COMS30035, Machine learning:

Classification and Neural Networks

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Textbooks

We will follow parts of the Chapter 4 and 5 of the Bishop book:

- Bishop, C. M., Pattern recognition and machine learning (2006). Available for free here.

Agenda

- Discriminant functions
- Logistic regression
- Perceptron
- Neural networks (multi-layer perceptron)
  - Architecture
  - The backpropagation algorithm
  - Gradient descent

See: [Chapter 5, Bishop]

Classification

- It is the classical example of **supervised learning**
- Goal: Classify input data into one of K classes

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- Goal: Classify input data into one of K classes
- Model: *Discriminant function*:
  - A function that takes an input vector x and assigns it to class C_k. For simplicity we will focus on $K = 2$ and will first study linear functions (see Bishop for the general cases).

Linear discriminant function

- The simplest linear discriminant (LD) is $\boxed{y(x) = w_0 + \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}}$
  - where y is used to predicted class C_k, x is the input vector (feature values)
  - w_0 is a scalar, which we call *bias*
  - w_T is our vector of parameters, which we call *weights*

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- For $K = 2$: An input vector x is assigned to class C_1 if $y(x) \geq 0$ and to class C_2 otherwise.
- Optimisation: least-squares (as for regression) [1], where we want to minimise the cost or error function:

$\boxed{E = \frac{1}{2}\sum_{n=1}^{N}(\boldsymbol{w}^T\boldsymbol{x}_n + w_0 - t_n)^2}$ where t_n are the targets/labels (e.g. $t_1 = C_1$).

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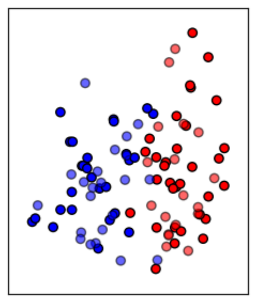
LD and linear separability

Example

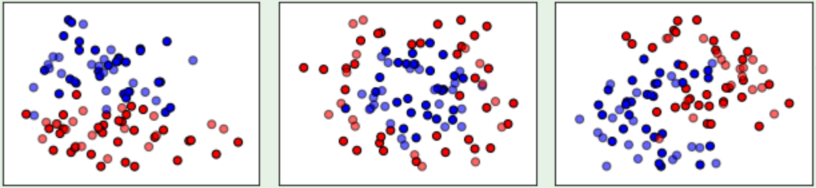
Linear separability is when two sets of points are separable by a line. We generated two sets of points using two Gaussians to illustrate this point, which can easily be fit by a LD. A *decision boundary* is the boundary that separates the two given classes, which our models will try to find.



Linear separability vs nonlinear separability

Example

Which datasets **are** and **are not** linearly separable[2]?



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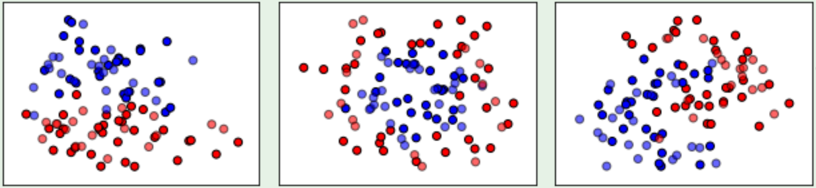


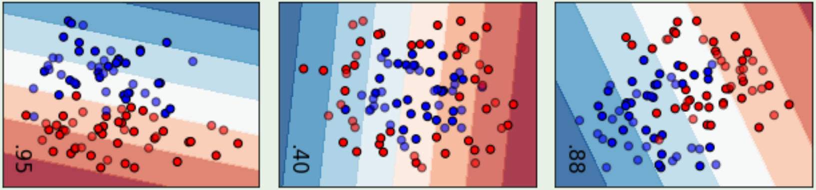
Only the first dataset is linearly separable!

[2] Example from Sklearn here.

Linear discriminant

Example

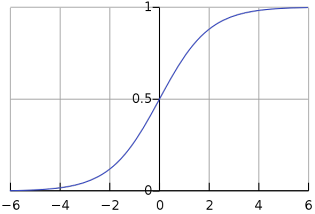
Using sklearn we fitted a LD to the data:



As expected, the LD model only does a good job in finding a good separation in the first dataset.

Logistic regression

- We use a logistic function to obtain the probability of class C_k: $\boxed{y(\boldsymbol{x}) = \sigma(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x})}$ where σ denotes the logistic sigmoid function (s-shaped), for example:



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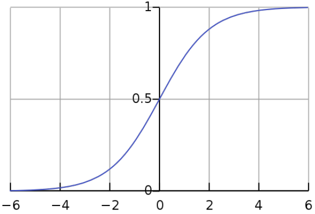

- such that when $y \to 0$ we choose class 1 and $y \to 1$ class 2.
- Taking a probabilistic view: $p(C_1|\boldsymbol{x}) = y(\boldsymbol{x})$, and $p(C_2|\boldsymbol{x}) = 1 - p(C_1|\boldsymbol{x})$.

Logistic regression – maximum likelihood estimation

Follow MLE recipe:

1. Define likelihood: For a data set $\{x_n, t_n\}$, where the targets $t_n \in \{0, 1\}$ we have $p(\boldsymbol{t}|\boldsymbol{w}) = \prod_{n=1}^{N} y_n^{t_n}(1 - y_n)^{1-t_n}$ where $y_n = p(C_1|x_n)$. [3]

[3] The exponent selects the probability of the target class (i.e. if $t_n = 1$ we get y_n; if $t_n = 0$ we get $1 - y_n$).

[4] Note that we used the logarithm product and power rule.

[5] This solution makes sense since we want to optimise the difference between the model output y and the desired targets t.

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2. Take negative logarithm of the likelihood [4]:
   $$-ln\, p(\boldsymbol{t}|\boldsymbol{w}) = -\sum_{n=1}^{N}\{t_n ln\, y_n + (1 - t_n) ln(1 - y_n)\}$$

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4. Now we can use Eq. above to directly update $\boldsymbol{w}$ using the data x.

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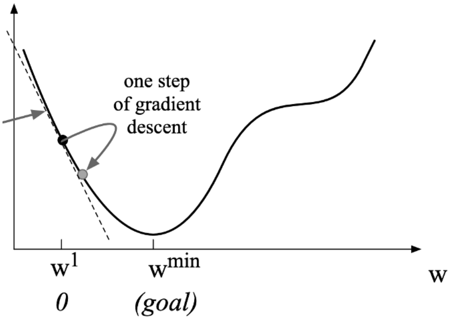
MLE using Gradient Descent



- Start with random weight values
- We want to adjust each weight w to minimise negative log likelihood: move downhill to the minimum
- The derivative represents the slope: $\frac{d \ln p(\mathbf{t}|\mathbf{w})}{d\mathbf{w}} = \sum_{n=1}^{N} (y_n - t_n) x_n$
- Increase or decrease w by a small amount in the downward direction

Logistic regression – maximum likelihood estimation

More details on calculating the derivative:

1. From here $-\ln p(\boldsymbol{t}|\boldsymbol{w}) = -\sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$

[6] We used the chain rule and $d\,ln(x) = 1/x$. We also used the derivative of the sigmoid $dy_n = y(1-y_n)$.

[7] You can find the full derivation here.

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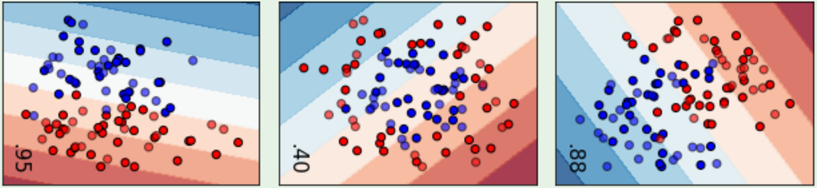
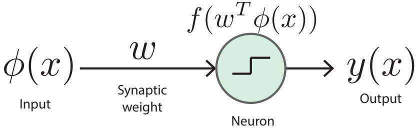


As you can see the results are very similar to LD, but because of probabilistic formulation we have an explicit probability of belonging to one or the other class (not shown); this can be very useful in real-world applications (e.g. self-driving cars or cancer detection).

Perceptron – a simplified neural network

- It is the very beginning of neural network models in ML!
- It is directly inspired on how neurons process information:



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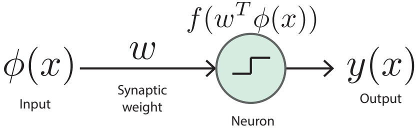

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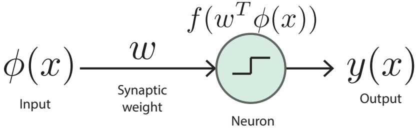

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  with a nonlinear *activation function* $f(a) = \begin{cases} +1, & a \geq 0 \\ -1, & a < 0 \end{cases}$
- Here the target $t = \{+1, -1\}$.
- And we aim to mimimise the following error $-\sum_{n=1}^{N} \boldsymbol{w}^T\phi_n t_n$ [8]

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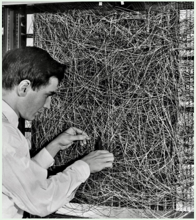


The Perceptron of Rosenblatt (1962)

The perceptron played an important role in the history of machine learning (Rosenblatt 1962). Indeed it represents the very start of the current *deep learning* revolution. Frank Rosenblatt used IBM and special-purpose hardware for a parallel implementation of perceptron learning. Rosenblatt's work was criticized by Marvin Minksy, who showed that such models could only learn *linearly separable problems*. However, this limitation is only true in the case of single layers!

source: Bishop p193.

Quiz and video time!

Watch this very cool video about the perceptron [9].

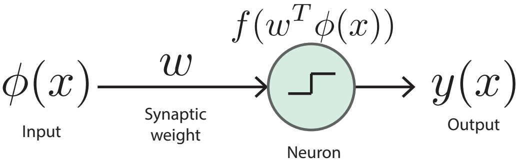
Go to Blackboard unit page » Quizzes » Week 1 » Classification and neural networks

[Should take you less than 5 minutes]

[9] Note the comment at the end – it underlies all the recent successes using deep learning!

Neural networks

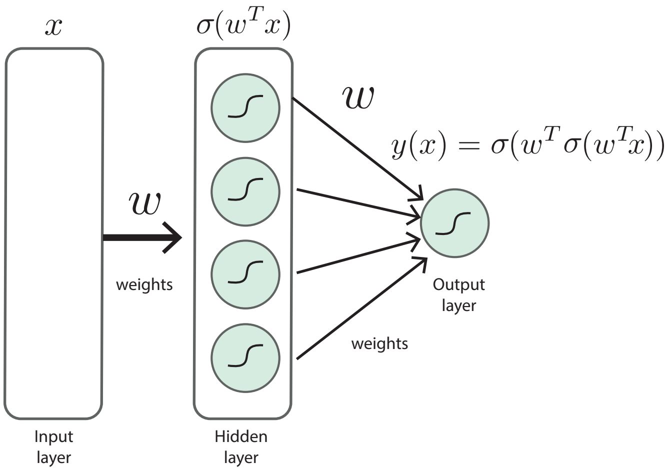
From a single layer perceptron:



However these and other linear (or near-linear) models have limited expressibility due to the *curse of dimensionality*.

Neural networks

To a Multiple Layer Perceptron (MLP) [10]:



[10] Although, we call it perceptron, it typically uses logistic sigmoid activation functions (continous nonlinearities), instead of step-wise discontinous nonlinearities.

Neural networks

- Neural networks are at heart composite functions of linear-nonlinear functions.
- **Deep learning**[11] refers to neural networks (or MLPs) with more than 1 hidden layer
- They can be applied in any form of learning, but we will focus on supervised learning and classification in particular

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- They can be applied in any form of learning, but we will focus on supervised learning and classification in particular
- MLP recipe [12]:
  - Define architecture (e.g. how many hidden layers and neurons) [13]
  - Define cost function (e.g. mean squared error)
  - Optimise network using backprop:
    1. Forward pass – calculate activations; generate y_k
    2. Calculate error/cost function
    3. Backward pass – use backprop to update parameters

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Neural networks – forward pass step-by-step

1. Calculate activations of the hidden layer h: $a_j = \sum_{i=1}^{D} w_{ji} x_i^{(h)} + w_{j0}^{(h)}$ [linear]
2. Pass it through a nonlinear function: $z_j = \sigma(a_j)$ [nonlinear[14]]

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[15] For classification problems we use a sigmoid at the output, where each output neuron codes for one class.

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4. Compute predictions using a sigmoid: $y_k = \sigma(a_k)$ [nonlinear[15]]
5. All together: $y_k = \sigma\left(\sum_{i=1}^{D} w_{kj}\, \sigma\left(\sum_{i=1}^{D} w_{ji} x_i^{(h)} + w_{j0}^{(h)}\right) + w_{k0}^{(o)}\right)$

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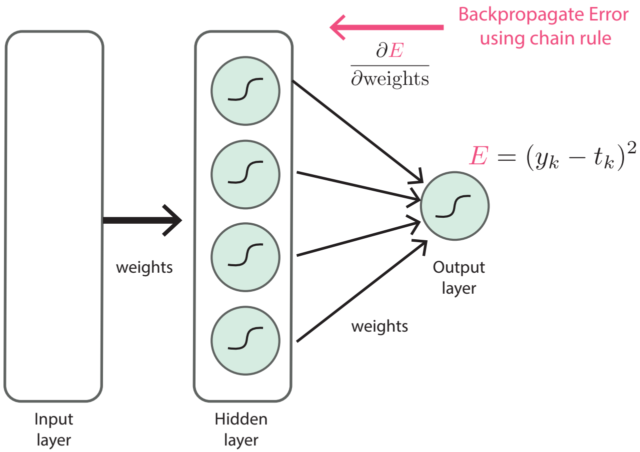
We now need to optimise our weights, and as before we use derivatives to find a solution. Effectively backpropagating the output error signal across the network – backpropagation algorithm.



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$$\frac{\partial E}{\partial w_{kj}} = \frac{\partial E}{\partial y_k}\frac{\partial y_k}{\partial \sigma}\frac{\partial \sigma}{\partial w_{kj}} = \sigma'(y_n - t_n)z_j$$ [16]

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Neural networks – gradient descent [19]

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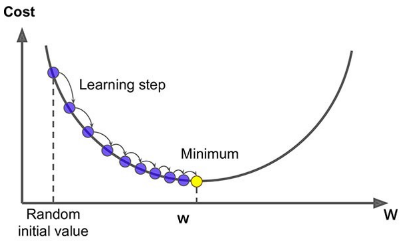

[18]

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[18] Figure from https://mc.ai/an-introduction-to-gradient-descent-2/

[19] Its called descent because we are minimising the cost function, so descending on the function landscape, which can be quite hilly!

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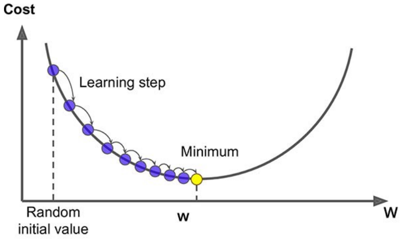


[18]

In our neural network this means to update the weights using:

- $w_{ji} = w_{ji} - \Delta w_{ji}$, where $\Delta w_{ji} = \sigma'(y_n - t_n) w_{kj}^T \sigma' x_i$
- $w_{kj} = w_{kj} - \Delta w_{kj}$, where $\Delta w_{kj} = \sigma'(y_n - t_n) z_j$
- This is often done in mini-batches – using a small number of samples to compute Δw.

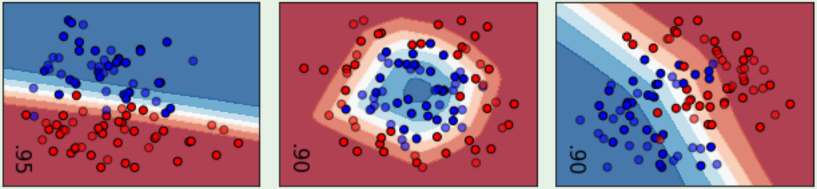
[18] Figure from `https://mc.ai/an-introduction-to-gradient-descent-2/`

[19] Its called descent because we are minimising the cost function, so descending on the function landscape, which can be quite hilly!

Neural networks

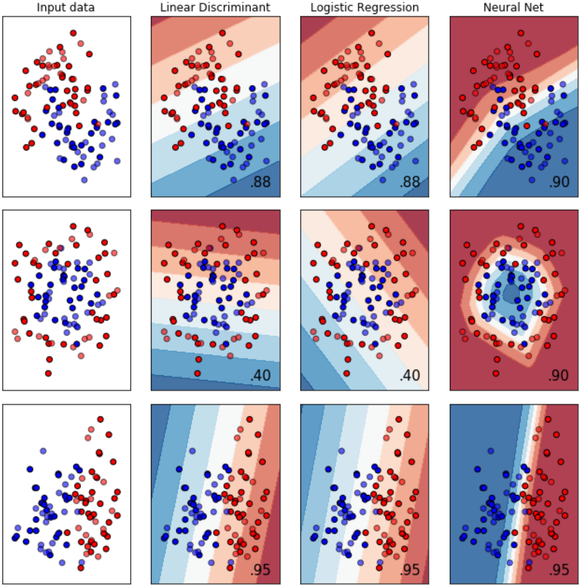
Example

Using sklearn we fitted a MLP classifier to the data:

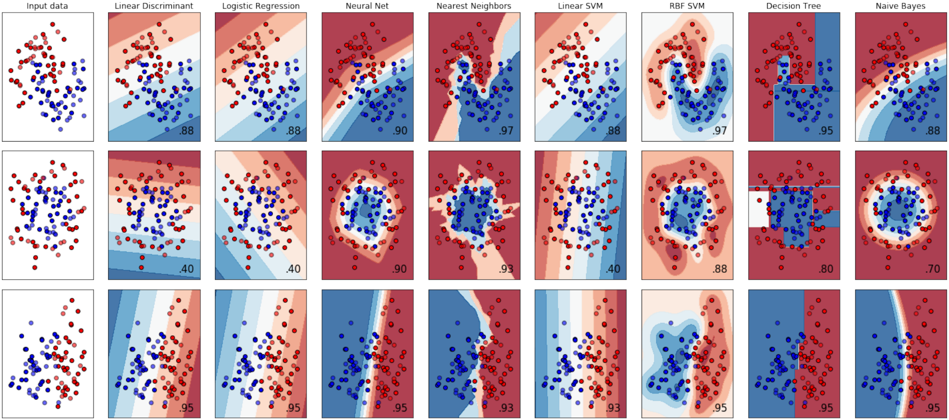


As you can see a MLP (with one hidden layer) can indeed perform very well in nonlinear classification problems. Note, however, because MLPs are highly flexible models they can easily *overfit* the data. To prevent this methods such as *early stopping* (stop when test performance starts decreasing) and *dropout* (randomly drop units in the network) are used.

Classification methods – overall comparison



Classification methods – overall comparison [including methods from the upcoming lectures]



Tasks

- Post questions Teams > QA channel or bring them to the next lecture

Tasks

- Post questions Teams > QA channel or bring them to the next lecture
- Next lab (Week 2): Neural nets and SVMs
  1. See link to lab 2 on BB