



MACHINE LEARNING IN R:

supervised
classification

“I think we should be very careful about artificial intelligence. If I had to guess at what our biggest existential threat is, it’s probably that. So we need to be very careful,”

Elon Musk

Machine Learning

network, graphs

focus on prediction

weights

learning

generalization

supervised learning

unsupervised learning

large grant = \$1,000,000

nice place to have a meeting:
Snowbird, Utah, French Alps

Statistics

model

focus on inference

parameters

fitting

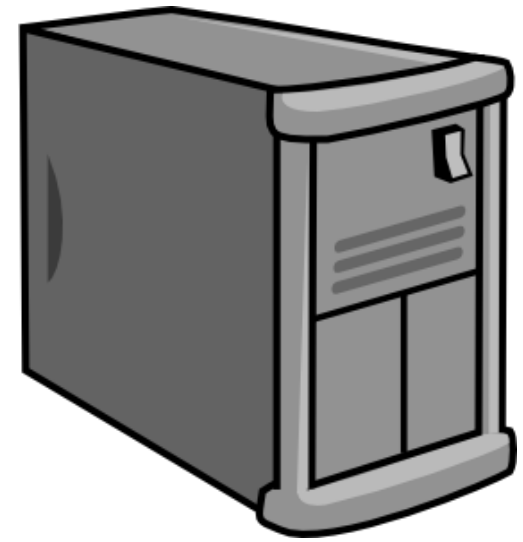
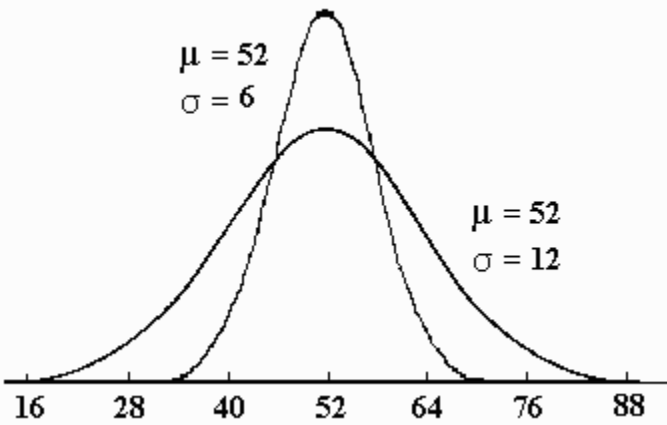
test set performance

regression/classification

density estimation, clustering

large grant = \$50,000

nice place to have a meeting:
Las Vegas in August



Statistics

Machine Learning

T-Test

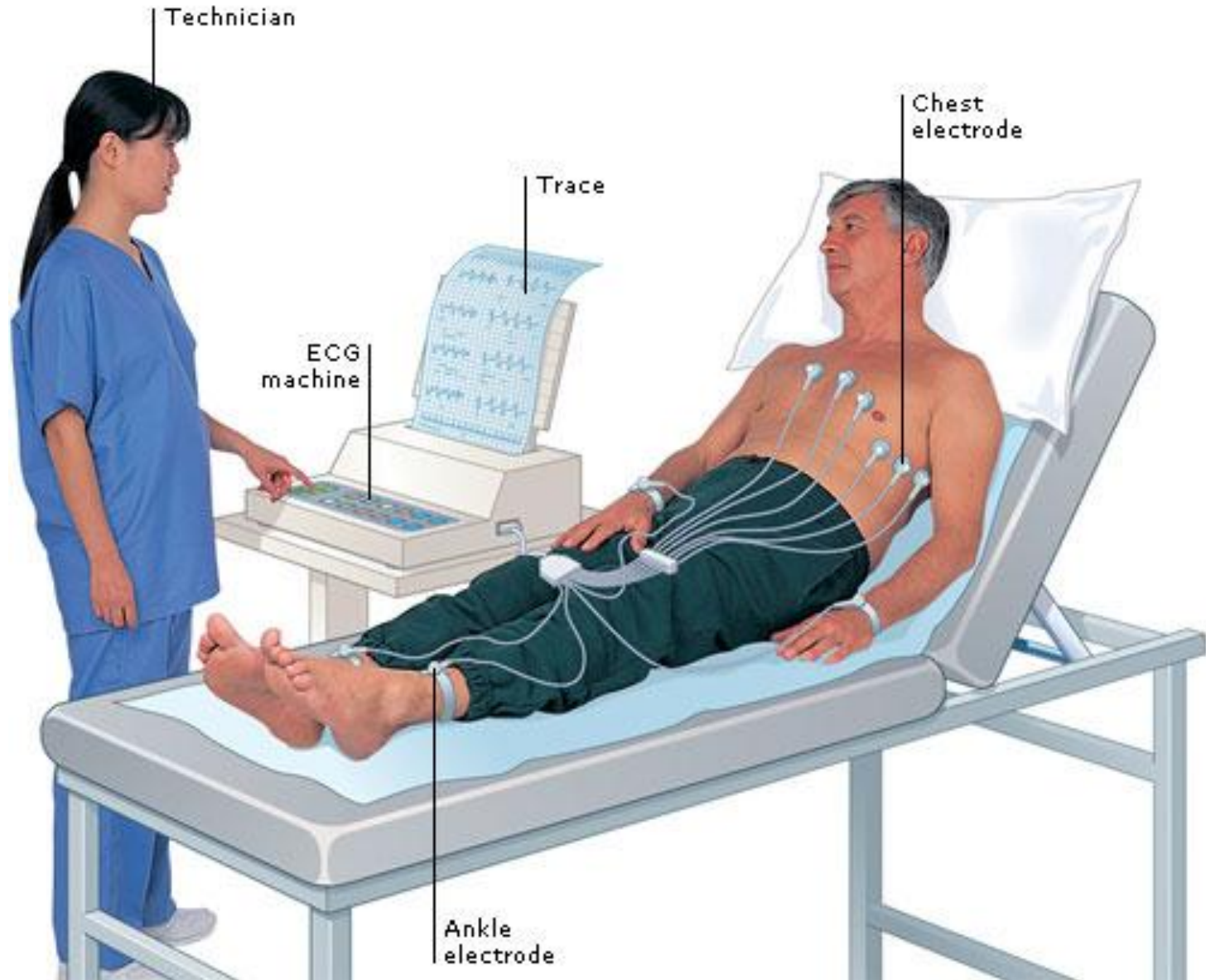
Logistic Regression

Elastic Net

Gradient Boosting

Deep Learning

Arrhythmia Data

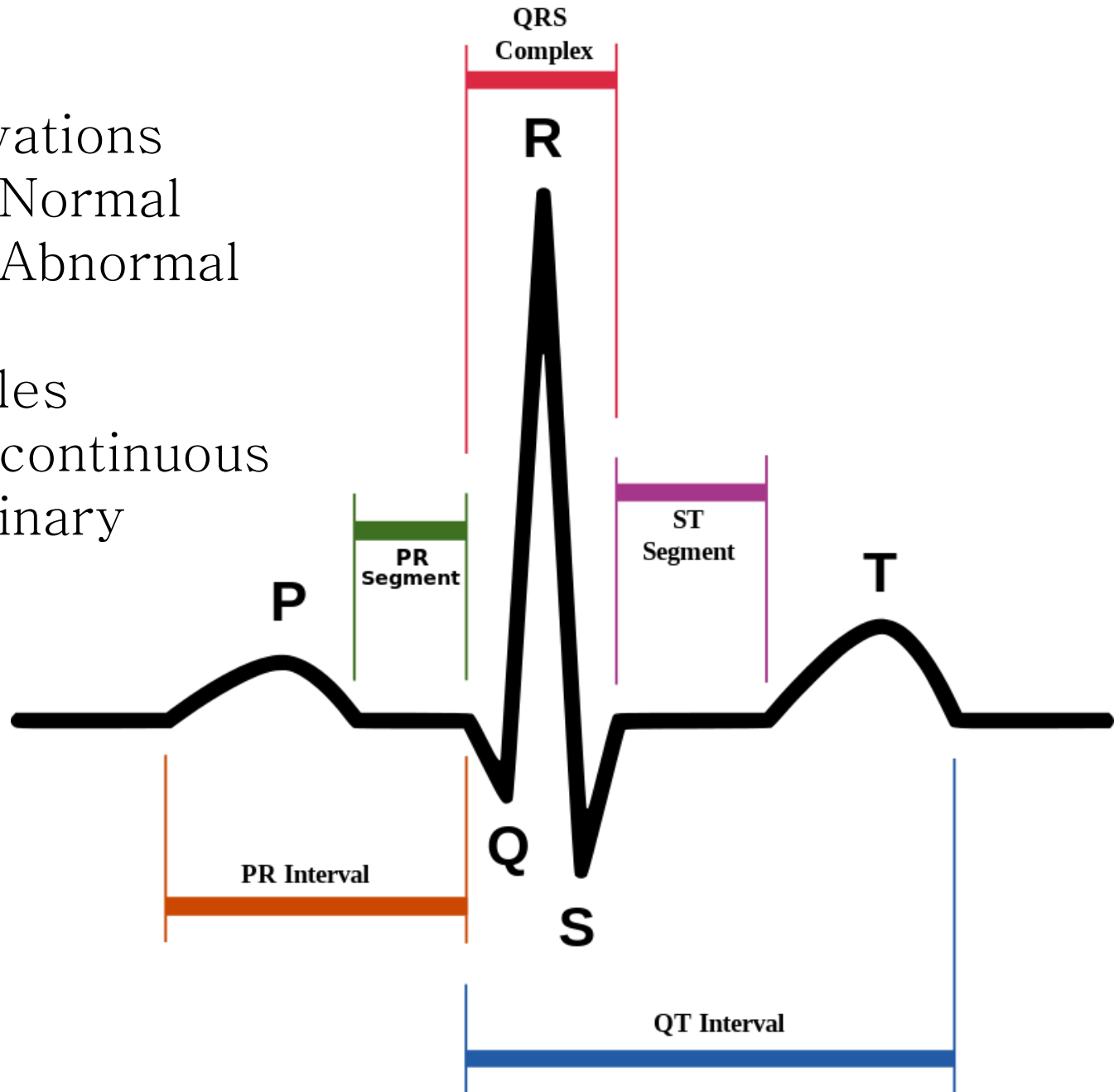


<http://archive.ics.uci.edu/ml/datasets/Arrhythmia>

Data

451 observations
245 Normal
206 Abnormal

263 variables
198 continuous
65 binary



Data pre-processing

```
arrhythmia = read.csv('arrhythmia.csv')

set.seed(120)

# Make folds vector to specify holdout set
folds = sample(1:10, nrow(arrhythmia ), replace = TRUE)
response = arrhythmia$abnormal

# Formula for use in model matrix function
fmla <- abnormal ~ sex + di_width_ragged_r_wave +
di_width_diphasic_derivation_of_r_wave + ...

# Make sparse model matrix
mm = Matrix::sparse.model.matrix( fmla, data =
arrhythmia)
```

Logistic regression

10 events per variable?

Choose 20 'best variables'

```
#fit a logistic regression
glm1 = glm(fmla2,
           data = arrhythmia[folds < 9, , drop = TRUE],
           family = binomial())

#make predictions
p_logistic = predict(glm1,
                     arrhythmia[folds >= 9, ],
                     type = "response")

#get predictive accuracy
auc(p_logistic, response[folds >= 9] )
accuracy(p_logistic > 0.5, response[folds >= 9] )
```

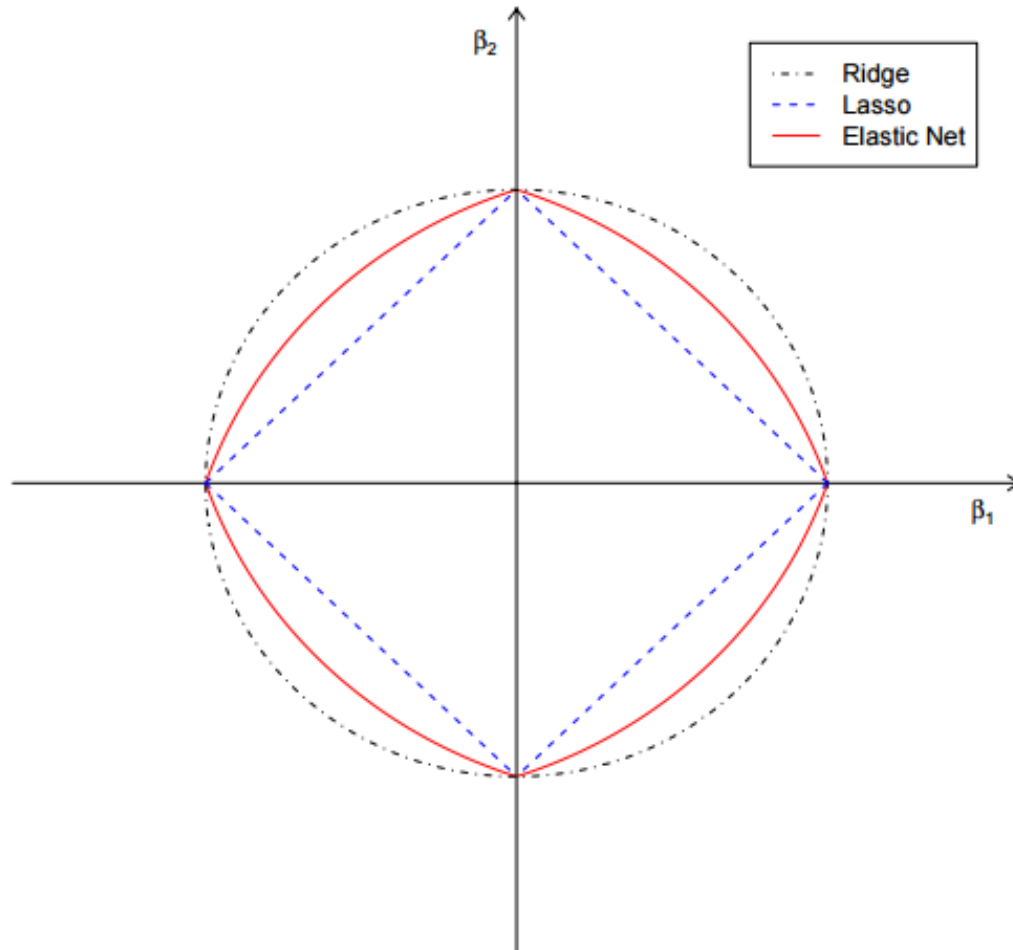
AUC = 70%

THE ELASTIC NET

INTERPRETABLE MODELS
GOOD WHEN $p \gg n$

Elastic Net

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} (\|y - X\beta\|^2 + \lambda_2 \|\beta\|^2 + \lambda_1 \|\beta\|_1)$$



Elastic Net in R

```
library(glmnet)
#fit model on training set
e_net_default = glmnet( x = mm[folds < 9,],
                        y = response[folds < 9],
                        family = "binomial")

#make predictions on test set
p_e_net_default = predict(e_net_default,
                          newx = mm[folds >= 9,],
                          type = "response")

str(p_e_net_default )
# num [1:98, 1:100] 0.467 0.467 0.467 0.467 0.467 ...
# - attr(*, "dimnames")=List of 2
# ..$ : chr [1:98] "11" "12" "15" "17" ...
# ..$ : chr [1:100] "s0" "s1" "s2" "s3" ...
```

Elastic Net in R

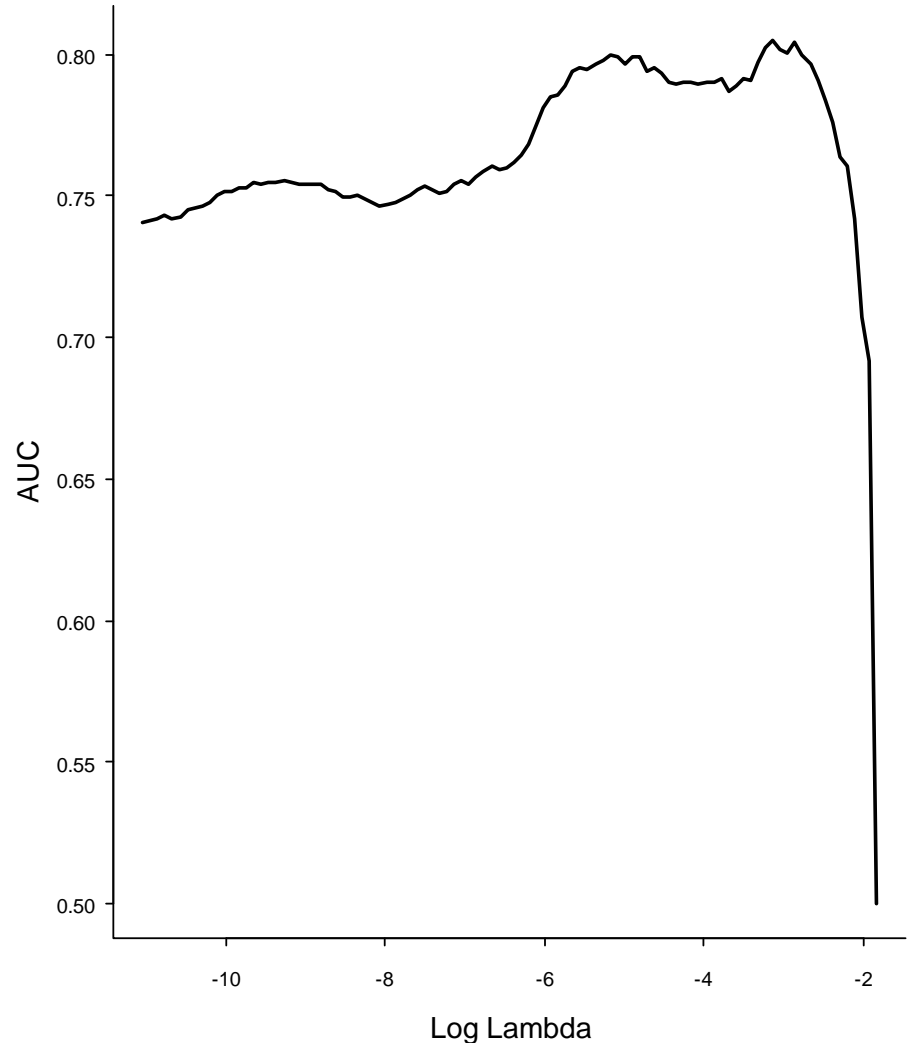
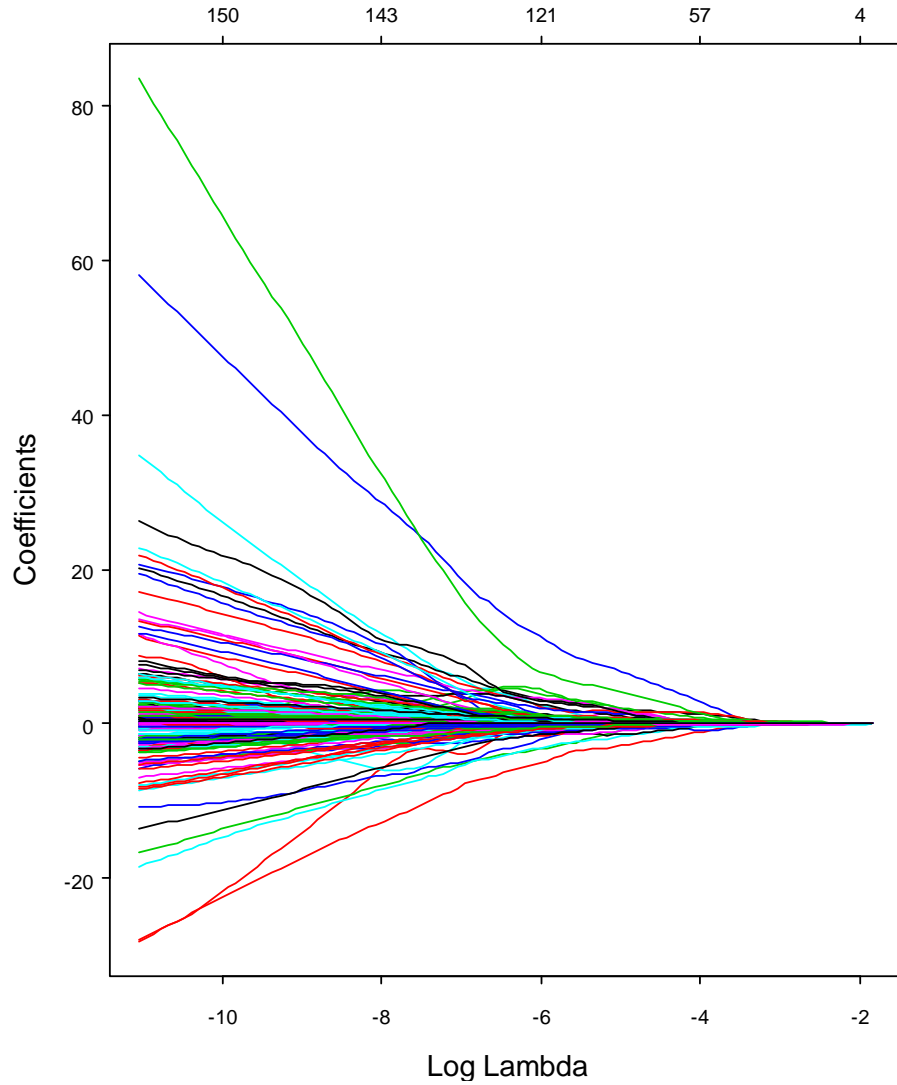
```
#get auc for each prediction
```

```
e_net_default_auc = aaply(p_e_net_default, 2,  
  function(.x) {  
    auc(y = response[ folds >= 9], prob = .x)  
  })
```

```
#plot these results
```

```
par(mfrow = c(1,2))  
plot(e_net_default, xvar = "lambda")  
plot(y = e_net_default_auc ,  
  x = log(e_net_default$ lambda ),  
  xlab = 'Log Lambda',  
  ylab = 'AUC', type = 'l', lwd = 2)
```

Elastic net plots



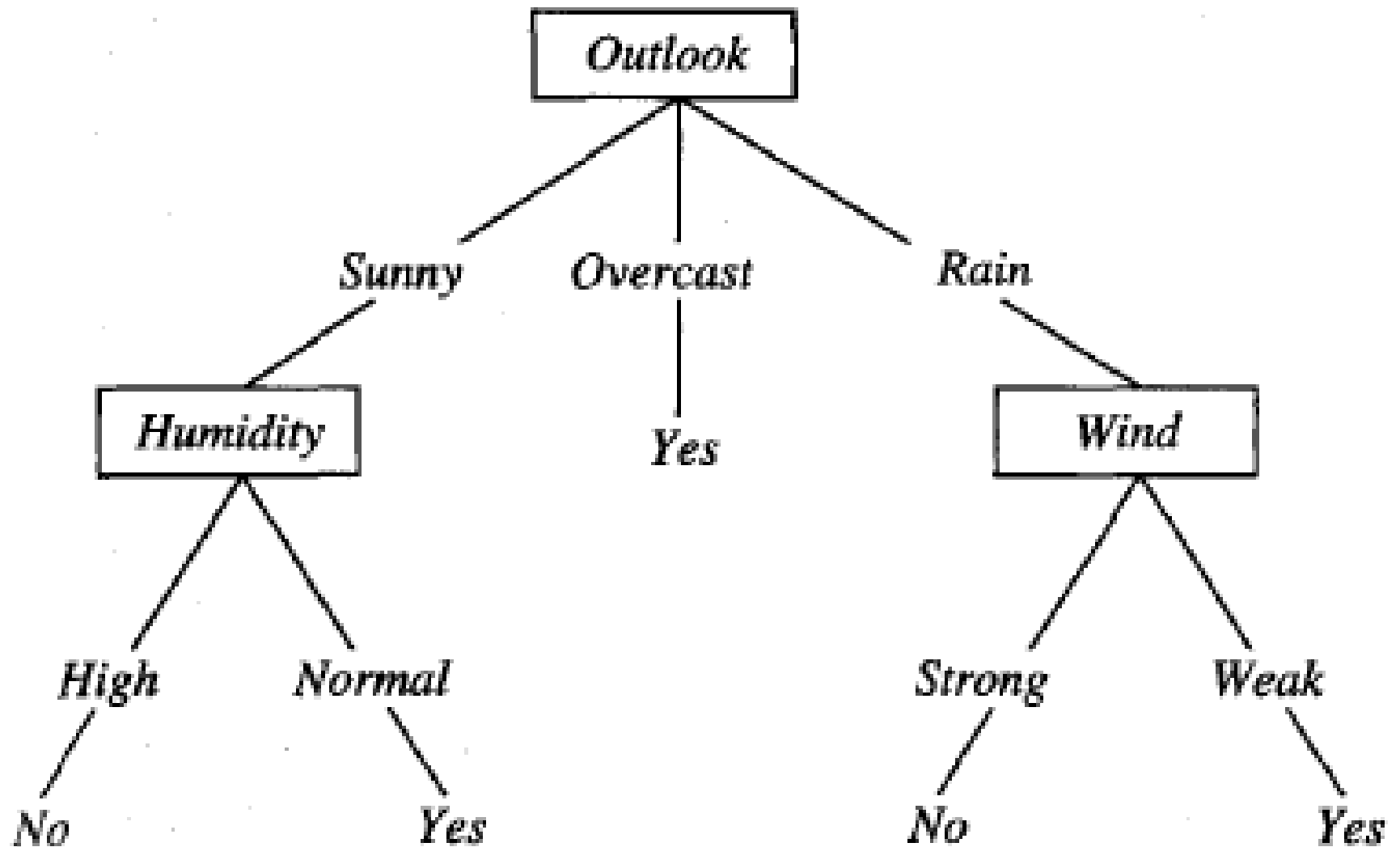
AUC = 80%

A photograph of the Space Shuttle Columbia during its ascent. The shuttle is positioned vertically, with its external tank and solid rocket boosters visible. A large, bright plume of fire and white smoke is being emitted from the base, indicating a powerful launch. The shuttle is moving upwards, leaving a trail of smoke behind it. The background is a clear blue sky with some scattered clouds.

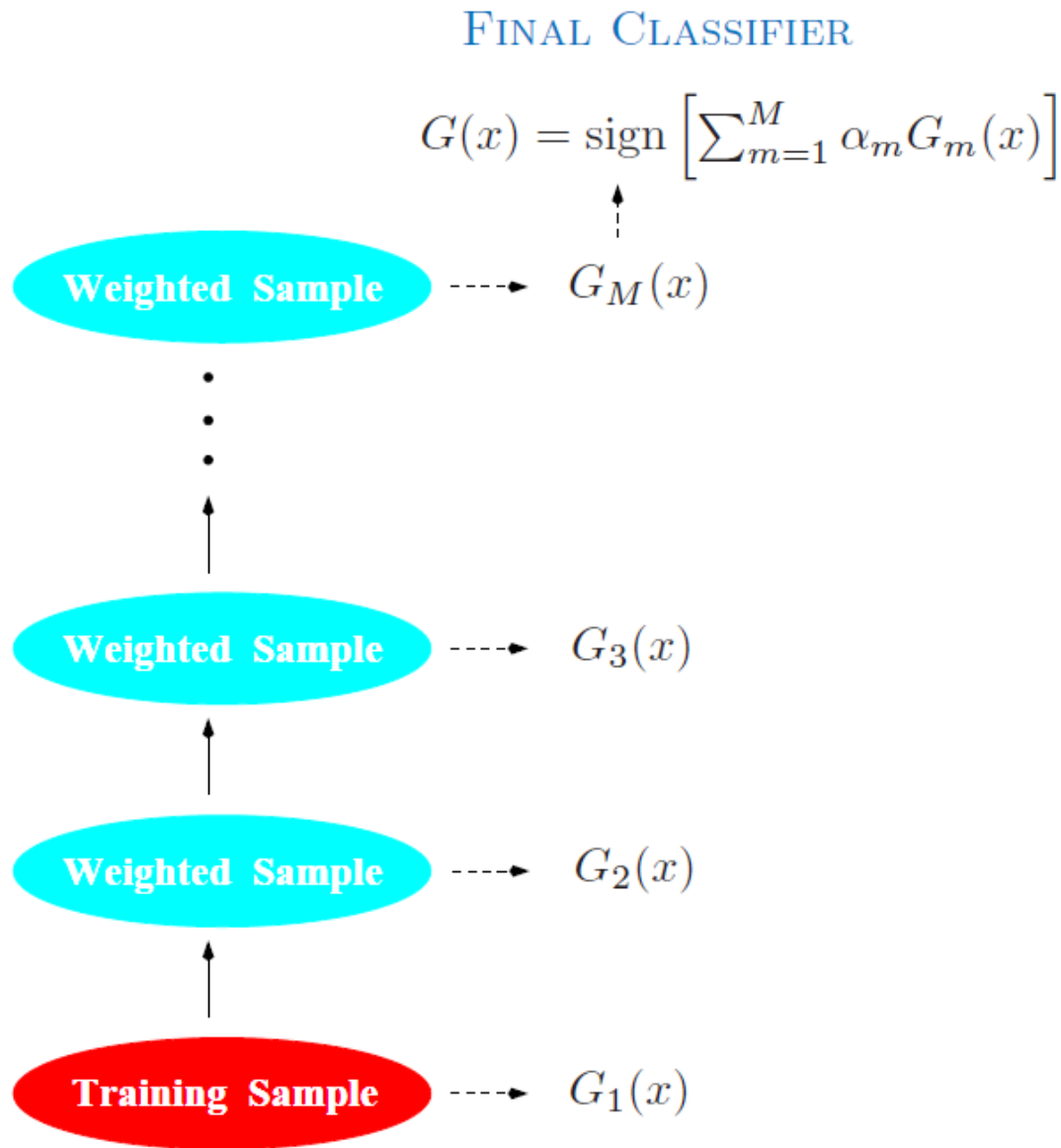
GRADIENT BOOSTING!

**THE BEST OFF-THE-SHELF
CLASSIFIER IN THE WORLD!**

Trees



Boosting



Gradient Boosting in R

```
library(xgboost)

#fits model
boost_default = xgboost(data = mm[folds < 9,],
                        label = response[folds < 9],
                        nrounds = 50,
                        objective = "binary:logistic")

#makes predictions
p_boost_default = predict(boost_default,
                          mm[folds >= 9,])

auc (p_boost_default, response[folds >= 9] )
accuracy (p_boost_default > 0.5, response[folds >= 9] )
```

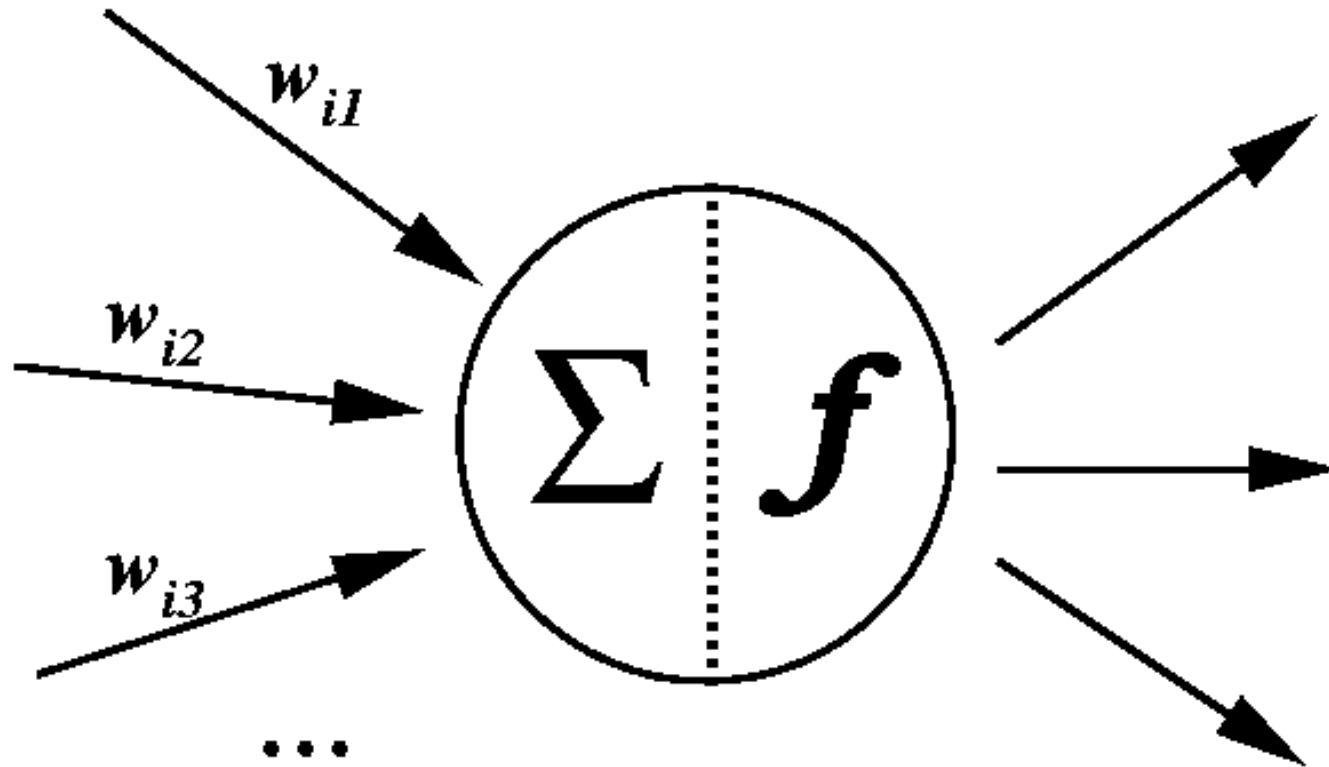
AUC = 83%



DEEP LEARNING IS LIKE LOVE

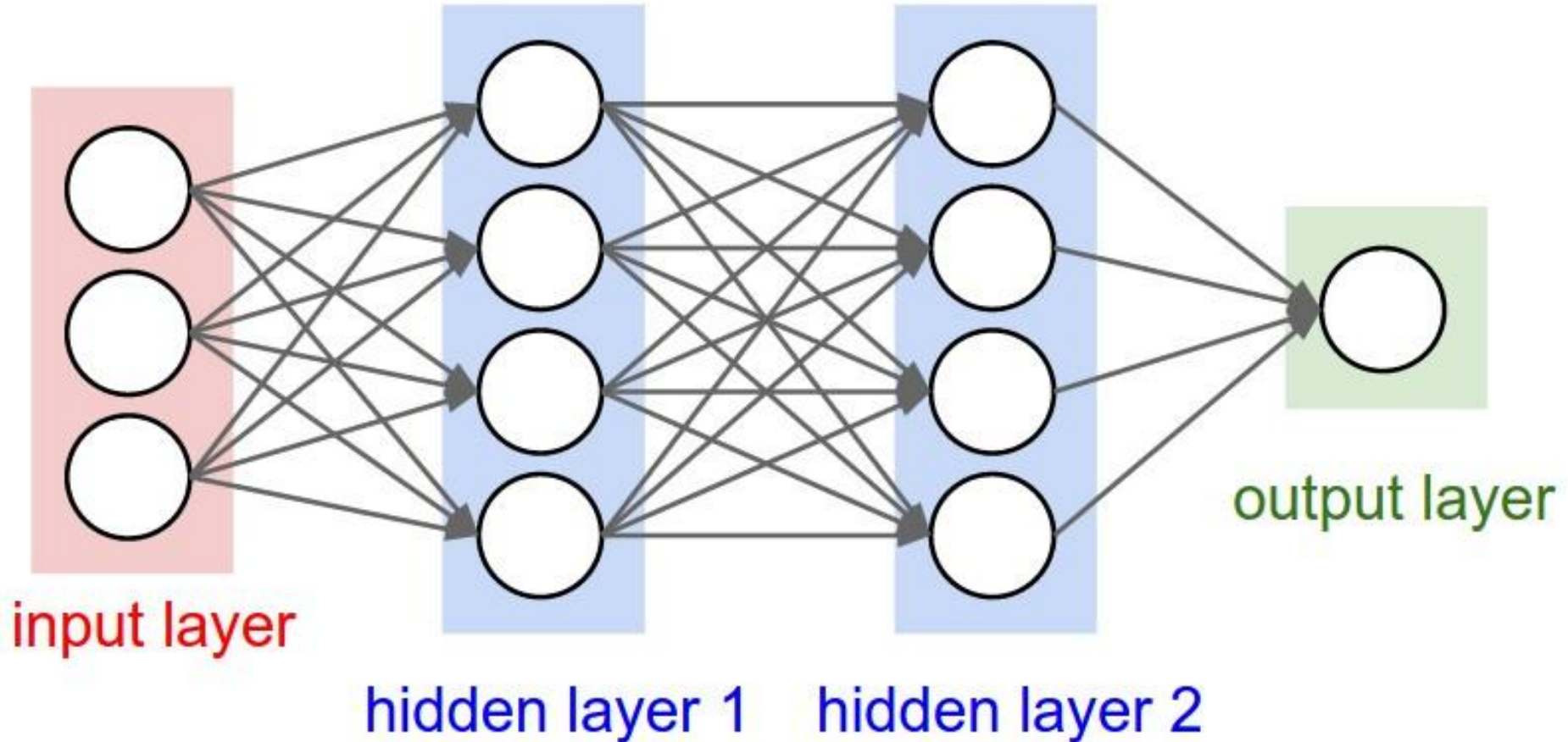
**NO ONE IS SURE WHAT IT IS,
BUT EVERYONE WANTS IT**

Neural Networks



$$y_i = f(\text{net}_i)$$

'Deep' Neural Networks



Deep Learning in R

```
library(h2o)

# initialise h2o
localH2O <- h2o.init(ip = "localhost",
                     port = 54321, startH2O = TRUE)

# get data in h2o format
dat_h2o <- as.h2o(arrhythmia)

# get vector of predictor locations
predictors = which(!names(arrhythmia) %in%
                  c("arrhythmia", "abnormal" ))
```

Deep Learning

```
#fit model
dl_fit <- h2o.deeplearning(x = predictors,
  y = 'abnormal',
  training_frame = dat_h2o[which(folds < 9),],
  epochs = 50)

#make predictions
pred_dl <- h2o.predict(dl_fit,
  dat_h2o[which(folds >= 9) , 1])

pred_dl <- as.data.frame(pred_dl)

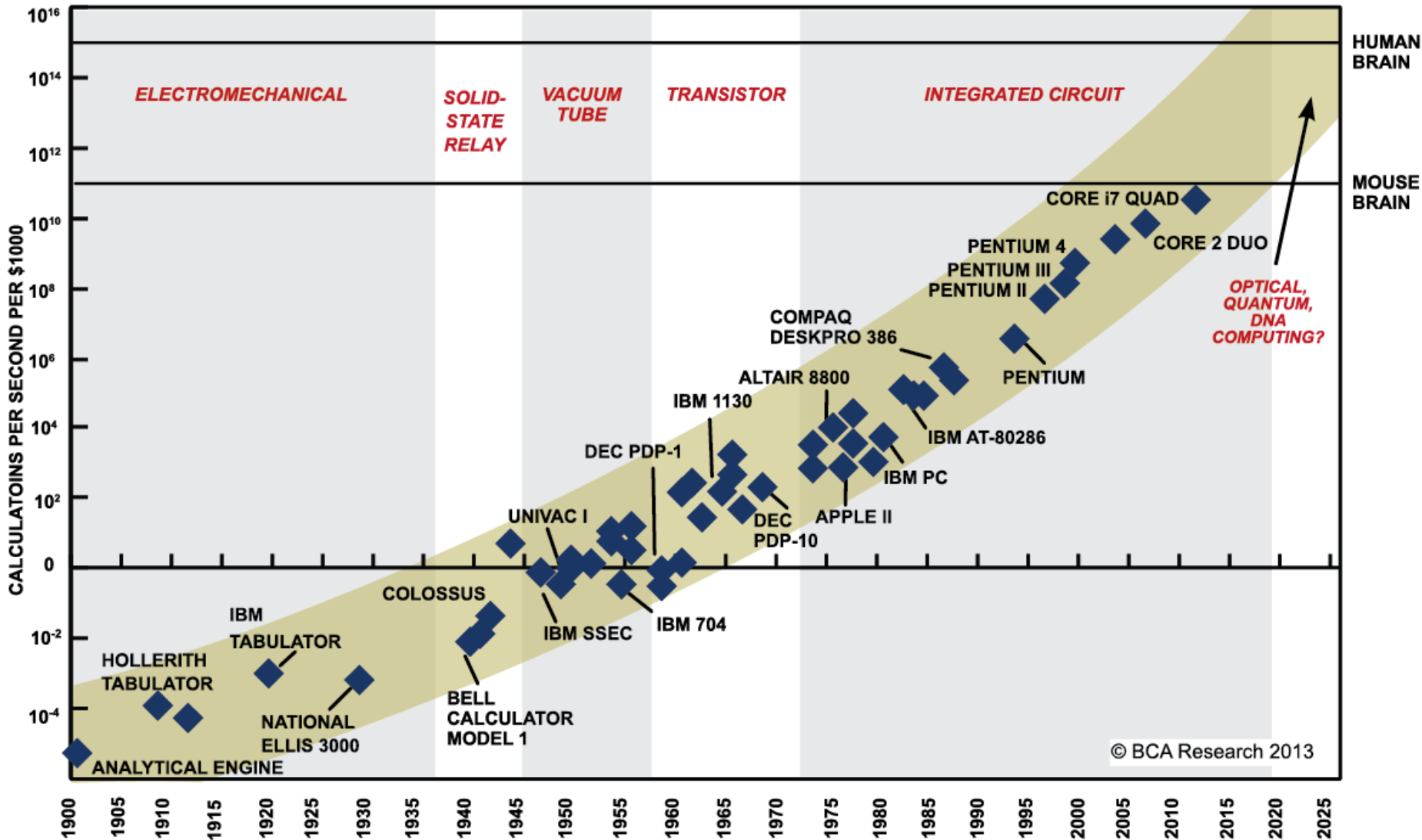
auc( pred_dl$`TRUE.` , response[folds >= 9])
accuracy( pred_dl$`TRUE.` , response[folds >= 9])
```

AUC = 84%

Results

Model	AUC
Logistic Regression	70
Elastic Net	80
Gradient Boosting	83
Deep Learning	84
Combined model	85

THE SINGULARITY IS NEAR?



SOURCE: RAY KURZWEIL, "THE SINGULARITY IS NEAR: WHEN HUMANS TRANSCEND BIOLOGY", P.67, THE VIKING PRESS, 2006. DATAPPOINTS BETWEEN 2000 AND 2012 REPRESENT BCA ESTIMATES.

Other topics

- **Cross validation**
- **Tuning parameters**
- **Bias/Variance trade-off**
- **Distributed learning/big data**
- **Unsupervised Learning**
- **Unstructured data**

- **... many more...**

Thanks!

Scripts and data available here:

https://github.com/tomliptrot/Machine_Learning_ManchesterR/