## UiO: University of Oslo

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
- $10^{11}$ Neurons
- $10^{14}$ Synapses
- The strength is the interactions
- Neural Networks



## 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


Input Layer

## 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


Input Layer

## Going forwards (predictions)

- There is one input node for each feature/dimension in an input vector: $\left(x_{1}, x_{2}, \ldots, x_{m}\right)$
- 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.)


Input Layer

## One hidden unit

1. First sum of weighted inputs :

- $\mathrm{z}=\sum_{i=0}^{m} w_{i} x_{i}=\boldsymbol{w} \cdot \boldsymbol{x}$

2. Then the result is run through an activation function, $g$ to produce $g(z)=g(\boldsymbol{w} \cdot \boldsymbol{x})$

- 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
- $y=\sigma(z)=\frac{1}{1+e^{-\vec{w} \cdot \vec{x}}}$
- Differentiable
- $y^{\prime}=y(1-y)$
- (There are alternative activation functions.)



## One hidden node

1. First sum of weighted inputs:

- $\mathrm{z}=\sum_{i=0}^{m} w_{i} x_{i}=\boldsymbol{w} \cdot \boldsymbol{x}$

2. Then

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



## 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


Input Layer


## 1. Regression

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


Input Layer

## 2. Binary classification

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


Input Layer

## 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


Input Layer

# 8.2 Matrix representations 

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## Representing the connections

$\left.\begin{array}{l}{\left[\begin{array}{llll}x_{0} & x_{1} & x_{2} & \cdots\end{array} x_{m}\right.}\end{array}\right]\left[\begin{array}{rrrr}w_{0,1} & w_{0,2} & \cdots & w_{0, n} \\ w_{1,1} & w_{1,2} & \cdots & w_{1, n} \\ w_{2,1} & w_{2,2} & \cdots & w_{2, n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m, 1} & w_{m, 2} & \cdots & w_{m, n}\end{array}\right]=\left[\begin{array}{llll}z_{1} & z_{2} & \cdots & z_{n}\end{array}\right] \quad$ - We use a matrix to represent the connections

- (Beware, some texts do it differently)


## Connections going into a node

$\left[\begin{array}{lllll}x_{0} & x_{1} & x_{2} & \cdots & x_{m}\end{array}\right]\left[\begin{array}{rrrrr}w_{0,1} & w_{0,2} & \cdots & w_{0, n} \\ w_{1,1} & w_{1,2} & \cdots & w_{1, n} \\ w_{2,1} & w_{2,2} & \cdots & w_{2, n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m, 1} & w_{m, 2} & \cdots & w_{m, n}\end{array}\right]=\left[\begin{array}{llll}z_{1} & z_{2} & \cdots & z_{n}\end{array}\right]$


## Connections going out of a node

$$
\left[\begin{array}{llll}
x_{0} & x_{1}
\end{array} x_{2} \quad \cdots \quad x_{m}\right]\left[\begin{array}{rrrr}
w_{0,1} & w_{0,2} & \cdots & w_{0, n} \\
w_{1,1} & w_{1,2} & \cdots & w_{1, n} \\
\hline w_{2,1} & w_{2,2} & \cdots & w_{2, n} \\
\vdots & \vdots & \ddots & \vdots \\
w_{m, 1} & w_{m, 2} & \cdots & w_{m, n}
\end{array}\right]=\left[\begin{array}{llll}
z_{1} & z_{2} & \cdots & z_{n}
\end{array}\right]
$$



## 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: $y_{i, j}=g\left(z_{i, j}\right)$
- In NumPy this can be done by one operation: $g(X W)$
- Reminder: $g$ may be the logistic function, but doesn't have to
- i.e., $g\left(z_{i, j}\right)=\sigma\left(z_{i, j}\right)=\frac{1}{1+e^{-z_{i, j}}}$


## 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 | $w_{i, j}$ | $w_{j, i}$ |
| Data and weights | $X W$ | $W X$ |
| Applying activation function | $g(X W)$ | $g(W X)$ |

- 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 $f^{\prime}(x)=x$
2. If $f(x)=c$ then $f^{\prime}(x)=0$
3. If $f(x)=h(g(x))$ then $f^{\prime}(x)=h^{\prime}(g(x)) g^{\prime}(x)$ (the chain rule) He forgot
4. If $y=\sigma(z)=\frac{1}{1+e^{-\bar{w} \cdot \bar{x}}}$, then $y^{\prime}=y(1-y)$

## 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
- $\left\{\left(\boldsymbol{x}_{1}, t_{1}\right),\left(\boldsymbol{x}_{2}, t_{2}\right), \ldots,\left(\boldsymbol{x}_{N}, t_{N}\right)\right\}:$
- Forwards:
- Run them forwards and get predictions
- $\left\{y_{1}, y_{N}, \ldots, y_{N}\right\}$
- Backwards


Input Layer

- Use a suitable loss function and compare these to the target values
- $\left\{t_{1}, t_{2}, \ldots, t_{N}\right\}$
- Apply gradient descent to update the weights (partial derivatives)


## 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 $\mathbf{V}$ be the connections from input to hidden and $\mathbf{W}$ from hidden to output
- $\operatorname{dim}(V)=((m+1) \times k)$
- $\operatorname{dim}(W)=((k+1) \times n)$


Input Layer

- Activation functions:
- Hidden layers: $g$
- Hidden output layer: $f$
- Let us in the following consider SGD where we update for one input $\boldsymbol{x}=\left(x_{1}, x_{2}, \ldots x_{m}\right)$


## Forwards (notation)

- Add bias and send
- $\boldsymbol{x}^{+}=\left(x_{0}, x_{1}, \ldots x_{m}\right)$
- through the first layer to get
- $\boldsymbol{h}=\boldsymbol{x}^{+} \boldsymbol{V}=\left(h_{1}, h_{2}, \ldots, h_{k}\right)$, where
- $h_{j}=\sum_{i=0}^{m} x_{i} v_{i, j}$
- $k$ is the number of hidden nodes
- Apply activation function to get
- $\boldsymbol{a}=g(\boldsymbol{h})=\left(a_{1}, a_{2}, \ldots, a_{k}\right)$,
- where $a_{j}=g\left(h_{j}\right)$
- Add bias and send
- $\boldsymbol{a}^{+}=\left(a_{0}, a_{1}, a_{2}, \ldots, a_{k}\right)$
- through the second layer to get
- $\boldsymbol{z}=\boldsymbol{a}^{+} \boldsymbol{W}=\left(z_{1}, z_{2}, \ldots, z_{n}\right)$, where
- $z_{j}=\sum_{i=0}^{k} a_{i} w_{i, j}$
- $n$ is the number of output nodes
- Apply activation function to get
- $\boldsymbol{y}=f(\mathbf{z})=\left(y_{1}, y_{2}, \ldots, y_{n}\right)$,
- where $y_{j}=f\left(z_{j}\right)$


## 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


Input Layer

## Backwards: Update last layer

- For loss, we use MSE, or , as Marsland, the simpler

Sum of Squares Error (SE): $L_{S E}(\mathbf{t}, \boldsymbol{y})=\frac{1}{2} \sum_{j=1}^{N}\left(t_{j}-y_{j}\right)^{2}$

- (The index $j$ here, runs over the input items. There is only one output node)
- We have seen that
- $\frac{\partial}{\partial w_{i, 1}} L_{S E}(\mathbf{t}, \boldsymbol{y})=\frac{\partial}{\partial \boldsymbol{y}} L_{S E}(\mathbf{t}, \boldsymbol{y})\left(\frac{\partial}{\partial w_{i, 1}} \boldsymbol{y}\right)=\sum_{j=1}^{N}\left(\left(t_{j}-y_{j}\right)\left(-a_{j, i}\right)\right)$
- For SGD where we update for one input $\boldsymbol{x}=\left(x_{1}, x_{2}, \ldots x_{m}\right)$
- $\frac{\partial}{\partial w_{i, 1}} L_{S E}(\mathrm{t}, y)=\frac{\partial}{\partial y} L_{S E}(\mathrm{t}, y)\left(\frac{\partial}{\partial w_{i, 1}} y\right)=(t-y)\left(-a_{i}\right)=(y-t)\left(a_{i}\right)$


## Backwards: Update last layer, ctd.

- $\frac{\partial}{\partial w_{i, 1}} L_{S E}(\mathrm{t}, y)=(y-t)\left(a_{i}\right)$
- We know from lect. 6 how to update this ( $\boldsymbol{a}$ corresponds to $\boldsymbol{x}$ then)
- But wait!
- We first have to find how to update the first layer.



## Backwards: Update first layer: V, 1

- $\boldsymbol{y}=f(\mathbf{z})=\mathbf{z}$, where $\mathbf{z}=\boldsymbol{a}^{+} \boldsymbol{W}$
- $\boldsymbol{a}=g(\boldsymbol{h})$, where $\boldsymbol{h}=\boldsymbol{x}^{+} \boldsymbol{V}$
- $\frac{\partial}{\partial v_{i, j}} L_{S E}(\mathrm{t}, y)=$
- $\frac{\partial}{\partial \boldsymbol{a}} L_{S E}(\mathrm{t}, y)\left(\frac{\partial}{\partial v_{i, j}} \boldsymbol{a}\right)=$
- $\frac{\partial}{\partial a_{j}} L_{S E}(\mathrm{t}, y)\left(\frac{\partial}{\partial v_{i, j}} a_{j}\right)$
- 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

- $\boldsymbol{y}=f(\mathbf{z})=\mathbf{z}$, where $\mathbf{z}=\boldsymbol{a}^{+} \boldsymbol{W}$
- $\frac{\partial}{\partial a_{j}} L_{S E}(\mathrm{t}, y)=\frac{\partial}{\partial y} L_{S E}(\mathrm{t}, y)\left(\frac{\partial}{\partial a_{j}} y\right)=$ $(t-y)\left(-w_{j, 1}\right)=(y-t)\left(w_{j, 1}\right)$
- Observe similarities and differences to
- $\frac{\partial}{\partial w_{i, 1}} L_{S E}(\mathrm{t}, y)=(y-t)\left(a_{i}\right)$
- We call the common part: $(y-t)$ for the delta term, $\delta_{o}(\kappa)$ of the end node $\kappa$.


Input Layer

## Backwards: Update first layer: V, 3

- $\boldsymbol{a}=g(\boldsymbol{h})$, where $\boldsymbol{h}=\boldsymbol{x}^{+} \boldsymbol{V}$
- $\left(\frac{\partial}{\partial v_{i, j}} a_{j}\right)=\left(\frac{\partial}{\partial \boldsymbol{h}} g\right)\left(\frac{\partial}{\partial v_{i, j}} \boldsymbol{h}\right)=$
$=\left(\frac{\partial}{\partial h_{j}} g\right)\left(\frac{\partial}{\partial v_{i, j}} h_{j}\right)$
- $\frac{\partial}{\partial v_{i, j}} h_{j}=x_{i}$
- If $a_{j}=g\left(h_{j}\right)=\sigma\left(h_{j}\right)$, then
- $\left(\frac{\partial}{\partial h_{j}} g\right)=a_{j}\left(1-a_{j}\right)$
- $\left(\frac{\partial}{\partial v_{i, j}} a_{j}\right)=a_{j}\left(1-a_{j}\right) x_{i}$


Input Layer

## Backwards: Update first layer: V, 4

- $\boldsymbol{y}=f(\mathbf{z})=\mathbf{z}$, where $\mathbf{z}=\boldsymbol{a}^{+} \boldsymbol{W}$
- $\boldsymbol{a}=g(\boldsymbol{h})$, where $\boldsymbol{h}=\boldsymbol{x}^{+} \boldsymbol{V}$
- $\frac{\partial}{\partial v_{i, j}} L_{S E}(\mathrm{t}, y)=\frac{\partial}{\partial a_{j}} L_{S E}(\mathrm{t}, y)\left(\frac{\partial}{\partial v_{i, j}} a_{j}\right)=$


## $\delta_{0}(\kappa)$

- $(y-t)\left(w_{j, 1}\right) a_{j}\left(1-a_{j}\right) x_{i}$


Input Layer

## 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: $\delta_{o}\left(\kappa_{1}\right)=(y-t)$
- 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: $\delta\left(\right.$ hidden $\left._{j}\right)=\delta_{o}\left(\kappa_{1}\right)\left(w_{j, 1}\right) a_{j}\left(1-a_{j}\right)$
- Update the weights by the deltas:
- $w_{i, 1}=w_{i, 1}-\eta \delta_{o}\left(\kappa_{1}\right) a_{i}$
- $v_{i, j}=v_{i, j}-\eta \delta\left(\right.$ hidden $\left._{j}\right) x_{i}$


## 2. Binary classification, take one

- Like Marsland, and regression, for loss use (SE):

$$
L_{S E}(\mathbf{t}, \boldsymbol{y})=\frac{1}{2} \sum_{j=1}^{N}\left(t_{j}-y_{j}\right)^{2}
$$

- 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
- $\delta_{o}\left(\kappa_{1}\right)=(y-t) y(1-y)$
- The rest is as for regression


Input Layer

## 2. Binary classification, take two

- Use instead cross-entropy loss (cf. Lecture 7, Marsland 4.6.6)
- $\frac{\partial}{\partial y} L_{C E}(\mathrm{t}, y)=-\frac{(t-y)}{y(1-y)}$
- Logistic activation
- $\delta_{o}\left(\kappa_{1}\right)=-\frac{(t-y)}{y(1-y)} y(1-y)=$ $(y-t)$
- The rest is as for regression and take one



## 3. Multi-label classification

- Several output nodes
- Logistic activation function
- The model Marsland considers
- $L_{S E}(\mathbf{t}, \boldsymbol{y})=\frac{1}{2} \sum_{j=1}^{N}\left(t_{j}-y_{j}\right)^{2}$
- (The index $j$ here, runs over the output nodes.)
- We still look at one input only


Input Layer

## 3. Multi-label classification

- (SE loss, logistic output activation)
- We compute a delta term at each output node, $\kappa_{j}$ :
- $\delta_{o}\left(\kappa_{j}\right)=\left(y_{j}-t_{j}\right) y_{j}\left(1-y_{j}\right)$



## 3. First layer

- (SE loss, logistic output activation)
- $\delta\left(\right.$ hidden $\left._{j}\right)=$
- $a_{j}\left(1-a_{j}\right) \sum_{i=1}^{n} \delta_{o}\left(\kappa_{i}\right) w_{j, i}$
- 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: $\delta_{o}\left(\kappa_{j}\right)=\left(y_{j}-t_{j}\right) y_{j}\left(1-y_{j}\right)$ for each node $\kappa_{j}$ for $j=1, \ldots, n$
- Compute the delta terms for each node in the hidden layer,
- here: $\delta\left(\right.$ hidden $\left._{j}\right)=a_{j}\left(1-a_{j}\right) \sum_{i=1}^{n} \delta_{o}\left(\kappa_{i}\right) w_{j, i}$ for $j=1, \ldots, k$
- Update the weights by the deltas in both layers
- $w_{i, j}=w_{i, j}-\eta \delta_{o}\left(\kappa_{j}\right) a_{i}$
- $v_{i, j}=v_{i, j}-\eta \delta\left(\right.$ hidden $\left._{j}\right) x_{i}$


## By the way:



## 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 $\mathbf{z}=\boldsymbol{w} \cdot \boldsymbol{x}$ 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 $i$ : $X_{i}=\left\{x_{1 i}, x_{2 i}, \ldots x_{N i}\right\}$.
- Let $m$ be the mean value:
- $m=\frac{1}{N} \sum_{j=1}^{N} x_{j, i}$
- Let $s$ be the standard deviation
- Define $\operatorname{scale}_{i}\left(x_{j i}\right)=\frac{x_{j i}-m}{s}$
- 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



## Early stopping

- The loss on the training data will decrease during training
- There is a danger of overfitting by training for too long:

- 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
- 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.)


Input Layer

## Alternative activation functions in the hidden layer




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



### 8.5 More on evaluation

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## Evaluation measures



- Accuracy: (tp+tn)/N
- Precision:tp/(tp+fp)
- Recall: tp/(tp+fn)
- F-score combines P and R
- $F_{1}=\frac{2 P R}{P+R}\left(=\frac{1}{\frac{\frac{1}{R}+\frac{1}{P}}{2}}\right)$
- $F_{1}$ called "harmonic mean"
- General form
- $F=\frac{1}{\alpha \frac{1}{P}+(1-\alpha) \frac{1}{R}}$
- for some $0<\alpha<1$


## Confusion matrix

| gold standard labels <br> gold positive |  |  |  |  |
| :--- | :--- | :--- | :--- | :---: |
| gold negative |  |  |  |  |

Digure 6.4 Contingency table

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


## Confusion matrix



Figure 6.5 Confusion matrix for a three-class categonization 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

