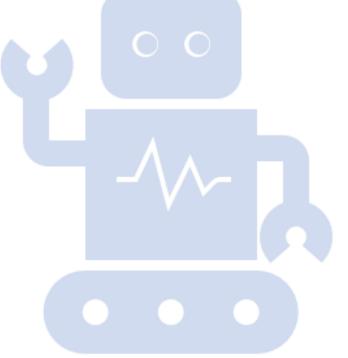


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IN3050/IN4050 -Introduction to Artificial Intelligence and Machine Learning Lecture 8



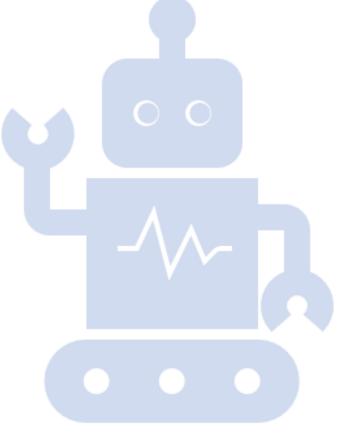
Multi-layer neural networks and backpropagation Jan Tore Lønning





# 8.1 Feed-forward Neural networks

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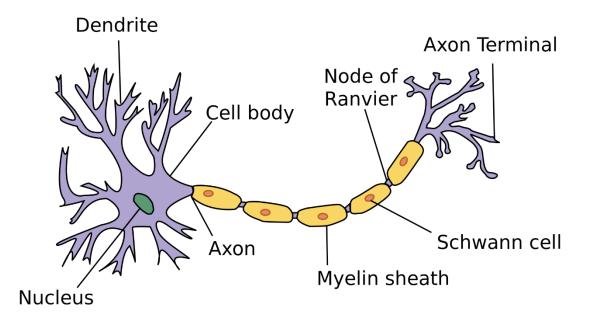


# Today

- 1. Feed-forward neural networks (Multi-layer Perceptron)
- 2. Matrix representations of neural networks
- 3. The Backpropagation Algorithm
- 4. Finer details
- 5. More on Evaluation

# The neural inspiration

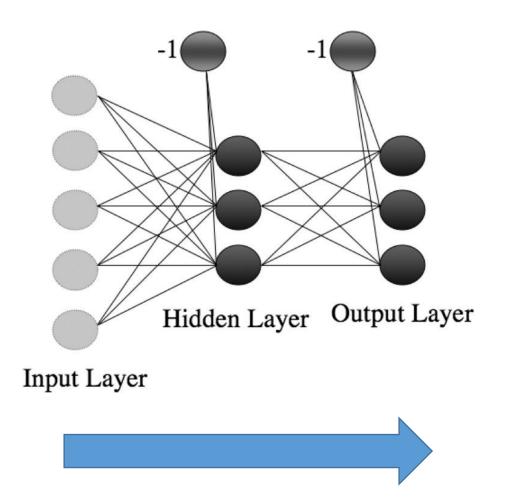
- So far inspired by one neuron
- That does not make intelligence
- The human brain, roughly
  - 10<sup>11</sup> Neurons
  - 10<sup>14</sup> Synapses
  - The strength is the interactions
- Neural Networks



https://simple.wikipedia.org/wiki/Neuron#/media/File:Neuron.svg

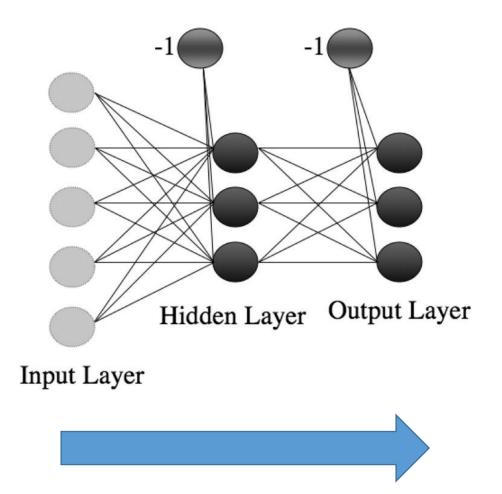
# Artificial Neural Networks

- Inspired by the brain
- Does not pretend to be a model of the brain
- The simplest model is the
  - Feed forward network, also called
  - Multi-layer Perceptron



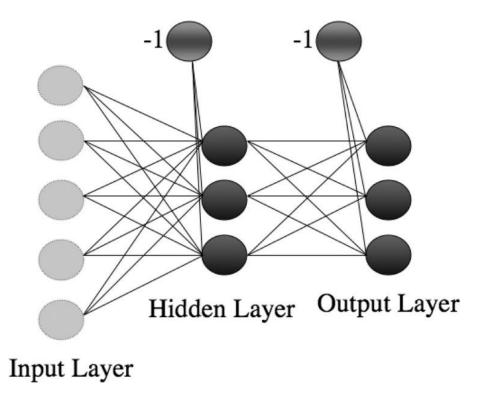
# Feed forward network

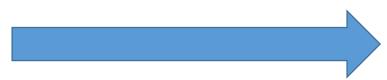
- An input layer
- An output layer: the predictions
- One or more hidden layers
- Connections from nodes in one layer to nodes in the next layer (from left to right)
- The connections are marked with weights



# Going forwards (predictions)

- There is one input node for each feature/dimension in an input vector:
   (x<sub>1</sub>, x<sub>2</sub>, ..., x<sub>m</sub>)
- In addition, an input bias node  $x_0 = -1$
- The input values are multiplied with the weights and summed into each hidden node.
- There is some processing in the hidden node.
- The output values of the hidden nodes are fed to the next layer.
- (etc.)



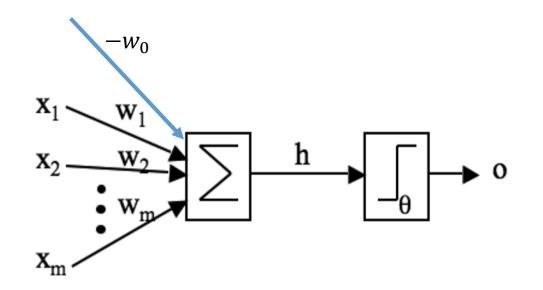


# One hidden unit

1. First sum of weighted inputs :

•  $z = \sum_{i=0}^{m} w_i x_i = \boldsymbol{w} \cdot \boldsymbol{x}$ 

- 2. Then the result is run through an activation function, g to produce  $g(z) = g(w \cdot x)$
- The activation function could be the step function,
  - c.f. the XOR-example:
    - Marsland sec 3.4..2 & start ch. 4



It is the non-linearity of the activation function which makes it possible for MLP to predict nonlinear decision boundaries

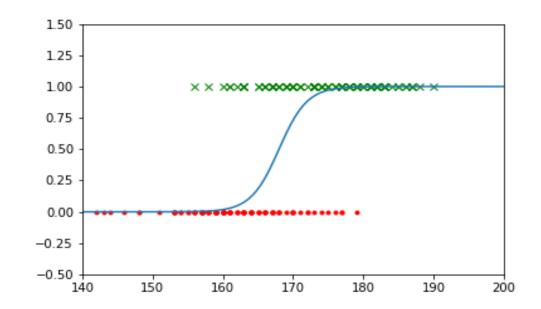
# A differentiable activation function

• It is unclear how to update the weights if g isn't differentiable

• One option is to use the logistic (sigmoid) function

• 
$$y = \sigma(z) = \frac{1}{1 + e^{-\overrightarrow{w} \cdot \overrightarrow{x}}}$$

- Differentiable
- y' = y(1-y)
- (There are alternative activation functions.)



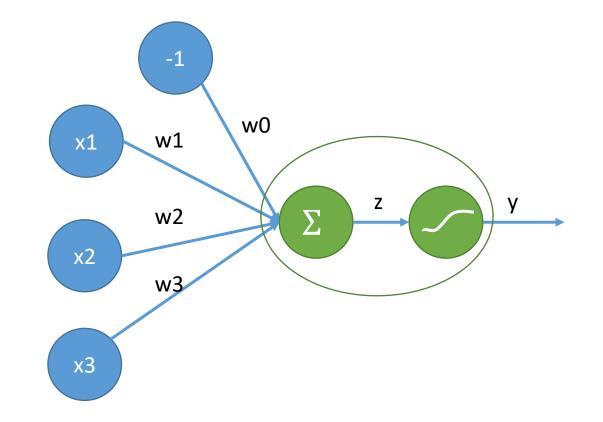
#### One hidden node

1. First sum of weighted inputs:

• 
$$z = \sum_{i=0}^{m} w_i x_i = \boldsymbol{w} \cdot \boldsymbol{x}$$

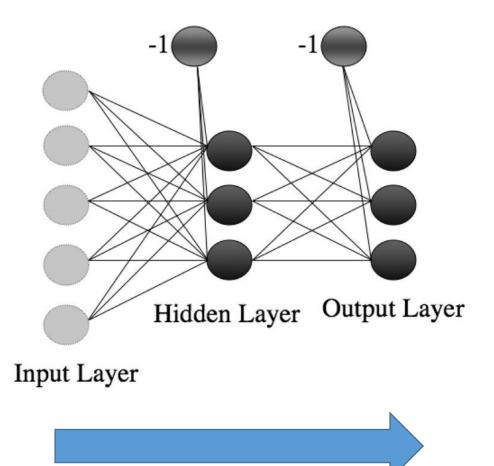
2. Then

• 
$$y = g(z) = \sigma(z) = \frac{1}{1 + e^{-\overrightarrow{w} \cdot \overrightarrow{x}}}$$



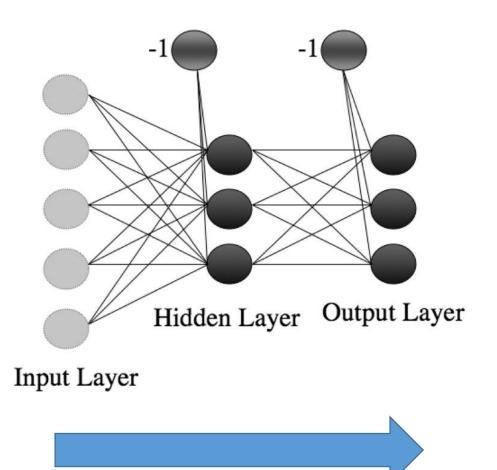
# Going forwards (predictions)

- After the processing in the hidden layer, the output is taken as input to the next layer
- One must also add a bias term at this layer.
  - Observe that this has to be done:
    - During processing
    - E.g., over again each time we process the same training item



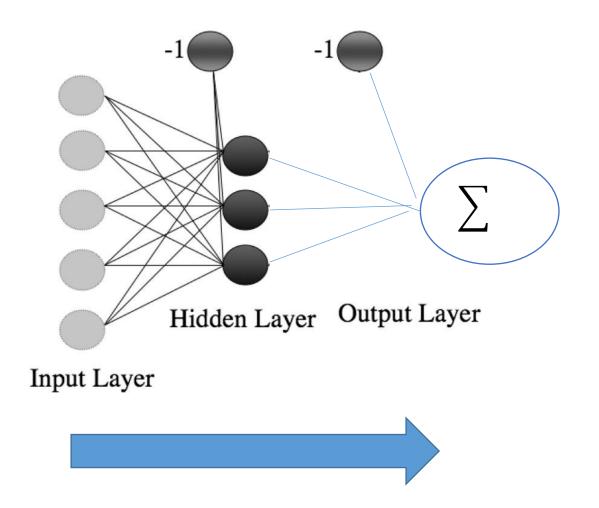
# Output layer

- Several possibilities, depending on the task, including:
  - Regression
  - Binary classification
  - Multi-label classification
  - Multi-class classification
- From the last layer to the output layer is like the same tasks without multiple layers!
- c.f. Marsland, sec. 4.2.3



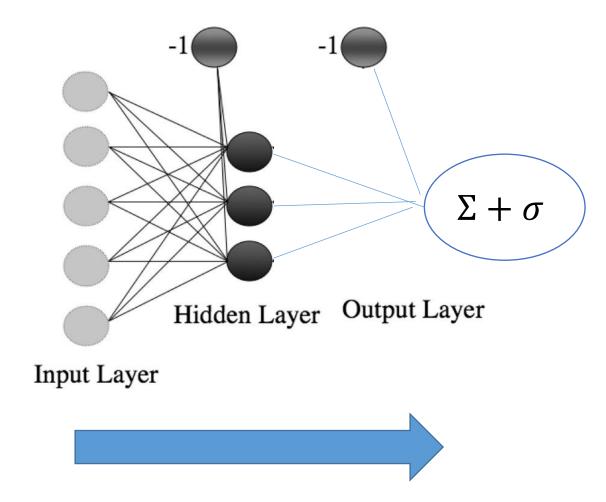
# 1. Regression

- One output node
- No activation function
  - activation function is the identity function
- Observe that this can predict non-linear functions!



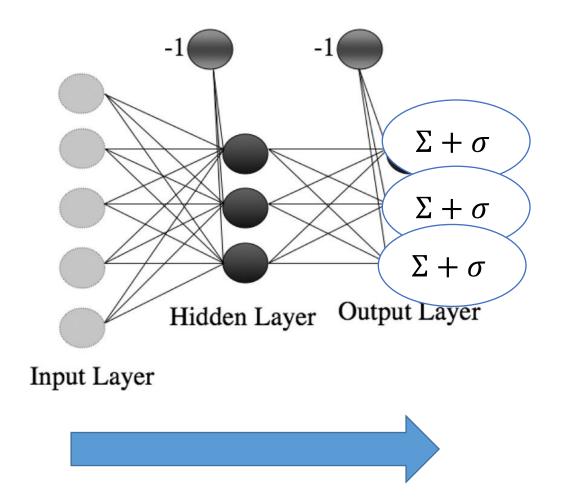
# 2. Binary classification

- One output node
- Logistic activation function
- Similar to logistic regression
- Can produce non-linear decision boundaries



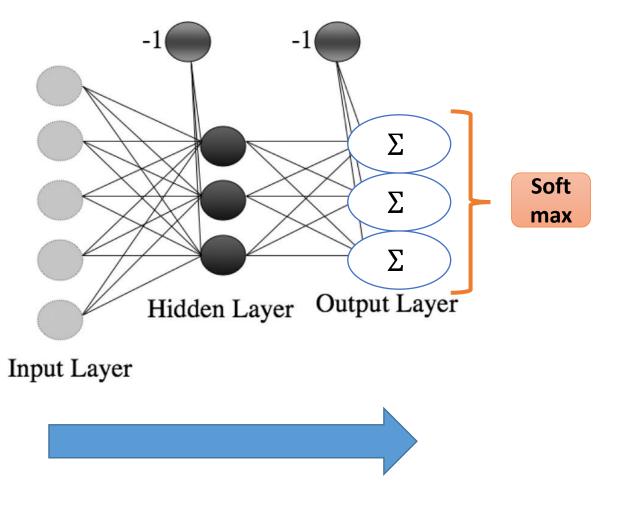
# 3. Multi-label classification

- Several output nodes
- Logistic activation function
- Can be made multi-class classification by one vs. rest.
- The model Marsland considers



# 4. Multi-class classification

- Several output nodes
- Sum the weighted inputs at each nodes
- The sums are brought together in the soft-max





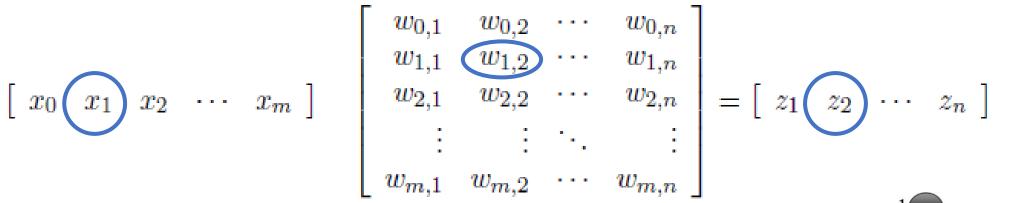


# 8.2 Matrix representations

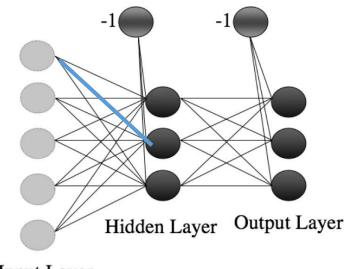
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and Machine Learning

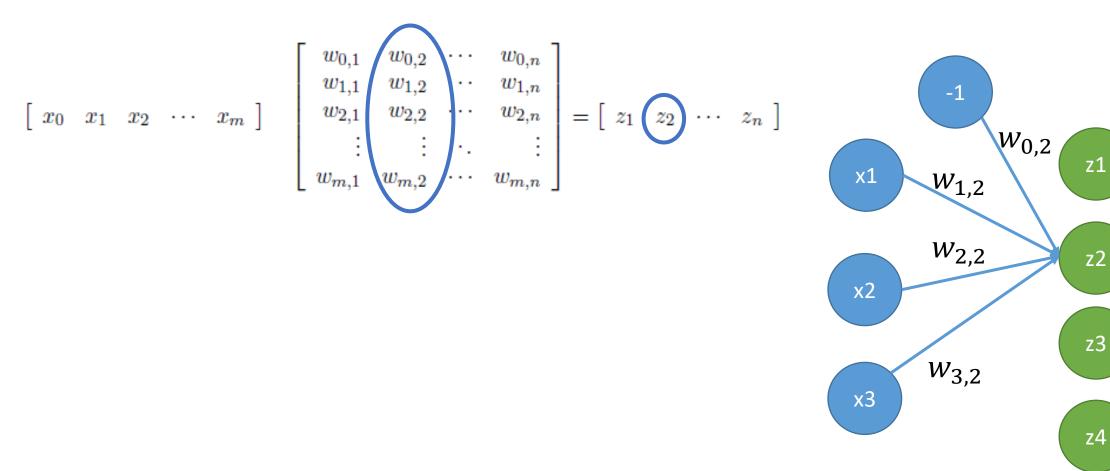
# Representing the connections



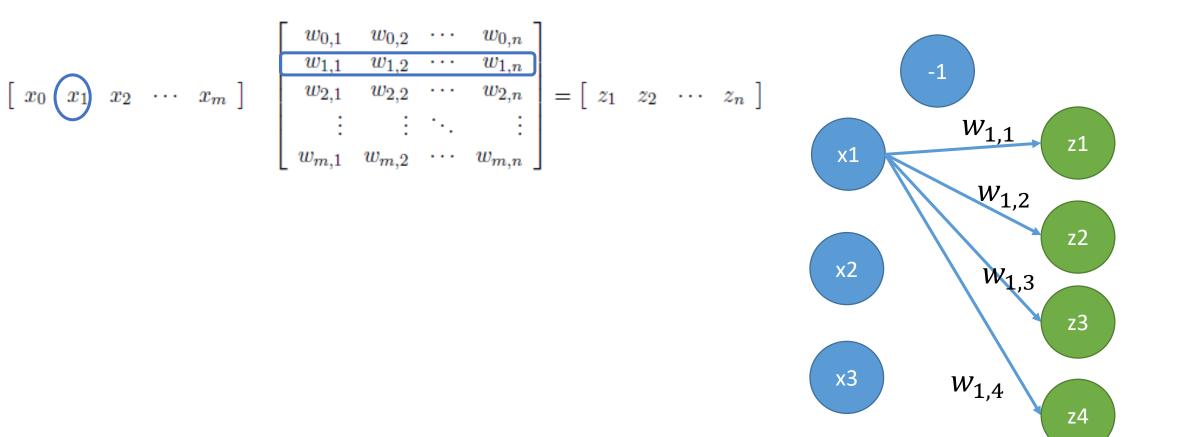
- We use a matrix to represent the connections
- Element  $w_{i,j}$  is the connection:
  - from node *i*
  - to node *j*
- (Beware, some texts do it differently)



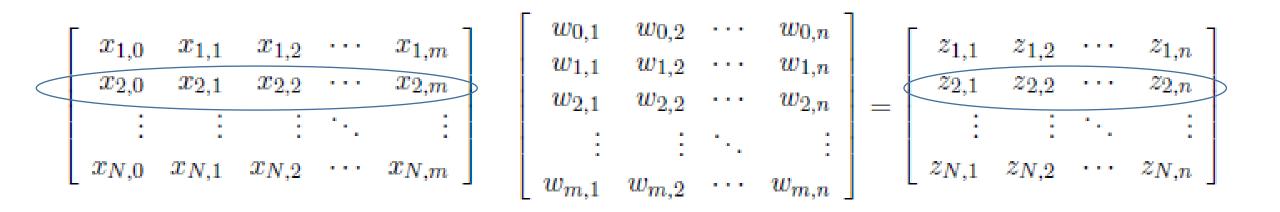
#### Connections going into a node



#### Connections going out of a node

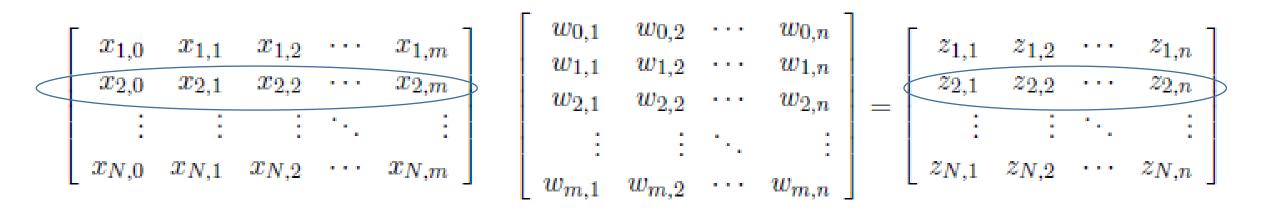


# Batch-processing



- In batch-processing we can multiply by weights and (i) sum the results for (iii) each input item, and (ii) each hidden node in one operation
- Three nested loops by just: XW

#### Activation function



- Each  $z_{i,j}$  is passed through the activation function:  $y_{i,j} = g(z_{i,j})$
- In NumPy this can be done by one operation: g(XW)
- Reminder: g may be the logistic function, but doesn't have to

• i.e., 
$$g(z_{i,j}) = \sigma(z_{i,j}) = \frac{1}{1 + e^{-z_{i,j}}}$$

### Footnote: Notation

- Half of all texts follow us and Marsland with respect to notation
- The other half does differently

|                                  | We               | Them             |
|----------------------------------|------------------|------------------|
| Connection from node i to node j | W <sub>i,j</sub> | W <sub>j,i</sub> |
| Data and weights                 | XW               | WX               |
| Applying activation function     | g(XW)            | g(WX)            |

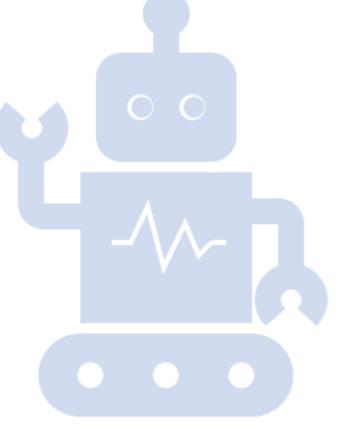
- It amounts to the same.
- But don't mix them up!





# 8.3 Learning by Back-propagation

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### Background

Marsland (p.74), "...just three things that you need to know...":

1. If 
$$f(x) = \frac{1}{2}x^2$$
 then  $f'(x) = x$   
2. If  $f(x) = c$  then  $f'(x) = 0$   
3. If  $f(x) = h(g(x))$  then  $f'(x) = h'(g(x))g'(x)$  (the chain rule)  
He forgot

4. If 
$$y = \sigma(z) = \frac{1}{1 + e^{-\vec{w} \cdot \vec{x}}}$$
, then  $y' = y(1 - y)$ 

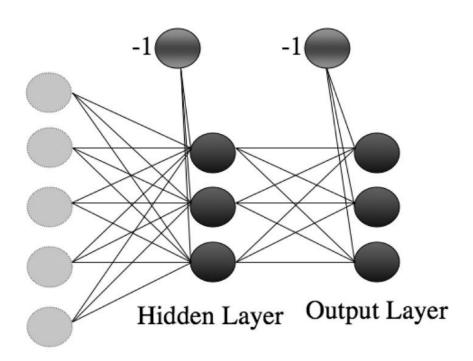
# In addition

We will make use of the following which we have already seen:

- The logistic regression model
- Gradient descent
- GD applied to
  - Linear regression
  - Logistic regression
- Loss-functions:
  - MSE, Cross-Entropy

# Training

- Given a set of training instances
  - { $(x_1, t_1), (x_2, t_2), ..., (x_N, t_N)$ }:
- Forwards:
  - Run them forwards and get predictions
    - $\{y_1, y_N, ..., y_N\}$
- Backwards
  - Use a suitable loss function and compare these to the target values
    - $\{t_1, t_2, ..., t_N\}$
  - Apply gradient descent to update the weights (partial derivatives)



Input Layer

# How do we update the weights

#### Last layer

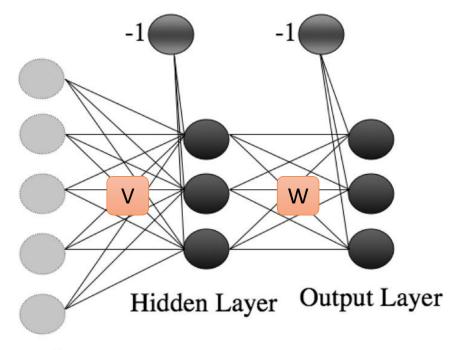
- (easy)
- Like the same problems for linear regression or logistic regression without a hidden layer

#### The first layer

- The big question:
- How do we update the first layer?
- We don't have a loss (error) here

# Solution: Backpropagation

- Let's be a little more formal
- Let the matrix V be the connections from *input* to *hidden* and W from *hidden* to *output*
  - dim(V) =  $((m+1) \times k)$
  - dim(W) =  $((k + 1) \times n)$
- Activation functions:
  - Hidden layers: *g*
  - Hidden output layer: f



Input Layer

• Let us in the following consider SGD where we update for one input  $\mathbf{x} = (x_1, x_2, \dots x_m)$ 

# Forwards (notation)

- Add bias and send
  - $x^+ = (x_0, x_1, ..., x_m)$
- through the first layer to get
  - $h = x^+ V = (h_1, h_2, ..., h_k)$ , where
  - $h_j = \sum_{i=0}^m x_i v_{i,j}$
  - k is the number of hidden nodes
- Apply activation function to get
  - $a = g(h) = (a_1, a_2, ..., a_k),$
  - where  $a_j = g(h_j)$

Add bias and send

• 
$$a^+ = (a_0, a_1, a_2, \dots, a_k)$$

- through the second layer to get
  - $z = a^+ W = (z_1, z_2, ..., z_n)$ , where

• 
$$z_j = \sum_{i=0}^k a_i w_{i,j}$$

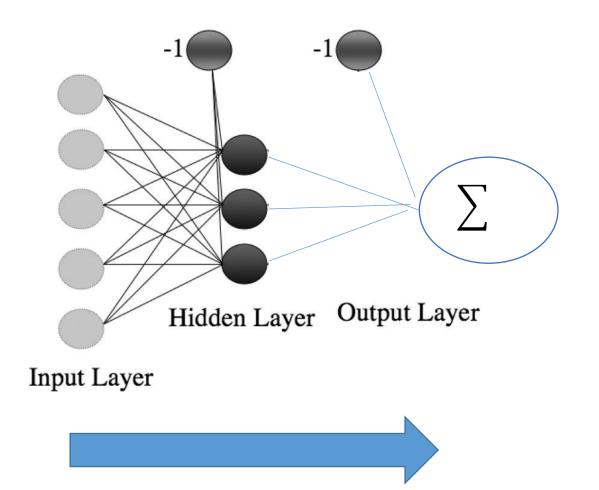
- *n* is the number of output nodes
- Apply activation function to get

• 
$$y = f(z) = (y_1, y_2, ..., y_n),$$

• where  $y_j = f(z_j)$ 

# Backwards: 1.Regression

- We will consider various output tasks, starting with the simple regression
- There is only one output node
- The output activation function, *f*, is identity



#### Backwards: Update last layer

- For loss, we use MSE, or , as Marsland, the simpler Sum of Squares Error (SE):  $L_{SE}(\mathbf{t}, \mathbf{y}) = \frac{1}{2} \sum_{j=1}^{N} (t_j - y_j)^2$ 
  - (The index *j* here, runs over the input items. There is only one output node)
- We have seen that

• 
$$\frac{\partial}{\partial w_{i,1}} L_{SE}(\mathbf{t}, \mathbf{y}) = \frac{\partial}{\partial \mathbf{y}} L_{SE}(\mathbf{t}, \mathbf{y}) \left(\frac{\partial}{\partial w_{i,1}} \mathbf{y}\right) = \sum_{j=1}^{N} \left( (t_j - y_j)(-a_{j,i}) \right)$$

• For SGD where we update for one input  $x = (x_1, x_2, ..., x_m)$ 

• 
$$\frac{\partial}{\partial w_{i,1}} L_{SE}(t,y) = \frac{\partial}{\partial y} L_{SE}(t,y) \left(\frac{\partial}{\partial w_{i,1}}y\right) = (t-y)(-a_i) = (y-t)(a_i)$$

# Backwards: Update last layer, ctd.

• 
$$\frac{\partial}{\partial w_{i,1}} L_{SE}(t, y) = (y - t)(a_i)$$

- We know from lect. 6 how to update this (*a* corresponds to *x* then)
- But wait!
- We first have to find how to update the first layer.



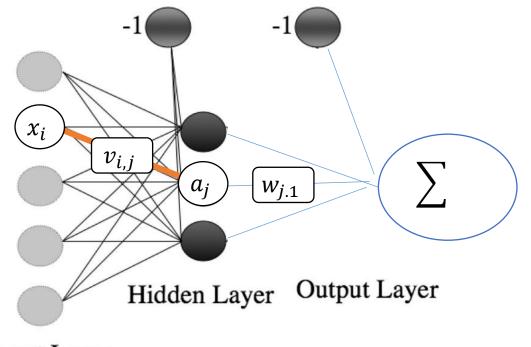
#### Backwards: Update first layer: V, 1

• 
$$y = f(z) = z$$
, where  $z = a^+ W$ 

- $\boldsymbol{a} = g(\boldsymbol{h})$ , where  $\boldsymbol{h} = \boldsymbol{x}^+ \boldsymbol{V}$
- $\frac{\partial}{\partial v_{i,j}} L_{SE}(t, y) =$
- $\frac{\partial}{\partial a} L_{SE}(\mathbf{t}, \mathbf{y}) \left( \frac{\partial}{\partial v_{i,j}} \mathbf{a} \right) =$

• 
$$\frac{\partial}{\partial a_j} L_{SE}(\mathbf{t}, \mathbf{y}) \left(\frac{\partial}{\partial v_{i,j}} a_j\right)$$

• because  $\left(\frac{\partial}{\partial v_{i,j}}a_k\right) = \mathbf{0}$  for  $k \neq j$ 



#### Input Layer



#### Backwards: Update first layer: V, 2

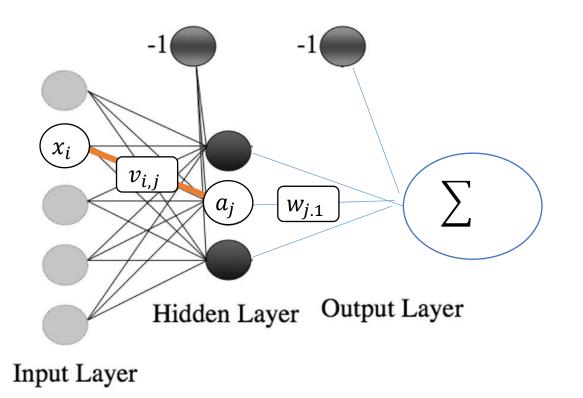
• 
$$y = f(z) = z$$
, where  $z = a^+ W$ 

• 
$$\frac{\partial}{\partial a_j} L_{SE}(t, y) = \frac{\partial}{\partial y} L_{SE}(t, y) \left(\frac{\partial}{\partial a_j} y\right) = (t - y)(-w_{j,1}) = (y - t)(w_{j,1})$$

• Observe similarities and differences to

• 
$$\frac{\partial}{\partial w_{i,1}} L_{SE}(t, y) = (y - t)(a_i)$$

• We call the common part: (y - t) for the delta term,  $\delta_o(\kappa)$  of the end node  $\kappa$ .



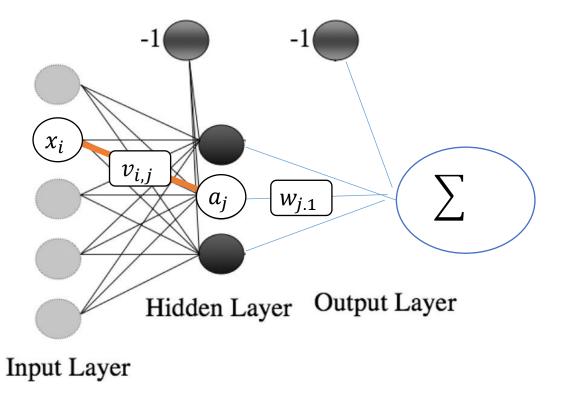
#### Backwards: Update first layer: V, 3

• 
$$\boldsymbol{a} = g(\boldsymbol{h})$$
, where  $\boldsymbol{h} = \boldsymbol{x}^+ \boldsymbol{V}$ 

• 
$$\left(\frac{\partial}{\partial v_{i,j}}a_j\right) = \left(\frac{\partial}{\partial h}g\right)\left(\frac{\partial}{\partial v_{i,j}}h\right) =$$
  
=  $\left(\frac{\partial}{\partial h_j}g\right)\left(\frac{\partial}{\partial v_{i,j}}h_j\right)$ 

• 
$$\frac{\partial}{\partial v_{i,j}} h_j = x_i$$

• If 
$$a_j = g(h_j) = \sigma(h_j)$$
, then  
•  $\left(\frac{\partial}{\partial h_j}g\right) = a_j(1 - a_j)$   
•  $\left(\frac{\partial}{\partial v_{i,j}}a_j\right) = a_j(1 - a_j)x_i$ 





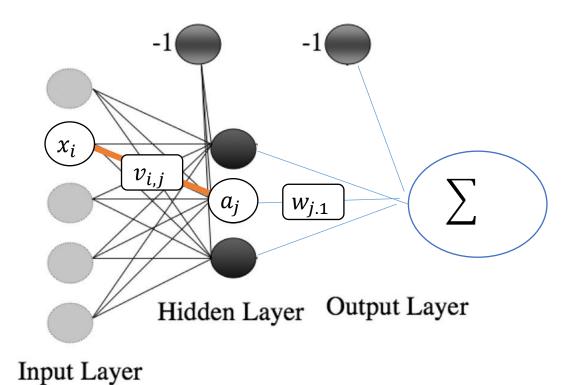
#### Backwards: Update first layer: V, 4

• 
$$y = f(z) = z$$
, where  $z = a^+ W$ 

• 
$$\frac{\partial}{\partial v_{i,j}} L_{SE}(t, y) = \frac{\partial}{\partial a_j} L_{SE}(t, y) \left(\frac{\partial}{\partial v_{i,j}} a_j\right) =$$

• 
$$(y-t)(w_{j,1})a_j(1-a_j)x_i$$

 $\delta$ -term at the node marked with  $a_j$ 

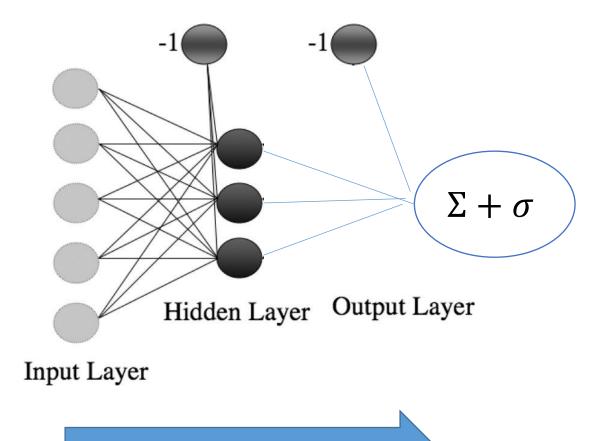


### Putting it together: the Algorithm

- Use the loss function and the derivative of the activation function to compute the delta term at the final node(s), here:  $\delta_o(\kappa_1) = (y t)$
- Compute the delta terms for each node in the hidden layer, from the delta term(s) and the hidden layer and the weights at the connections
  - here:  $\delta(hidden_j) = \delta_o(\kappa_1)(w_{j,1})a_j(1-a_j)$
- Update the weights by the deltas:
  - $w_{i,1} = w_{i,1} \eta \delta_o(\kappa_1) a_i$
  - $v_{i,j} = v_{i,j} \eta \delta(hidden_j) x_i$

#### 2. Binary classification, take one

- Like Marsland, and regression, for loss use (SE):  $L_{SE}(\mathbf{t}, \mathbf{y}) = \frac{1}{2} \sum_{j=1}^{N} (t_j - y_j)^2$
- The only difference to regression is the logistic activation function:  $y = \sigma(x) = \frac{1}{1+e^{-x}}$
- Since the derivative of this is y(1-y), we get
- $\delta_o(\kappa_1) = (y-t)y(1-y)$
- The rest is as for regression



#### 2. Binary classification, take two

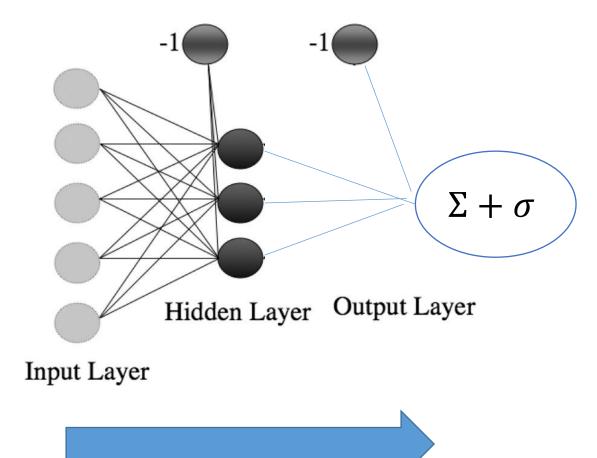
• Use instead cross-entropy loss (cf. Lecture 7, Marsland 4.6.6)

• 
$$\frac{\partial}{\partial y} L_{CE}(\mathbf{t}, y) = -\frac{(t-y)}{y(1-y)}$$

• Logistic activation

• 
$$\delta_o(\kappa_1) = -\frac{(t-y)}{y(1-y)}y(1-y) = (y-t)$$

• The rest is as for regression and take one

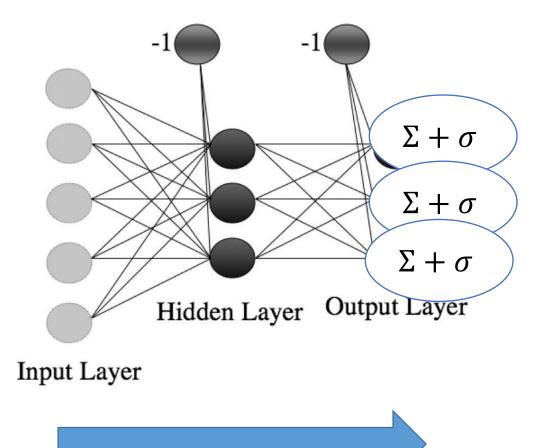


### 3. Multi-label classification

- Several output nodes
- Logistic activation function
- The model Marsland considers

• 
$$L_{SE}(\mathbf{t}, \mathbf{y}) = \frac{1}{2} \sum_{j=1}^{N} (t_j - y_j)^2$$

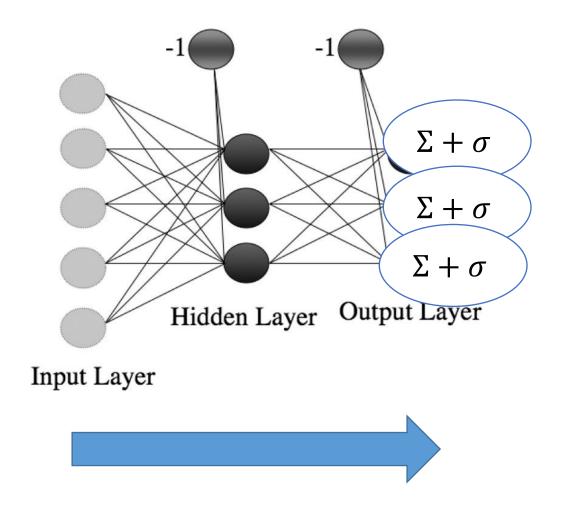
- (The index *j* here, runs over the output nodes.)
- We still look at one input only



### 3. Multi-label classification

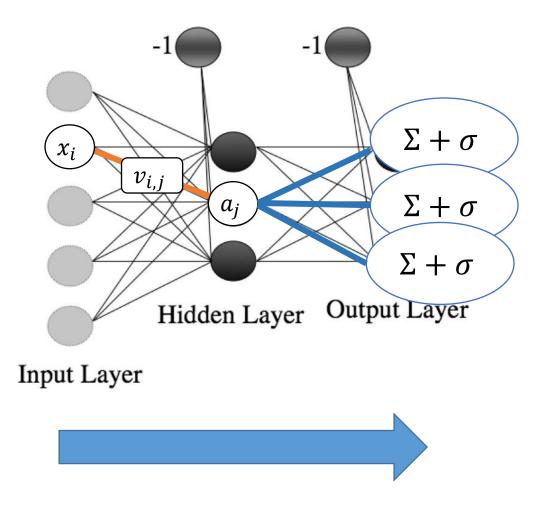
- (SE loss, logistic output activation)
- We compute a delta term at each output node, κ<sub>j</sub>:

• 
$$\delta_o(\kappa_j) = (y_j - t_j)y_j(1 - y_j)$$



### 3. First layer

- (SE loss, logistic output activation)
- $\delta(hidden_j) =$
- $a_j(1-a_j)\sum_{i=1}^n \delta_o(\kappa_i)w_{j,i}$
- i.e., sum of delta at output weighted by the connections between them
- The rest as for the others



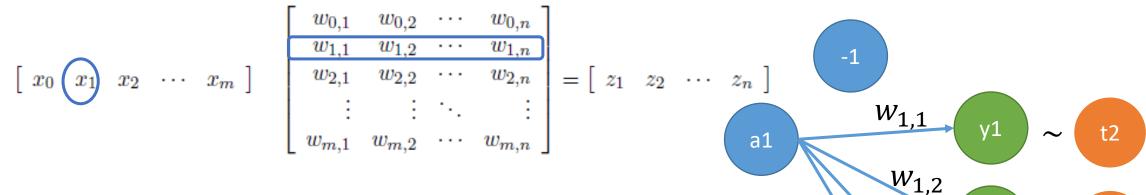
#### Putting it together: the Algorithm

• Use the loss function and the derivative of the activation function to compute the delta term at the final node(s),

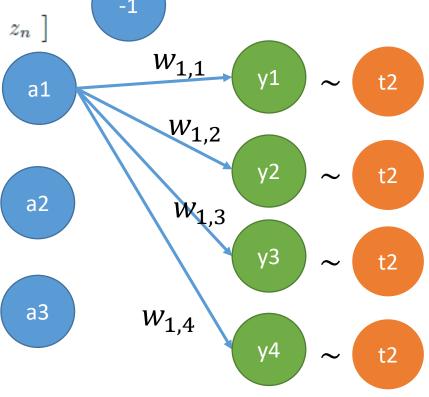
• here: $\delta_o(\kappa_j) = (y_j - t_j)y_j(1 - y_j)$  for each node  $\kappa_j$  for j = 1, ..., n

- Compute the delta terms for each node in the hidden layer,
  - here:  $\delta(hidden_j) = a_j(1-a_j)\sum_{i=1}^n \delta_o(\kappa_i)w_{j,i}$  for j = 1, ..., k
- Update the weights by the deltas in both layers
  - $w_{i,j} = w_{i,j} \eta \delta_o(\kappa_j) a_i$ •  $v_{i,j} = v_{i,j} - \eta \delta(hidden_j) x_i$

### By the way:



- To calculate  $\sum_{j=1}^{m} w_{l,j} \delta_j$  by matrices, use
- $[\delta(\kappa_1), \delta(\kappa_2), ... \delta(\kappa_n)] W^T$



### Congratulation!

- You just survived backpropagation!
- You now deserve a break and cake!

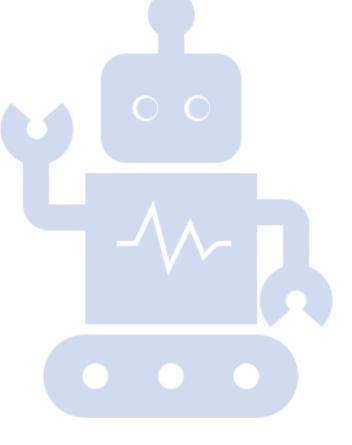






# 8.4 Finer details

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#### Practical advices

- Scaling
- Initializing the weights
- Local minima
- Early stopping
- Batch, stochastic, mini-batch
- Number of hidden nodes and hidden layers?
- Activation functions



## Scaling

- The  $z = w \cdot x$  shouldn't be too large for this to work, roughly |z|shouldn't be much more than 1
- For example, normalization (scikit: standardscaler) of each feature

#### Normalization

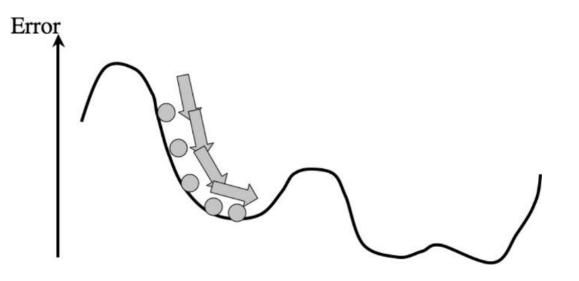
- Training data, dimension *i*:  $X_i = \{x_{1i}, x_{2i}, ... x_{Ni}\}.$
- Let *m* be the mean value: •  $m = \frac{1}{N} \sum_{j=1}^{N} x_{j,i}$
- Let s be the standard deviation
- Define  $scale_i(x_{ji}) = \frac{x_{ji} m}{s}$
- Use the same scaler on all test data!

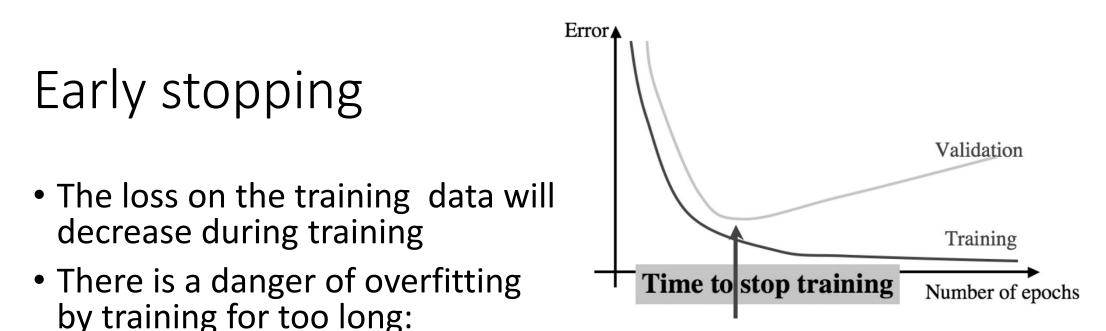
### Initializing the weights

- The weights:
  - should not be initialized to 0
  - should be initialized to random numbers
  - should be initialized to numbers between -1 and 1
- In addition, Marsland recommends to multiply with  $\frac{1}{\sqrt{m}}$ 
  - where m is the number of input nodes

### Local minima

- The loss function for MLP is not convex
- It can be caught in local minima
- Hence:
  - Make several runs with different initializations and compare the results (mean and std.dev.)
  - Consider methods for escaping local minima, cf. lecture 2 and adding momentum

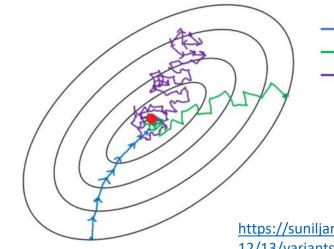




- The network knows the training set very well
- but does not generalize
  - Use a validation set V different from the training set.
  - After k rounds for some fixed k (e.g., 100):
    - check the loss on V
    - if the loss starts to increase, stop training!

### Variations of gradient descent

- Mini-batch training:
  - Pick a subset of the training set of a certain size
  - Calculate the loss for this subset
  - Make one move in the direction of this gradient
  - Repeat (an epoch)
- Batch training
  - Use the whole training set in each epoch
- Stochastic gradient descent:
  - Pick one datapoint at random and use in each epoch



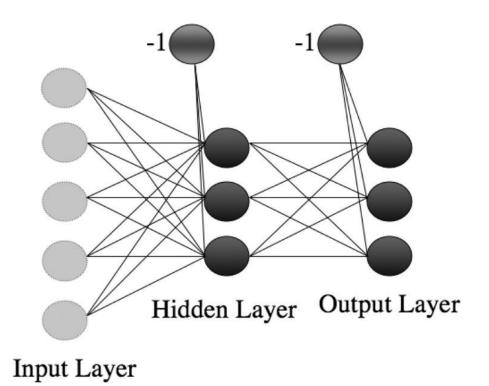
Batch gradient descent
 Mini-batch gradient Descent
 Stochastic gradient descent

https://suniljangirblog.wordpress.com/2018/ 12/13/variants-of-gradient-descent/

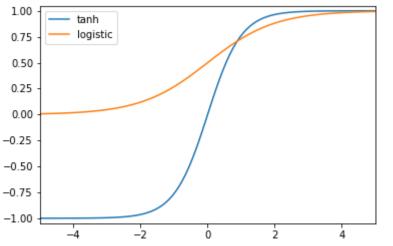
 SGD/Mini-batch can be a way to avoid local minima

### Number of hidden nodes and hidden layers?

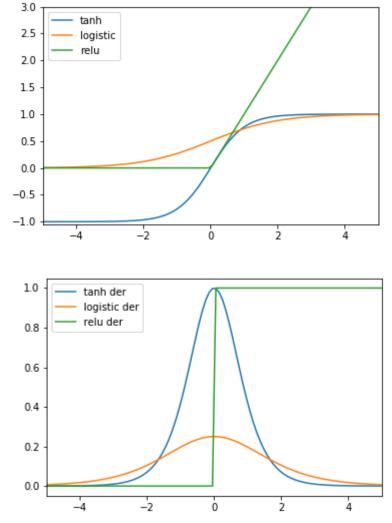
- Very much an empirical question
- Use an independent validation set
- Run with different settings and evaluate on the validation set
- Choose the settings which give the best result
- Called hyper-parameter tuning
  - (The hyper-parameters are the parameters that you have to set.)



#### Alternative activation functions in the hidden layer



- There are alternative activation functions
- One may use different functions at different layers
- $\tanh(x) = \frac{e^x e^{-x}}{e^x + e^{-x}}$
- $ReLU(x) = \max(x, 0)$
- ReLU is the preferred method in deep networks







# 8.5 More on evaluation

IN3050/IN4050 Introduction to Artificial Intelligence

and Machine Learning

### Evaluation measures

|       |     | Is in C |    |
|-------|-----|---------|----|
|       | _   | Yes     | NO |
| Class | Yes | tp      | fp |
| ifier | No  | fn      | tn |

- Accuracy: (tp+tn)/N
- Precision:tp/(tp+fp)
- Recall: tp/(tp+fn)

• F-score combines P and R

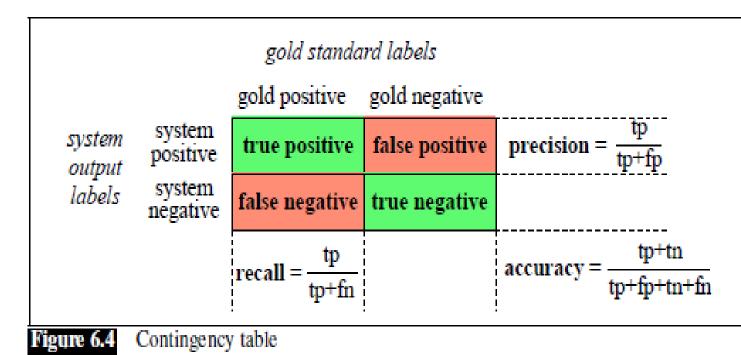
• 
$$F_1 = \frac{2PR}{P+R} \left( = \frac{1}{\frac{1}{\frac{1}{R} + \frac{1}{P}}} \right)$$

- F<sub>1</sub> called "harmonic mean"
- General form

• 
$$F = \frac{1}{\alpha \frac{1}{P} + (1 - \alpha) \frac{1}{R}}$$

• for some  $0 < \alpha < 1$ 

### Confusion matrix



- Beware what the rows and columns are:
  - Marsland swaps them

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#### Confusion matrix

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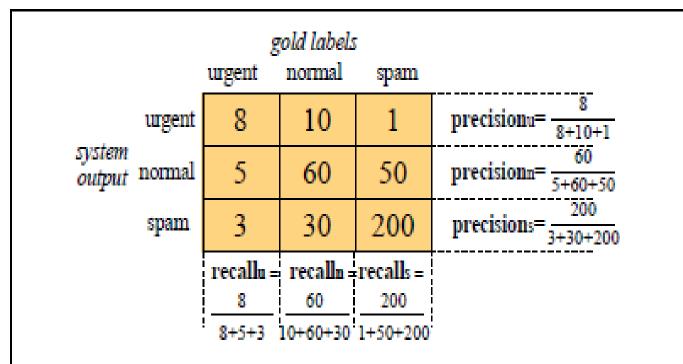


Figure 6.5 Confusion matrix for a three-class categorization task, showing for each pair of classes  $(c_1, c_2)$ , how many documents from  $c_1$  were (in)correctly assigned to  $c_2$ 

 Precision, recall and fscore can be calculated for each class against the rest