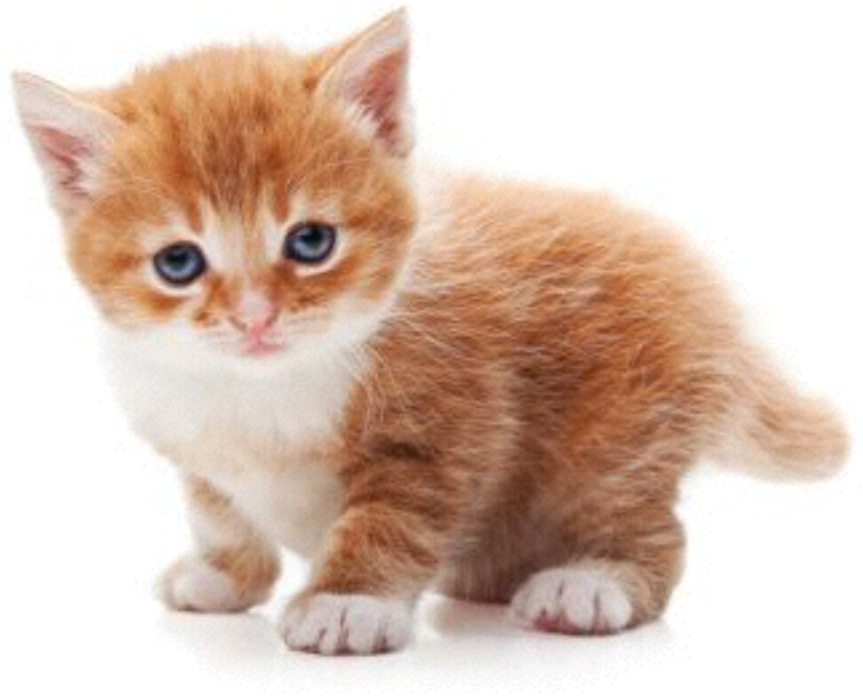
# Artificial Neural Networks

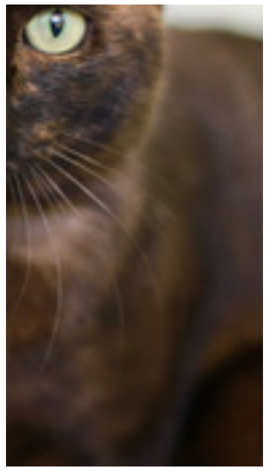
Roger Barlow

University of HUDDERSFIELD
International Institute for Accelerator Applications

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



## Classification

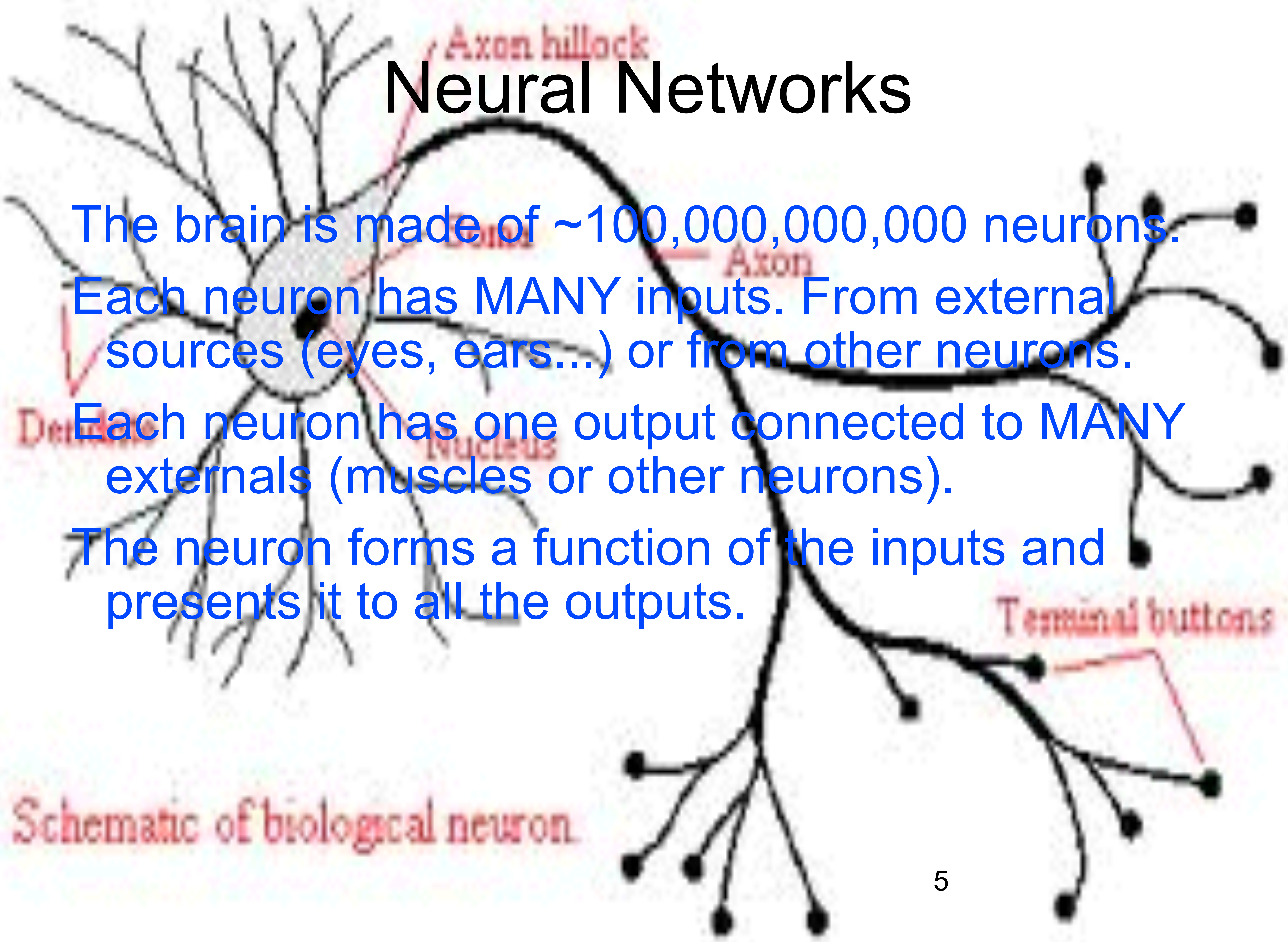
We recognise and classify objects -
- quickly
- robustly
- reliably

and we don’t use conventional logic (i.e. flow charts)

This attacks a very general statistics/data problem:

Physicist: is this event signal or background
 is the track a muon or a pion?
Astrnomer: is this blob a star or a galaxy?
Doctor: is this patient sick or well?
Banker: is this company a sound investment or junk?
Employer: is this applicant employable or a liability?

# Neural Networks



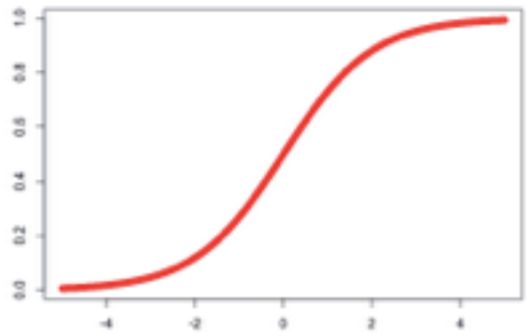
- The brain is made of ~100,000,000,000 neurons.
- Each neuron has MANY inputs. From external sources (eyes, ears...) or from other neurons.
- Each neuron has one output connected to MANY externals (muscles or other neurons).
- The neuron forms a function of the inputs and presents it to all the outputs.

# Artificial Neural Networks

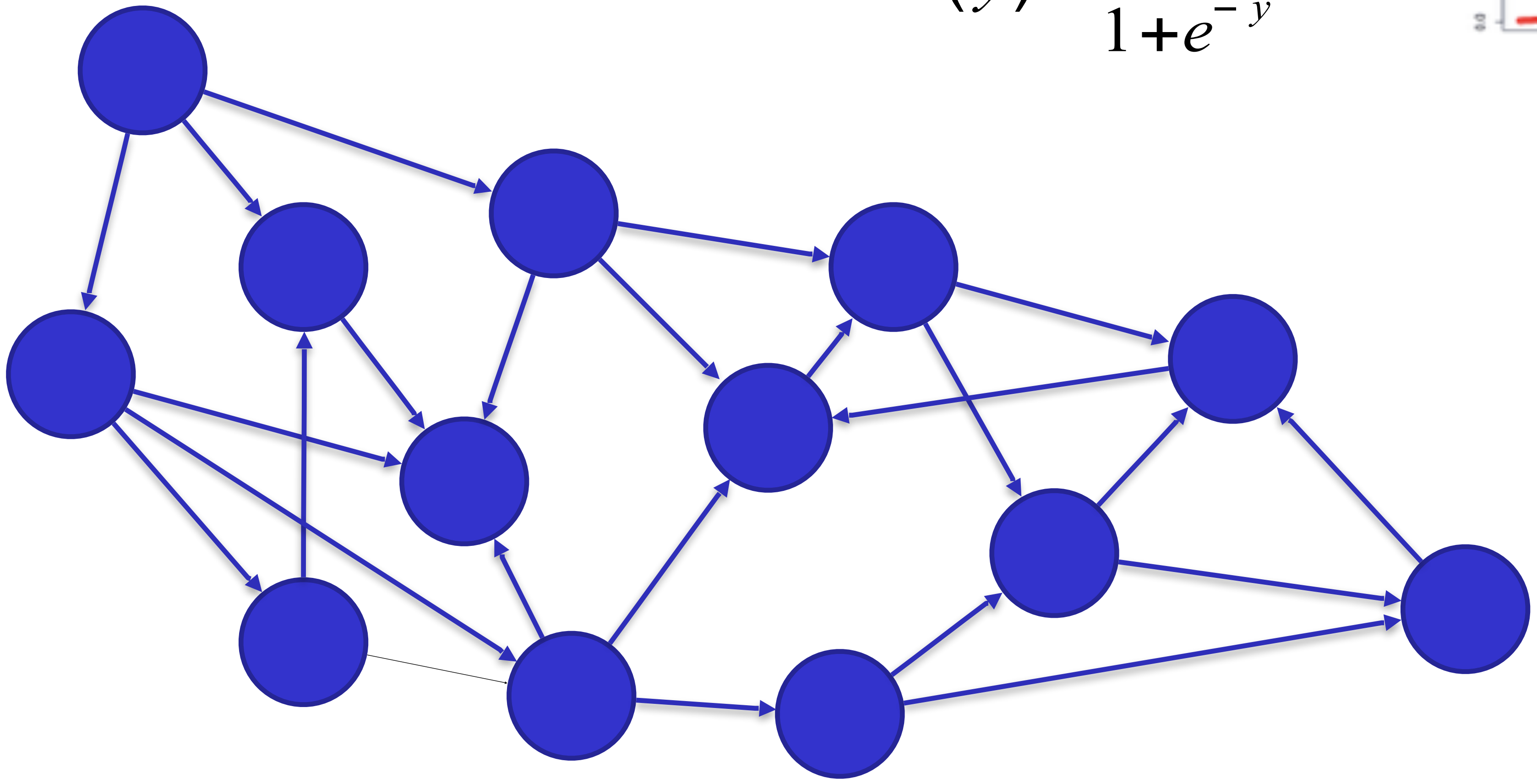
Tries to duplicate that processing in software

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

$F$ is thresholding function. Want output to increase monotonically. Linear central region but saturates at extremes.



Often use logistic (sigmoid) function $F(y) = \dfrac{1}{1+e^{-y}}$

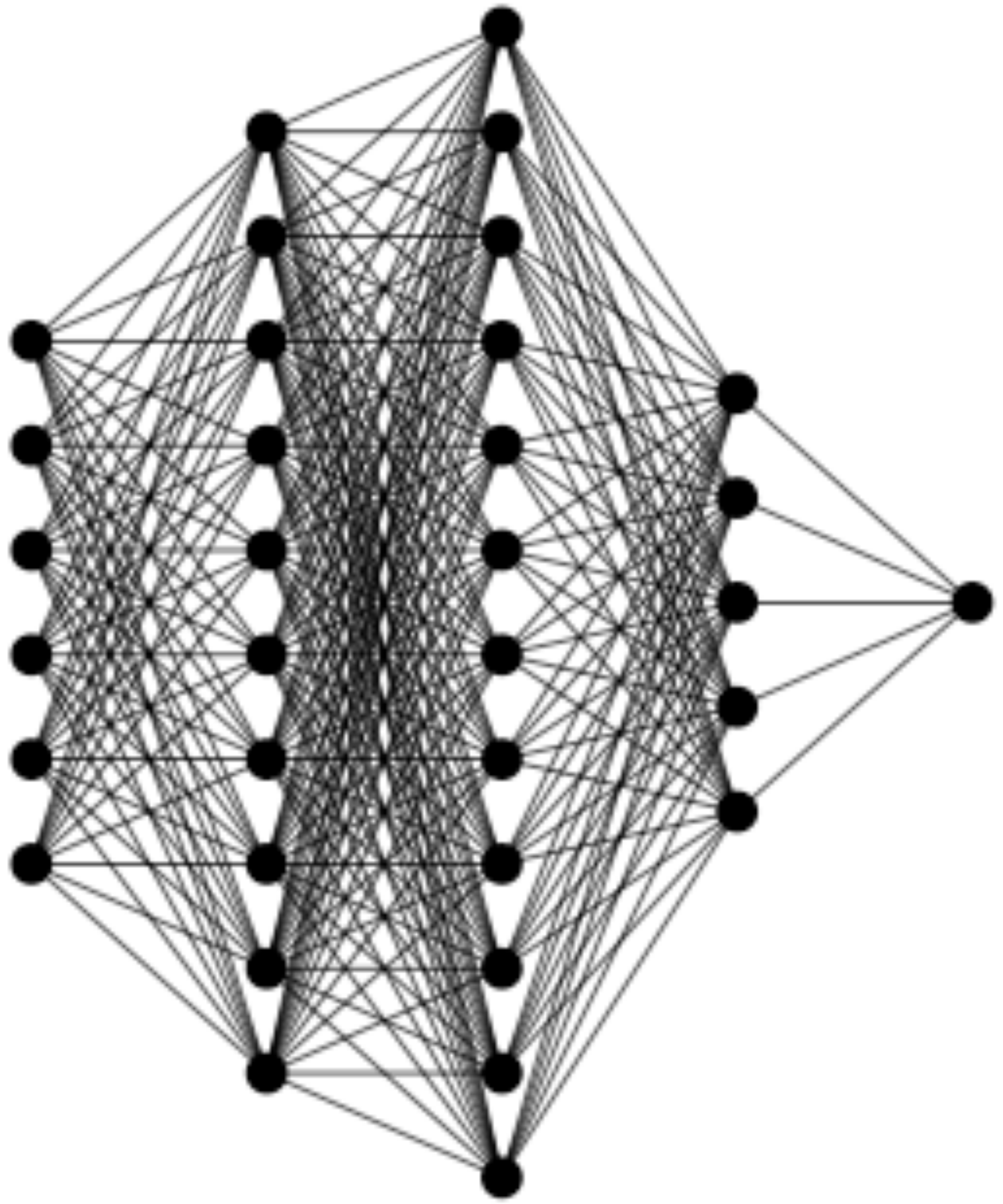


Sometimes use $F(y) = \tanh(y)$

Can simulate networks with various topologies

# The Multilayer Perceptron

A system for binary classification: recognise data ‘events’ (all of the same format) as belonging to one of 2 classes.
e.g. signal and background, S and 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

# How do we set the weights? Training:use samples of known events

Present events whose classification 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.

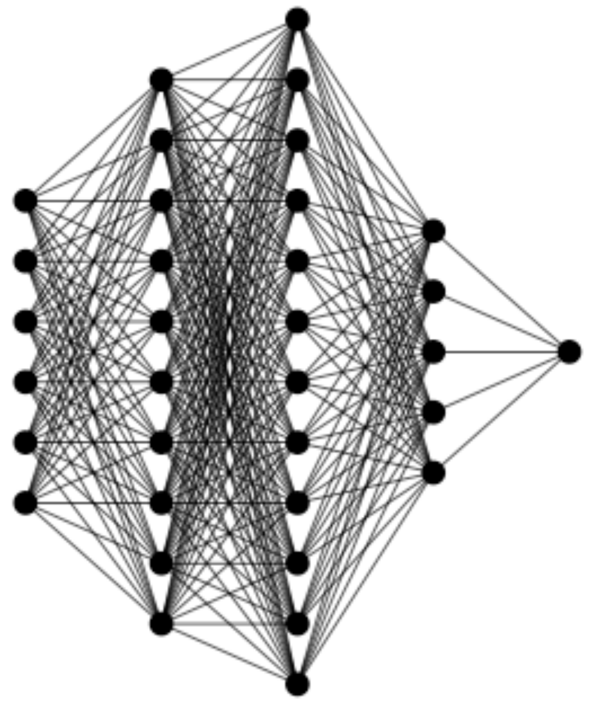
Strategy: change each weight $w_{ij}$ by step proportional to $-dB/dw_{ij}$ .

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')

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 $-\alpha\frac{\partial B}{\partial w}$
$\alpha$ 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, $l'$

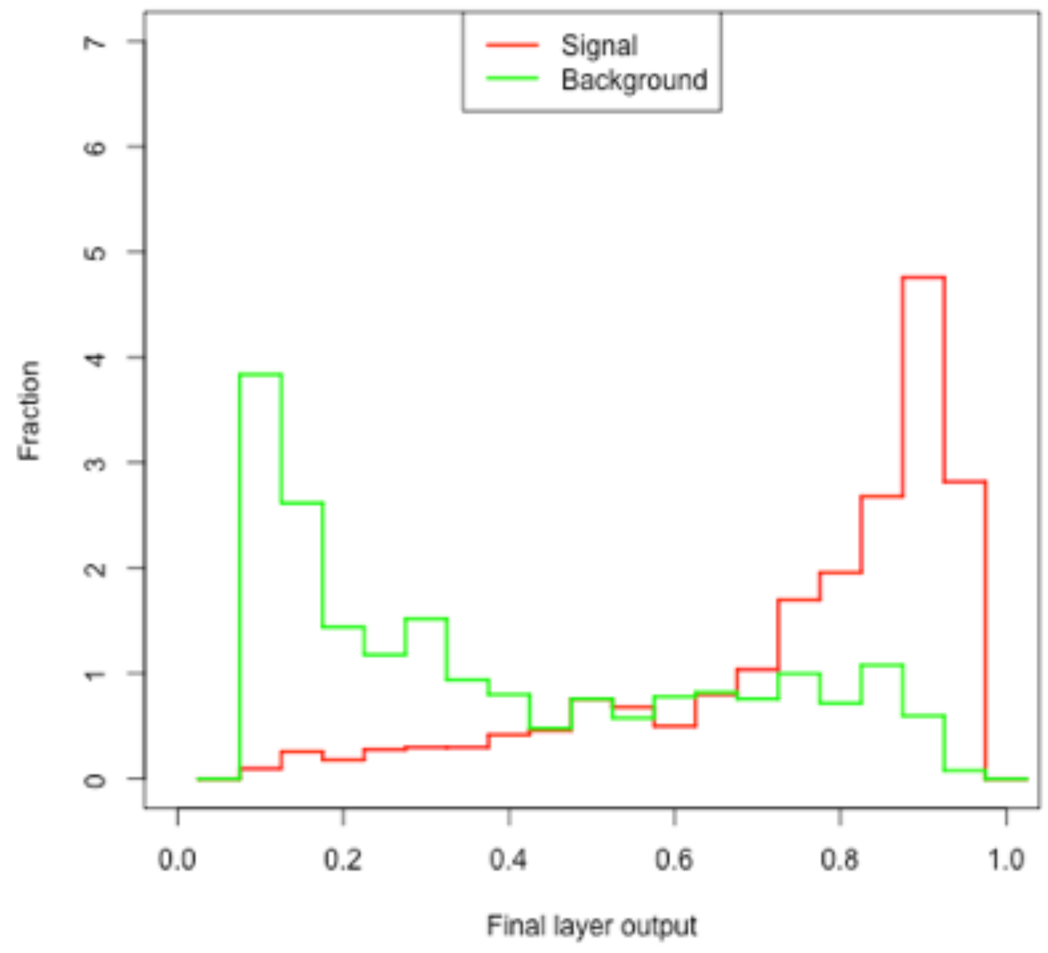
$$\frac{\partial B}{\partial w_{ll'}} = (U-T)\frac{\partial U}{\partial w_{ll'}} = (U-T)U(1-U)w_{1l}\frac{\partial U_l}{\partial w_{l'l'}}$$

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

Now $l''$

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

## Performance: Output histograms



After training the outputs from the S and B samples will look something like this

Select signal by requiring U>cut

Small cut value: high efficiency but high background

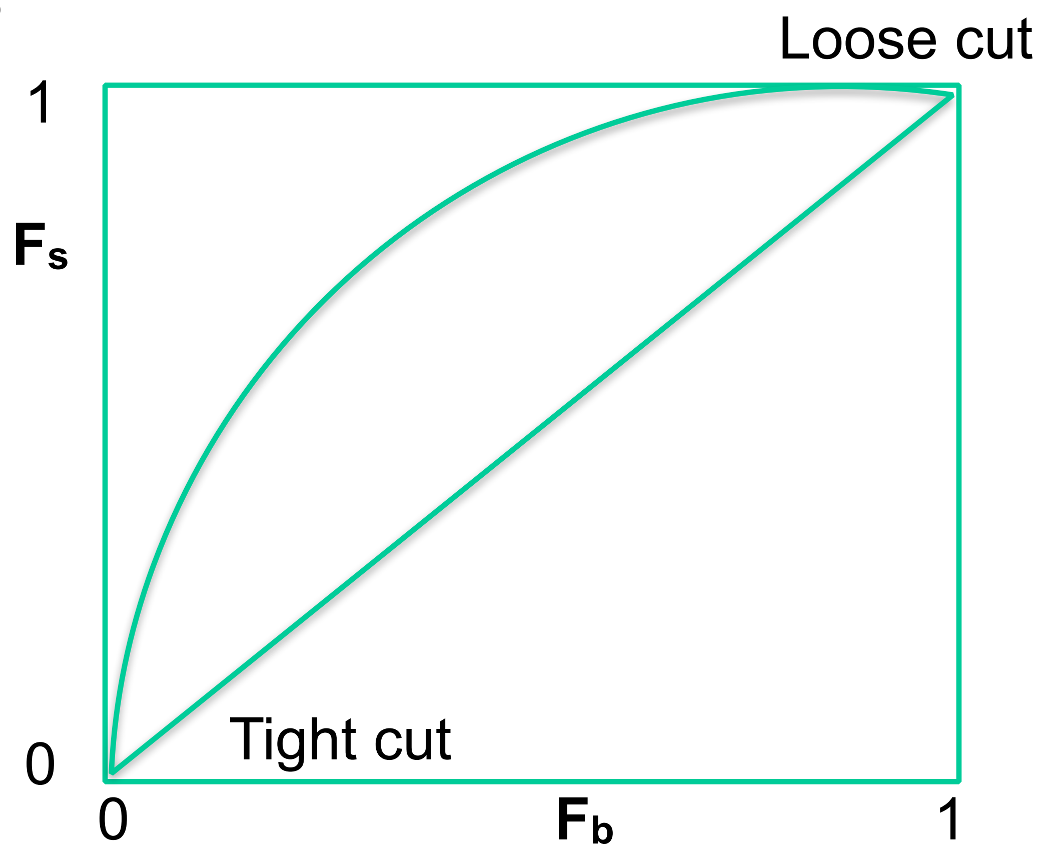
Large cut value: low background but low efficiency

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

## 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 generaly 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’)

## 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*

## Neural Network Regression

Not considered here but trivial extension -

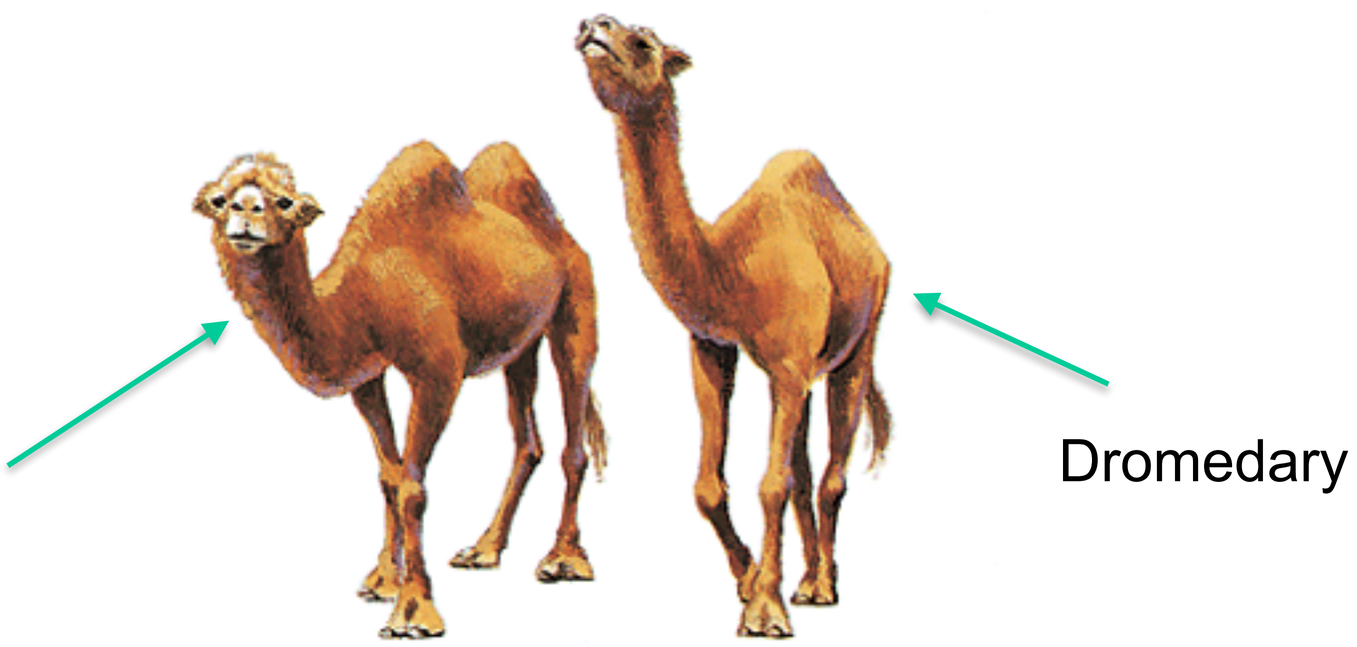
Desired output not simple true/false but numeric

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

NN classification is just a subset of NN regression

# Problem



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 samples to work on:

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

```
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
…

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
…
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
…
```

First column is 0 or 1 for C or D

Small added noise

Large added noise

Medium added noise plus some losses

## Write 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 download Fritsch & Günther's package

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

```
install.packages('neuralnet')
```

*Do this once. It asks you to choose a mirror. Tip - don't choose an https site*

```
library(neuralnet)
```

*Do this once per session*

```
help(neuralnet)
```

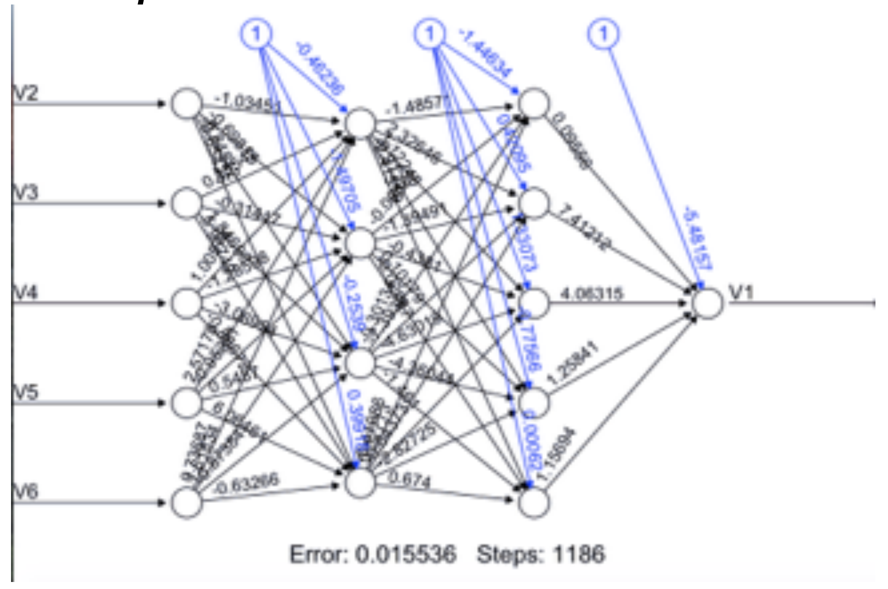
*Just do this! and read it all very carefully, twice*

```
df <- data.frame(truth,input1,input2)
nnet<-neuralnet(truth~input1+input2,df,c(4,5))
```

*Very basic example*

```
nnet<-neuralnet(truth~input1+input2,df,c(4,5),
     lifesign='full',
     algorithm='backprop',
     learningrate=0.05,
     linear.output=FALSE
     )
```

*less basic example*



```
plot(nnet)
```

*Nice picture of net*

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

*how it's used*

# Lab Session

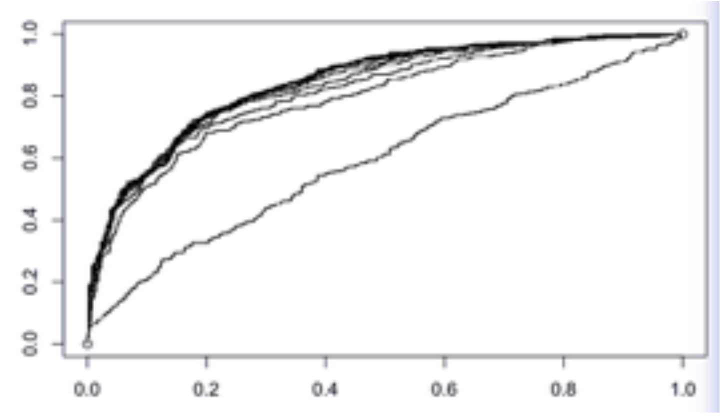
## 8 Questions

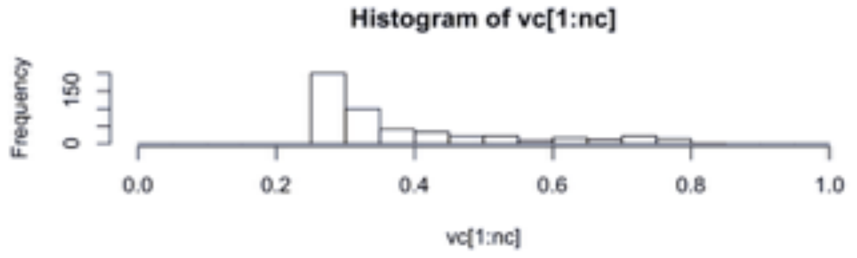
1. What is the effect of varying the learning parameter α?
2. What is the effect of using more, or fewer, nodes in the hidden layers?
3. What is the effect of using more, or fewer, hidden layers?
4. What is the effect of pre-processing the input data to give each data input mean zero and standard deviation 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?
7. Can you do a better job on sample 3 by separating the events with missing data values and analysing them separately?
8. Repeat the analysis using only 4 inputs, omitting input 5. How badly is the separation affected? Is that the same for all 5 inputs?

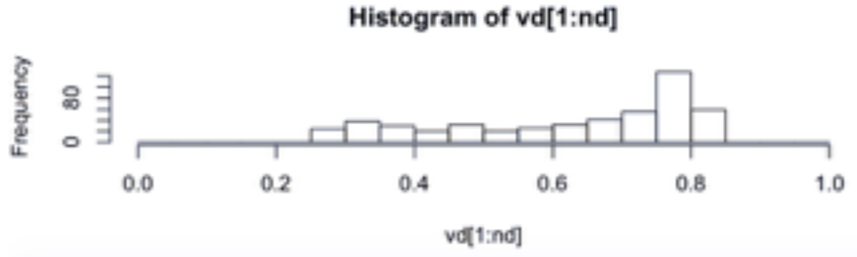
The 'what is the effect of…' questions, refer to both the eventual separation and the training time. Sample 2 and sample 3 can be used for this - sample 1 is too easy.

# Some (possibly) useful R stuff

```
sample <- read.table("Sample1.txt",header=FALSE)
Nsample <- dim(sample)[1]
print(head(sample))

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))
```







## Lab Session

Either write your own code, or download the neuralnet package, as directed

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.

Tackle your allocated question. Prepare a couple of slides to show your results, for presentation in the round-up session.

When you're done, if you've time, tackle any of the other problems that look interesting.