Artificial Neural Networks

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Outline

- Introduction
- Artificial Neural Networks
- Examples
- Lab exercise
- Presentation of your results

Data

- Everything can be data as long as it provides useful information.

- *Can you provide some examples?*

- *How do you analysis data?*

Data analysis paradigms

Statistics	Machine learning
Model	Network, Graphs
Data point	Examples/instances
Response	Label
Parameters	Weights
Covariate	Feature
Fitting/Estimation	Learning
Test set performance	Generalization
Regression/Classification	Supervised Learning
Density estimation, Clustering	Unsupervised Learning

From a machine (computer) only perspective, data can be structured or unstructured

Internet and data sharing

The main use of the internet is to share cute pictures of cats and dogs

The human brain is very good at recognising which is which

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Recognition and Classification

- Human brain is good at recognising and classifying objects:
  - This happens quickly, robustly and reliably. Also capable of learning

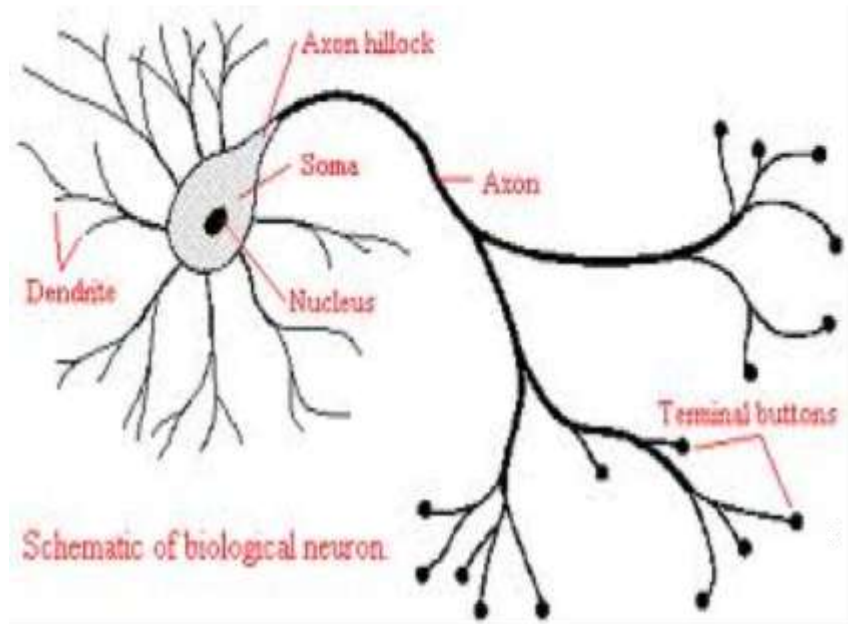
- This happens automatically without conventional logic (i.e. flow charts or sequential steps) even in the presence of other obscuring information.

- In our everyday activities, we process, classify information to make decisions
  - Physicists & Engineers: is this event signal or background noise?
  - Astronomers: is this blob a star or a galaxy?
  - Doctors: is this patient sick or well?
  - Economists & Bankers: is this company a sound investment or junk?
  - Employers: is this applicant employable or a liability?

The Human brain

- Recognition and Classification activities linked to over ~100,000,000,000 biological neurons arranged in a complex neural network.
- Each neuron has many inputs and only 1 output connected to MANY externals (neurons , muscles, etc)
- A neuron works by processing all it's inputs and if the internal function is satisfied triggers an electric impulse on its output, which is then distributed across the network.

Biological Neuron



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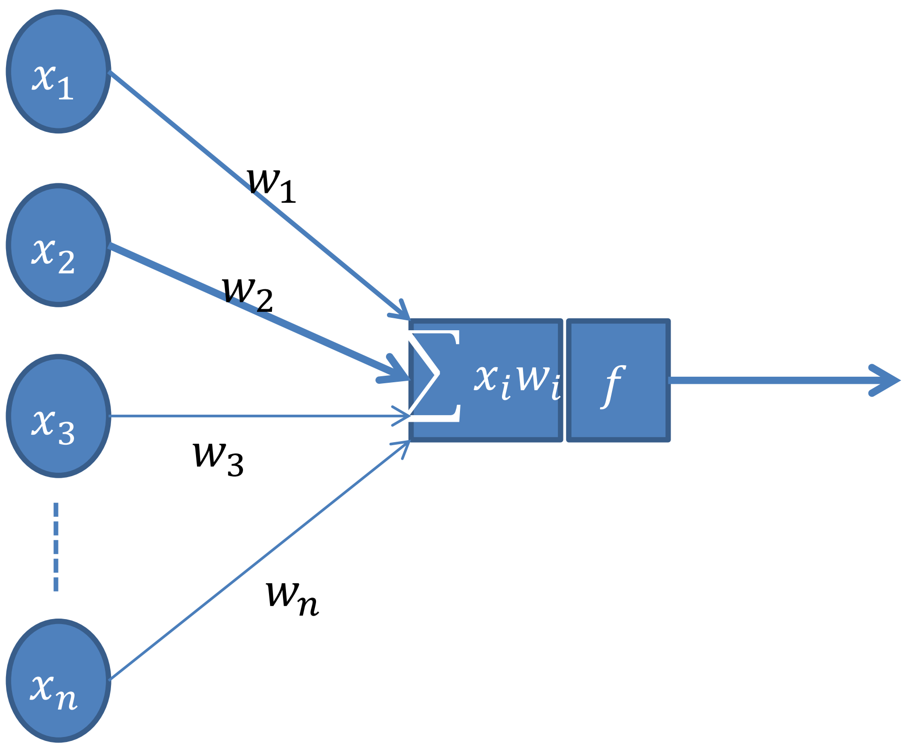
Modeling neurons artificially

Biological → Computational

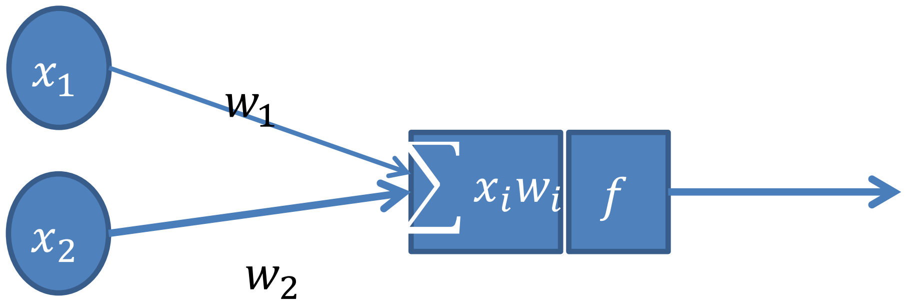
- Dendrites → inputs
- Synapses → weighted input
  - Synaptic strength → Weights
- Nucleus → Summation
  - Firing threshold → Activation-function (Step function)
- Axon → output
  - Bouton

Perceptron



Example perceptron

- Inputs
  - $x_1 = 0.6, x_2 = 1.0$
- Synaptic strengths
  - $w_1 = 0.5, w_2 = 0.7$
- Firing threshold ≥ 1
- Computation
  - Sum of synapses
    - $x_1 w_1 + x_2 w_2 =$
    - $0.6 * 0.5 + 1.0 * 0.7 =$
    - $0.3 + 0.7 = \mathbf{1.0}$



Discussion point: What is the effect of varying the synaptic strengths?

Class exercise 1

- Design the perceptron for implementing binary matching based on 3 different inputs?
  - Case 1: All 3 inputs must be equally present for a match
  - Case 2: Any 2 out of 3 inputs must be present for a match.
- Design the perception for implementing binary matching of two inputs only when either input is present but not when both are present.

Solutions

Exercise 1a

- Case 1
  - Synaptic strengths
    - $w_1 = {}^{1}/_{3}$,
    - $w_2 = {}^{1}/_{3}$,
    - $w_3 = {}^{1}/_{3}$
  - Firing threshold ≥ 1
- Case 2
  - Synaptic strengths
    - $w_1 = {}^{2}/_{3}$,
    - $w_2 = {}^{2}/_{3}$,
    - $w_3 = {}^{2}/_{3}$
  - Firing threshold ≥ 1

Exercise 1b

Input	input	output
0	0	0
0	1	1
1	0	1
1	1	0

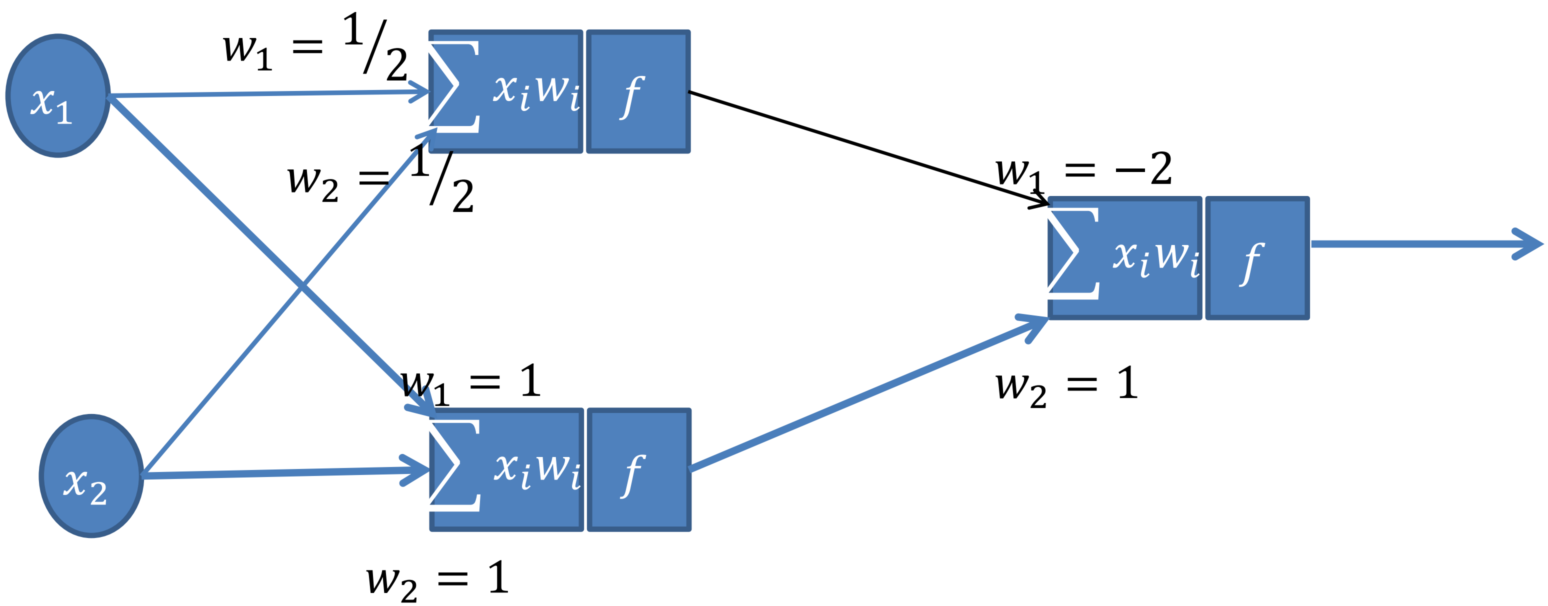
The required solution is not linear separable, so we shall come back to it later..

Neural Network Architecture

- Nodes: Main computational element that raises its output according to a preset activation or transfer function based on the sum up its set of inputs.
  - The activation or transfer function is non-linear in ANNs.
  - Bias nodes: Special nodes that generate a fixed output regardless of inputs
- Connections: Main element responsible for transferring output of a node to another node.
  - On input, each node has a distinct weight for each incoming connection.
- Layers: Nodes are arranged in blocks called layers
  - First layer (block of nodes) is also called the input layer. Nodes in this layer do not perform computations, they just passes information.
  - Last layer is the output layer.
  - Other layers in-between first and last are known as hidden layers, They are responsible for computations
  - The output of each node in a layer is connected as input to ALL nodes of next layer.
  - Each node in a layer receives the outputs of ALL nodes in previous layer.

Example 2: multilayer perceptron

- Firing threshold ≥ 1



Discussion points:

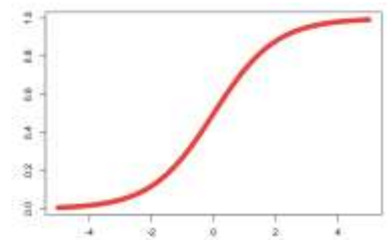
- *Is this the solution to exercise 1b?*
- *How were the weights obtained?*

Neural Networks

Duplicating the working of brain neurons

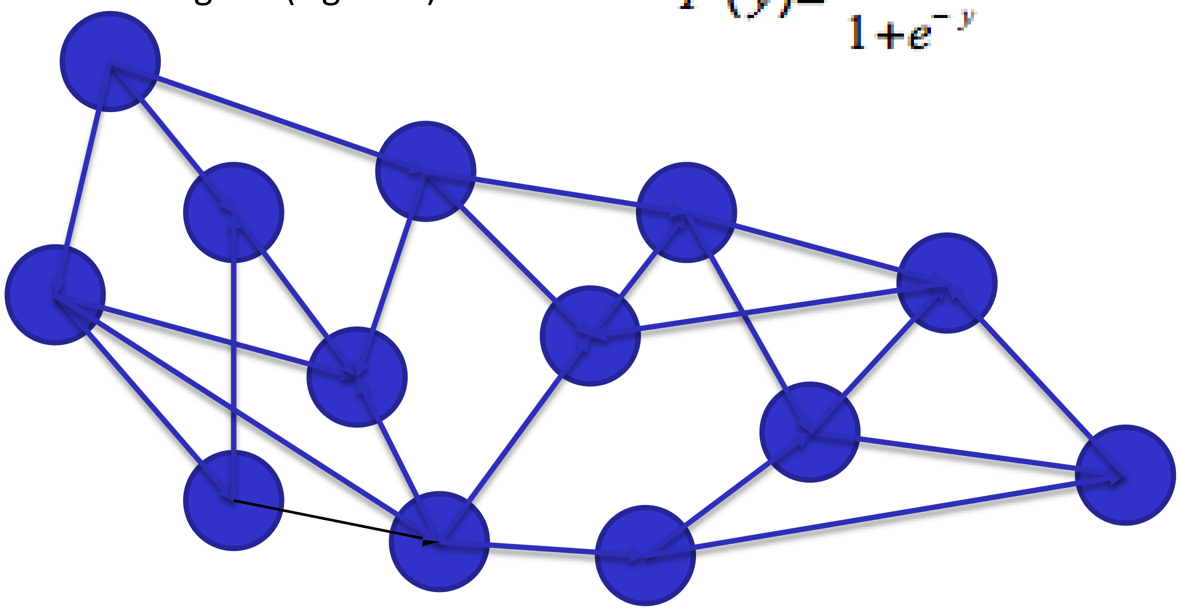
Neuron/node i has many inputs U_j. Apply weights, form $y_i = \sum w_{ij} U_j$ and generate output $U_i = F(y_i) = F(\sum w_{ij} U_j)$

F is thresholding function. Output increases monotonically from 0 to1. Linear central region but saturates at extremes.



Often use logistic (sigmoid) function

$$F(y) = \frac{1}{1+e^{-y}}$$



Sometimes use $F(y) = \tanh(y)$

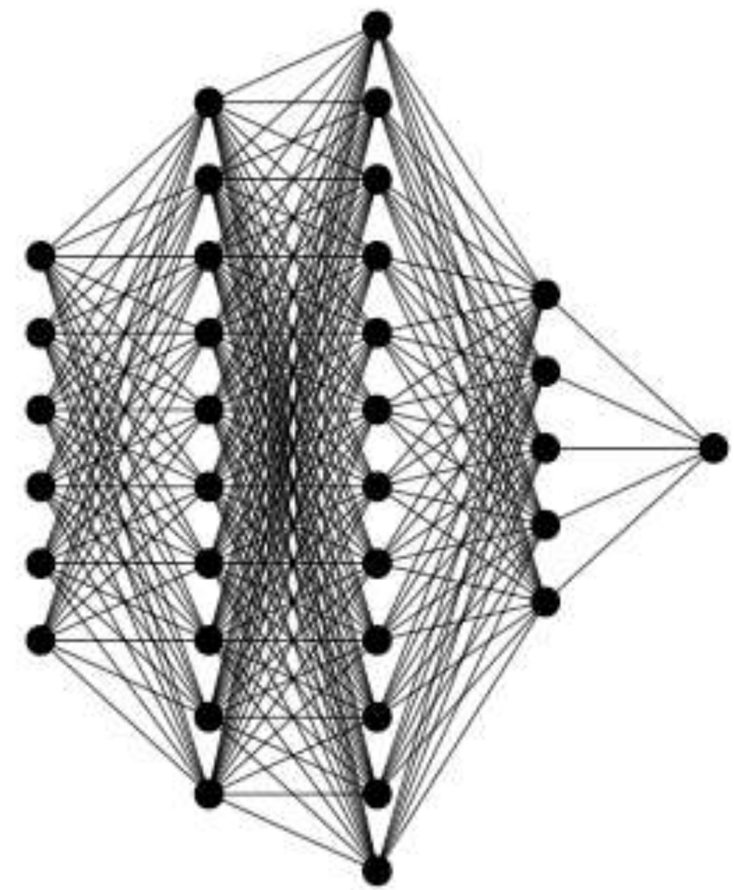
Can simulate networks with various topologies

Type of Neural Networks

- Feedforward Artificial Neural Networks
  - Single layer perceptron
  - Multi-layer perceptron
- Convolutional Neural Network (CNN)
  - Inspired by the visual cortex
  - Unit response can be approximated mathematically by a convolution operation
  - Variants of multilayer perceptron..
  - Mostly used for image and video recognition
- Recurrent neural networks (RNN)
  - Data is propagated in both forward and backward
  - Exhibits temporal memory useful for processing arbitrary sequences of inputs
  - Useful for handwriting recognition, speech recognition and other general sequence processors

Multilayer Artificial Neural Networks

A network architecture for binary classification: recognise data 'events' (all of the same format) as belonging to one of 2 classes.
e.g. Signal or Background? (S or B?)



- Nodes arranged in layers.
- First layer – input
- Last layer –single output, ideally 1 (for S) or 0 (for B)
- In between - 'hidden' layers
- Action is sychronised: all of first layer effects the second (effectively) simultaneously, then second layer effects third, etc

Learning in Neural Networks

- *Just like humans, Neural Networks can also learn in a crudely similar way to how we think biological learning works. That is implemented by changing and/or strengthening the connections of the Synapses.*
- Learning in artificial neural networks occurs through varying the network's weights, with some kind of learning algorithm.
  - There are many different algorithms with their own separate advantages and disadvantages.
  - *The aim is to find a set or matrix of weights which would map any input to a correct output.*

Types of learning

- Supervised learning: During supervised learning, the network is provide with both input and expected output.
- Unsupervised learning: The network is provided with only the inputs and is responsible for determining or classifying the outputs.
- Reinforcement learning: Similar to supervised learning but the network is provided with rewards rather than the expected output. Aim is to maximise reward through trial-and-error process.

The "deep" in deep learning refers to the number of (hidden + output) layers in the network. Training involves the process of back-propagation.

Perceptron learning rule

Steps

- For each weight/input
  - Calculate Error or difference between expected and real output
  - Change in weight is calculated as the product of an abritary learning-rate, the Error and the input
  - Calculate the new weight

- $E = T - U$
- $\Delta w_i = \alpha \, * E \, * x_i$
- (New) $w_i = \ w_i + \ \Delta w_i$
- Where
  - E = error
  - T = Target output
  - U = actual output
  - α = Learning rate
  - x_i = input
  - w_i= weight of input

ANN Deep Learning using samples of known events

- Present events whose type is known: has a desired output T, which is 0 or 1. Call the actual output U.
- Define 'Badness' $B = \frac{1}{2}(U-T)^2$. "Training the net" means adjusting the weights to reduce total (or average) B.
- Strategy: change each weight w_{ij} by step proportional to $-dB/dw_{ij}$.
- Do this event by event (or in batches, for efficiency).
- All we need do is calculate those differentials... start with final layer and work backwards ('back-propagation')

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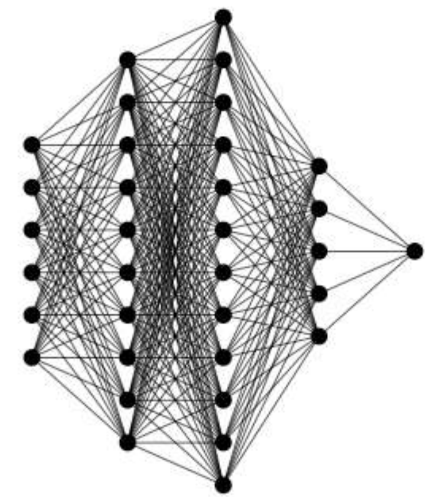
For a single event, let U be the output given by the net and T be the desired outcome.
Define Badness $B = \frac{1}{2}(U - T)^2$
Strategy: adjust all network weights w by an amount $-\alpha \frac{\partial B}{\partial w}$
α is a small fixed number
Consider a weight in the final layer, w_{1l} (1st index 1 as only 1 output node).

$$U = U(\sum_l w_{1l} U_l) \qquad U(y) = \frac{1}{1+e^{-y}} \qquad U'(y) = U(1-U)$$

$$\frac{\partial B}{\partial w_{1l}} = (U-T)\frac{\partial U}{\partial w_{1l}} = (U-T)U(1-U)U_l$$



Now consider the penultimate layer, l'

$$\frac{\partial B}{\partial w_{ll'}} = (U-T)\frac{\partial U}{\partial w_{ll'}} = (U-T)U(1-U)w_{1l}\frac{\partial U_l}{\partial w_{l'l'}}$$

$$= (U-T)U(1-U)w_{1l}U_l(1-U_l)U_{l'}$$

Now l''

$$\frac{\partial B}{\partial w_{l'l''}} = (U-T)U(1-U)\sum_l w_{1l}U_l(1-U_l)w_{ll'}U_{l'}(1-U_{l'})U_{l''}$$

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Performance analysis

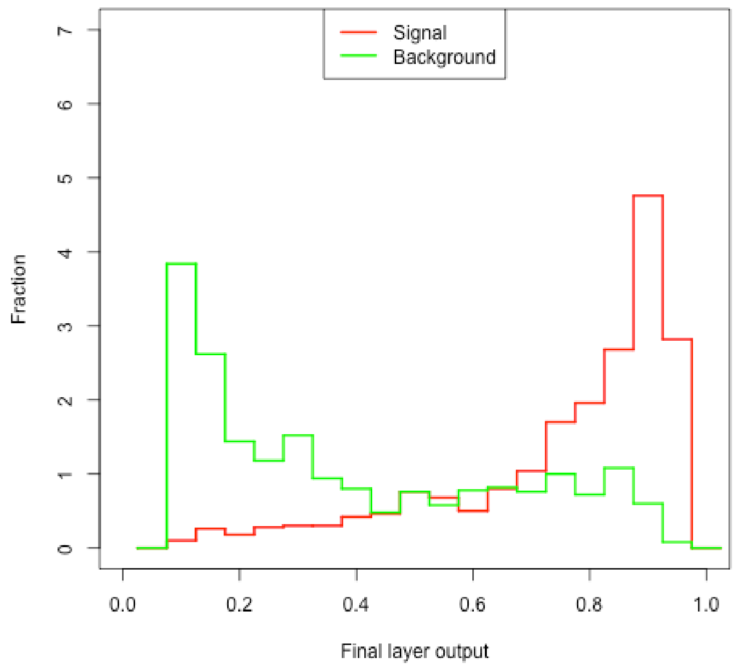
	Actual Positive	Actual Negative
True	True Positive (TP)	False Positive (FP)
False	False Negative (FN)	True Negative (TN)
	Positives (P)	**Negatives (N)**

P = TP + FN
N = FP + TN

Analysis

- Precision $= \frac{TP}{TP+FP}$
- Accuracy $= \frac{TP+TN}{P+N}$
- Sensitivity $= \frac{TP}{P}$
- Specificity $= 1 - \frac{FP}{N}$

Performance: Output histograms



After training - over the whole training sample many times - the outputs from the Signal and Background samples will look something like this

Select signal by requiring U>cut

Small cut value: high efficiency but high background

Large cut value: low background but low efficiency

$$Background = \frac{FP}{N} \text{ and } Signal = \frac{TP}{P}$$

Exactly where to put the cut depends on

(i) The penalties for Type I and Type II errors

(ii) The prior probabilities of S and B

Note the actual shape of the histograms means nothing. Any transformation of the x-axis does not affect the results

Reminder:
Type I error: excluding a signal event
Type II error: including a background event

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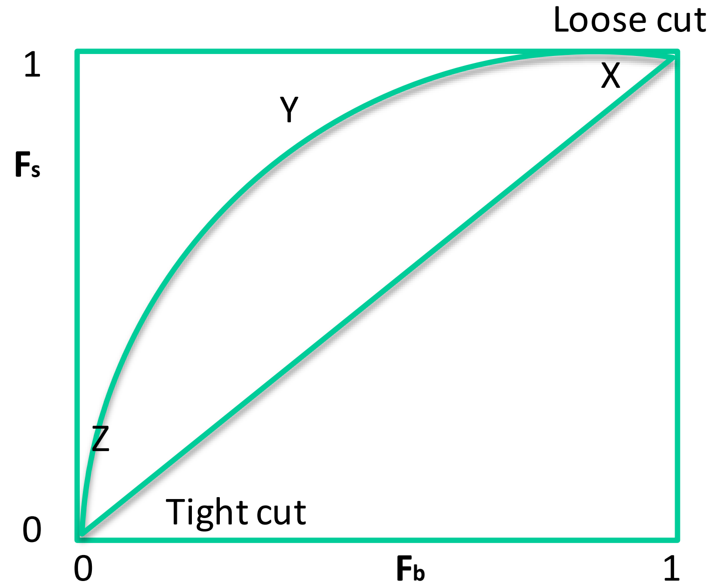
$$X\text{-}axis = \frac{FP}{N} \text{ and } y\text{-}axis = \frac{TP}{P}$$

Performance: ROC* plots



Plot fraction of background accepted against fraction of signal accepted, sliding the cut from 0 (nothing) to 1 (everything)

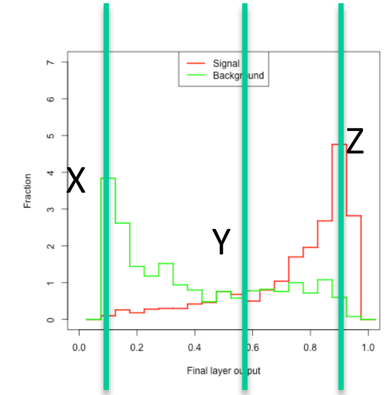
(Note that conventions vary on how to do this)

If net is working, background falls faster than efficiency

No discrimination gives 45 degree line

The bigger the bulge, the better

To draw ROC plot can use histograms, or go back to raw data, rank it according to the output (use R function order), and step through it



*Receiver Operating Characteristic

Training, over-training, testing, validating

Network is trained on the sample, and then re-trained, and then re-re-trained…getting better all the time, as measured by $\sum(T_i-U_i)^2$

An ‘over-trained’ network will select peculiarities of individual events in the sample. Improved performance on training sample but worse performance on other samples

Recommended procedure: have separate training sample (about 80% of data) and testing sample (remaining 20%). Train on training sample until performance on testing sample stops improving
Easy to do if you have lots of samples - which is generally the case for large Monte Carlo samples but not for real data

Validating. Given output X, what can you say about probability of S or B? (i.e. those histograms) Separate sample needed for validation.

Or cross-validation. For each event, train on the rest of the sample and compare truth and prediction, avoiding bias. (If too slow, use sub-samples ‘K-fold cross validation’)

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Warning! Language ambiguities

- Signal Efficiency

  Fraction of signal events remaining after the cut

- Background Efficiency

  (i) Fraction of background events remaining after the cut, OR
  (ii) fraction of background events removed by cut

- Contamination (or Contamination probability)

  (i) Fraction of background events remaining after cut
  OR (ii) fraction of selected events which are background

- Purity

  Fraction of selected events which are signal

- True positive rate

  Same as signal efficiency - not purity

- False positive rate

  Same as background efficiency (i) - not Contamination

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Neural Network Regression

Not considered here but trivial extension -

Desired output not simple true/false but numeric

Examples:

- House price from location, no. of rooms, etc
- Pupil progress from past performance+background

Train to minimise $^1/_2\ (T-U)^2$, test, predict as before, but T is a (scaled) number, not just 0 or 1.

NN classification is just a subset of NN regression

Now Lab work!!

Lab Problem

Camel

Dromedary

- Tell a camel from a dromedary:
- Given 5 inputs, and events of 2 types:
- either 1-2-3-2-1 (+ noise) or 0-4-1-4-0 (+noise)

ro

The camel has a single hump;
The dromedary , two;
Or else the other way around.
I'm never sure. Are you?

Ogden Nash

3 data samples to work on:

Download from http://barlow.web.cern.ch/barlow/Sample1.txt etc

First column is 0 or 1 for C or D

sample1
0 -0.05997873 3.881889 1.060744 4.022852 -0.05597012
1 0.881978 2.055923 3.158514 1.972982 1.190973
0 0.07778947 3.950015 0.9496442 3.976893 0.04745127
1 0.9759833 2.03223 2.990049 2.017683 1.062813
0 -0.001502924 3.862673 0.8942838 4.020337 -0.02683437
0 0.07309237 3.982063 1.043907 3.860677 -0.1394614
1 1.075466 1.973227 3.115331 1.935488 0.9712817
…

all ad
noise

sample2
0 1.587052 4.715568 -0.8595715 1.504009 2.145417
1 2.52062 2.682234 3.909693 0.2611399 0.3924642
1 -0.5450664 -1.449915 -0.2813677 4.057942 0.9299015
0 -1.047951 4.223808 3.068302 9.673196 3.915838
1 -2.863264 1.250906 0.293735 -0.2080808 -0.6673748
1 -0.2963963 2.988054 1.449716 2.326187 -0.5594592
1 4.581936 6.263028 5.522227 3.473845 -2.042601
…

ge ad
noise

sample3
0 -0.7064082 3.266121 0.2208592 4.825086 0
0 0.912854 3.48706 0.3057296 4.402847 -0.07224356
0 0.2116067 4.659067 0.9210807 4.95437 -0.7723788
1 0.7854812 2.079436 1.336324 2.16746 0.5728526
0 0.1380971 0 1.143737 4.632105 0.2767737
0 0.4398898 4.436032 1.55822 3.477277 0.3308824
1 0 1.320041 3.46353 1.087296 1.499402
…

um a
plus some

Download the datasets

http://barlow.web.cern.ch/barlow/Sample1.txt

http://barlow.web.cern.ch/barlow/Sample2.txt

http://barlow.web.cern.ch/barlow/Sample3.txt

Sample code for writing your own ANN -

```
ALPHA=0.05  #  learning parameter

nodes=c(5,7,10,1)       # 5 inputs, 2 hidden layers, with 7 and 10 nodes , 1 output
nlayers=length(nodes)  -1         # 3  sets of weights

net=list() # set up empty list
#  net[[ j ]] holds weight matrix feeding nodes of layer j+1 from nodes in layer j

#   make weights and fill with random numbers
for(j in 1:nlayers) net[[ j ]] <- matrix(runif(nodes[  j ]*nodes[  j +1 ]),nodes[j+1],nodes[j])

netsays <- function(x) { #  Returns net output for some input vector x
      for(j in 1:nlayers) x <- 1/(1+exp(-net[[  j ]] %*% x))
      return(x)
       }

 backprop <- function(layer,n1,n2,factor){ # recursive function  used for back-propagation
       if(layer>1) for(n in 1:nodes[layer-1])
            backprop(layer-1,n2,n,factor*net[[layer]][n1,n2]*r[[iayer]][n2]*(1-r[[layer]][n2]))
       net[[layer]][n1,n2]  <<-  net[[layer]][n1,n2]  - ALPHA*factor*r[[layer]][n2]
       }

netlearns <- function(x,truth) { # like netsays but changes weights
       r <<- list()   # to contain the outputs of all nodes in all layers
       r[[1]] <<- x     # the input layer
       for(layer in 1:nlayers) r[[layer+1]] <<- as.vector(1/(1+exp(-net[[layer]]  %*% r[[layer]])))
       u <- r[[nlayers+1]] # final answer, for convenience
       for(n in 1:nodes[nlayers]) backprop(nlayers,1,n,(u-truth)*u*(1-u))
       }
```

OR Use the R package

Package by S. Fitsch et al

- Installation *(To be performed only once)*

  install.packages("neuralnet")

- Loading *(To be performed once per session)*

  library(neuralnet)

- Obtaining help *(Please read carefully)*

  help(neuralnet)

Sample R code

```
library(neuralnet)

input1<- c(0,0,1,1)
input2<- c(0,1,0,1)
truth<- c(0,1,1,0)

df <- data.frame(truth,input1,input2)
nnet<-
neuralnet(truth~input1+input2,df,c(4,2))

plot(nnet)

test=compute(nnet,t(c(1,1)))
test$net.result
```

https://cran.r-project.org/web/packages/neuralnet/neuralnet.pdf

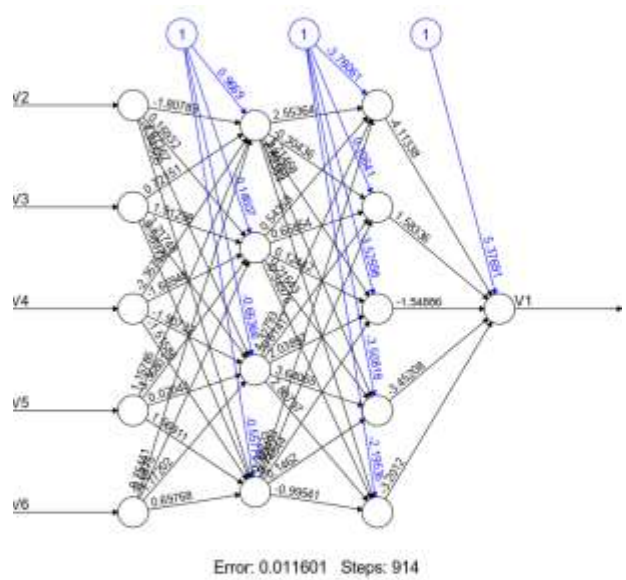
Another example

```
library(neuralnet)
df <- read.table("http://barlow.web.cern.ch/barlow/Sample1.txt",header=FALSE)
print(head(df))
V1 <- df[,1];V2 <- df[,2];V3 <- df[,3]
V4 <- df[,4];V5 <- df[,5];V6 <- df[,6]
nnet<-neuralnet(V1~V2+V3+V4+V5+V6,df,c(4,5), lifesign="full",
          algorithm="backprop", learningrate=0.05, linear.output=FALSE)

plot(nnet)

test=compute(nnet,t(c(0,3,1,4,1)))
test$net.result

test=compute(nnet,t(c(1,2,3,2,1)))
test$net.result
```

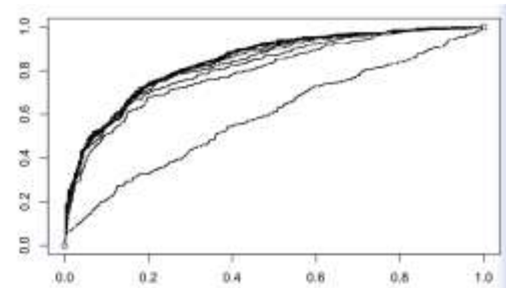


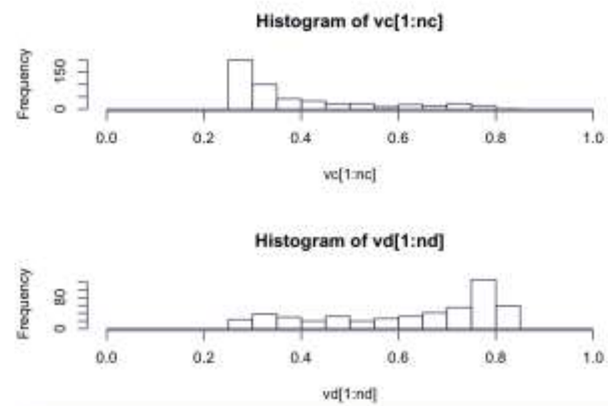
Some (possibly) useful R stuff

```
sample <- read.table(“Sample1.txt”,header=FALSE)
Nsample <- dim(sample)[1]
print(head(sample))
for (i in 1:Nsample) {print(sample[i,1]); print(sample[i,-1])}
plot(c(0,1),c(0,1))
v <- netsays(t(sample[,-1]))
p <- sample[order(v),1]
nc <- sum(sample[,1]==0)
nd <- Nsample-nc
nnc <- nc
nnd <- nd
for (i in 1:length(p)) {if(p[i]==1) {nd <- nd-1} else {nc <- nc-1}
 points(nc/nnc,nd/nnd,pch=‘.') }

vc <- rep(0,nnc)
vd <- rep(0,nnd)
nc <- 0
nd <- 0
for (i in 1:Nsample){
   itype <- sample[i,1]
   isay <- netsays(as.numeric(sample[i,-1]))
   if(itype==0) {nc <- nc+1;vc[nc] <- isay} else {nd<- nd+1;vd[nd] <- isay}
}

hc <- hist(vc,breaks=seq(0,1,.05))
hd <- hist(vd,breaks=seq(0,1,.05))
```





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Time to work on your own!!

Attempt all questions..

Lab Session

6 Questions

1. What is the effect of varying the learning parameter α?
2. What is the effect of using more, or fewer, nodes in the hidden layers?
3. What is the effect of using more, or fewer, hidden layers?
4. What is the effect of pre-processing the input data to give each data input mean zero and standard deviation 1? If you feel strong enough, also try Principal Component Analysis
5. *What is the effect of using a tanh function rather than a sigmoid ? (Use different differential)*
6. What happens if a network trained on one sample is applied to another sample?

The 'what is the effect of…' questions, refer to both the eventual separation and the training time. Sample 2 and sample 3 can be used for this - sample 1 is too easy.

More questions

Either write your own code, or use the neuralnet package to set up a network with 2 hidden layers, with 8 and 5 nodes

Train and test with the file sample1. It should achieve perfect separation. If not, keep trying till you do.

Train and test with sample2. Draw ROC plots to show the performance. Make sure you are not over-training.

Now try sample3 in the same way.

When done, Prepare a couple of slides to show your results, for presentation in the round-up session.

if you still have time, tackle any of the other problems that look interesting.