WEEK 7: MACHINE LEARNING 1

SECU0057

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Applied Data Science

WEEK 7: MACHINE LEARNING 1

MACHINE LEARNING?

- core idea: a system learns from experience
- no precise instructions

TODAY

- supervised learning
- performance metrics

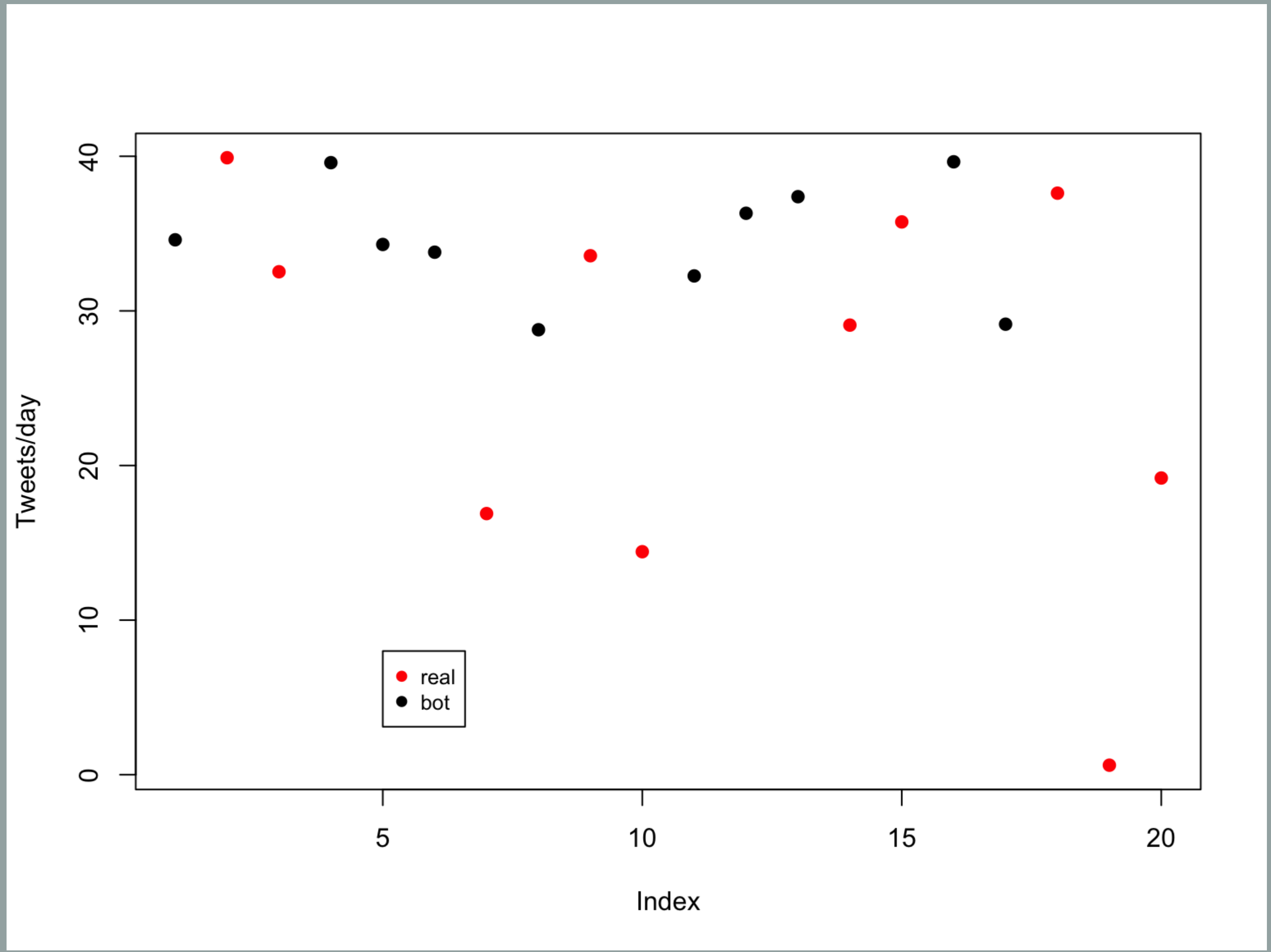
SUPERVISED LEARNING

- who is the supervisor?
- supervised = labelled data
- i.e. you know the outcome
- flipped logic

SIMULATED DATA

account	tweet_freq
bot	33.7960
bot	34.5973
bot	34.2955
bot	32.2615
real	19.1904
real	14.4237
real	37.6143
real	29.0793

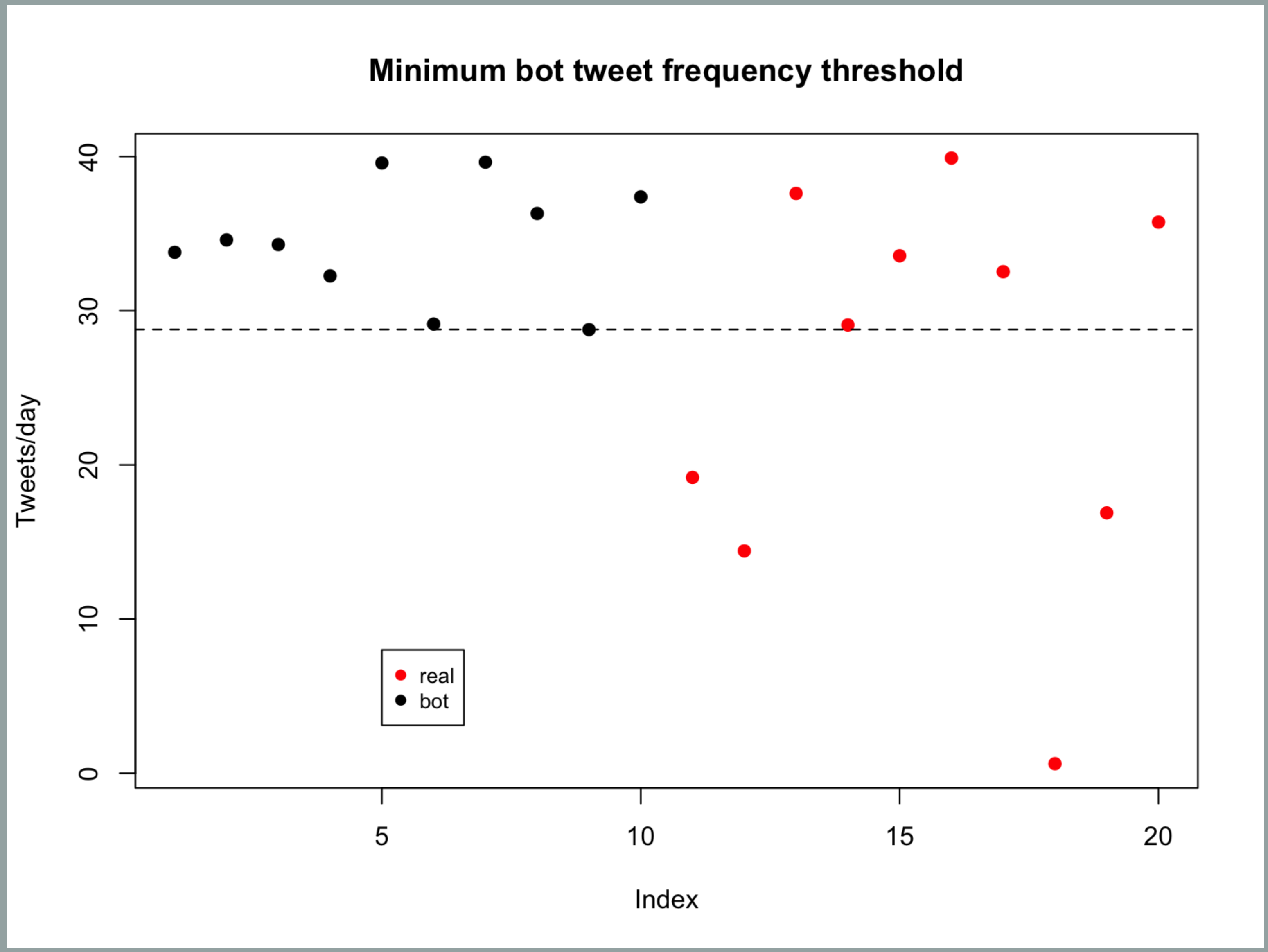
HOW TO BEST SEPARATE THE DATA INTO TWO GROUPS?



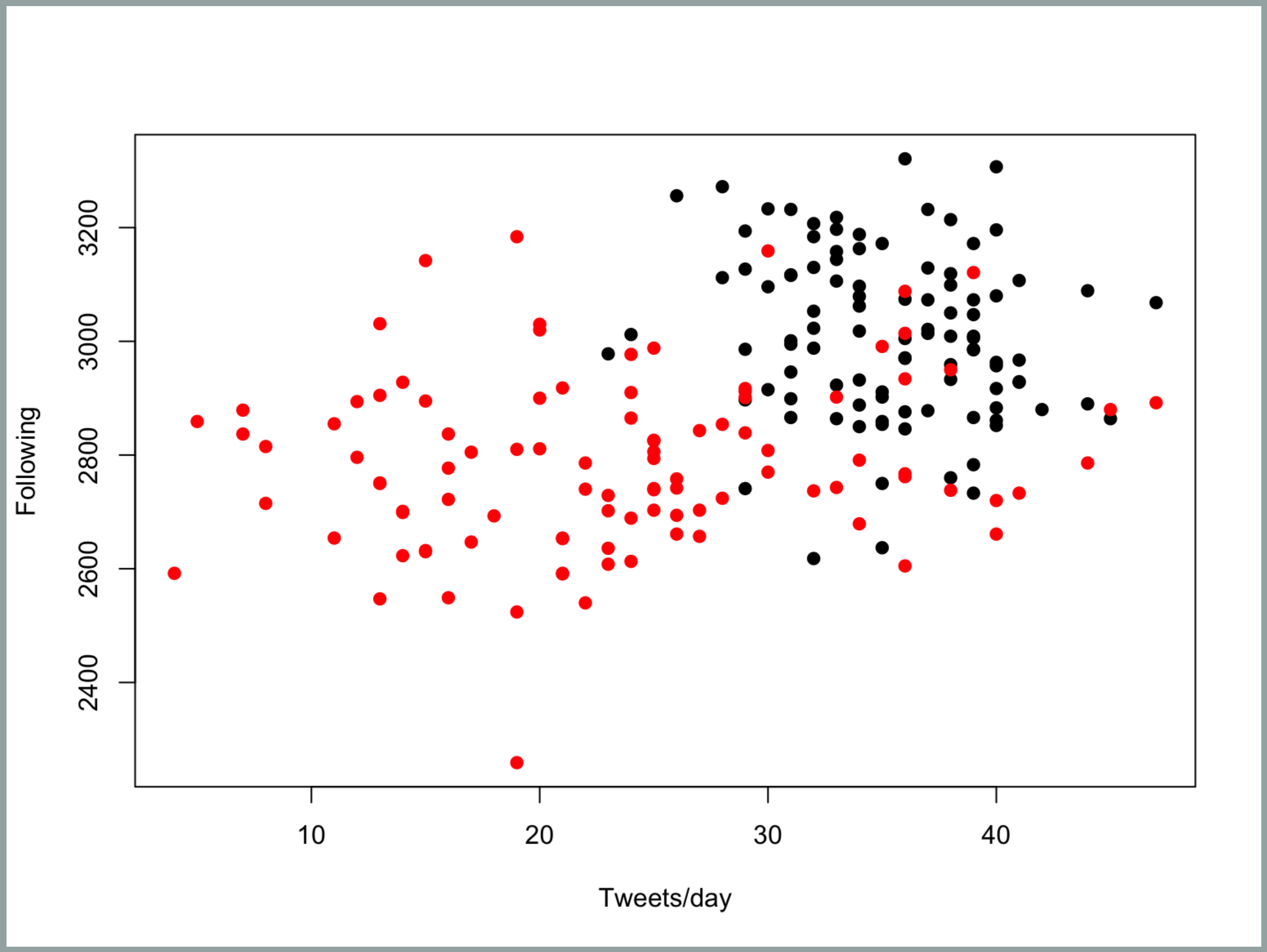
CORE IDEA

- learn relationship between
  - outcome (target) variable
  - features (predictors)
- “learning” is done through an algorithm
  - simplest algorithm: `if A then B`

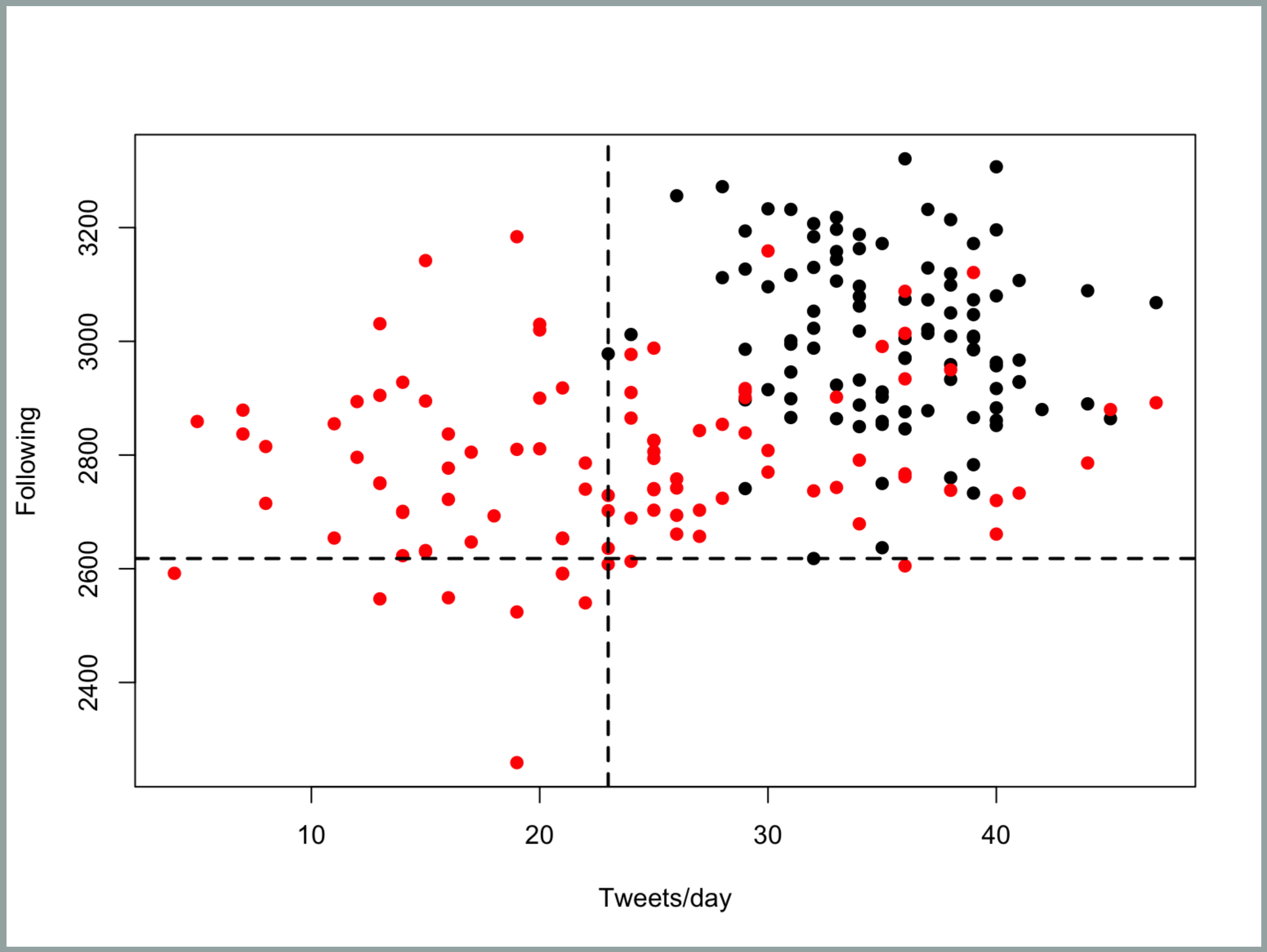
IDEA 1: MEAN THRESHOLDS

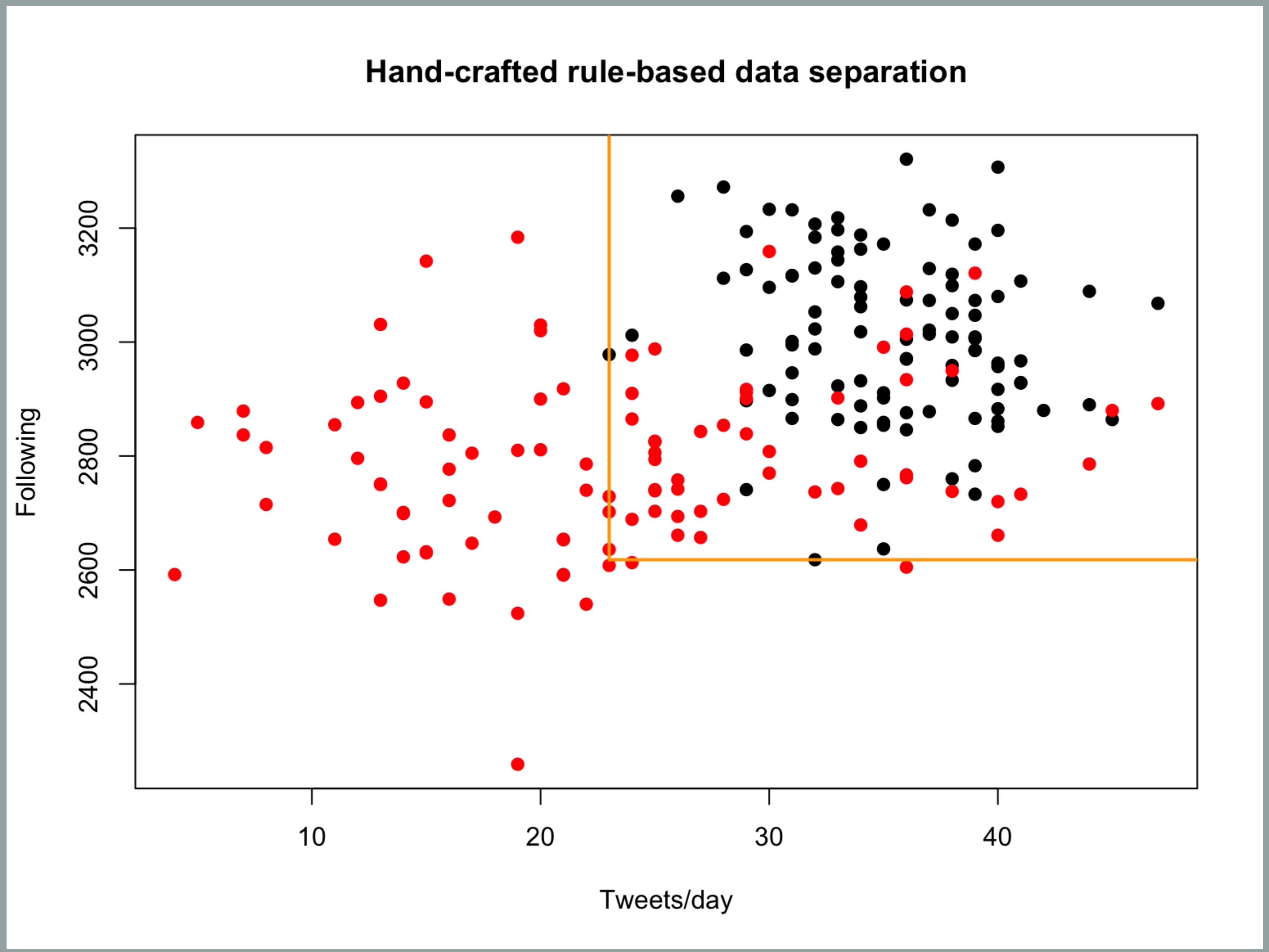


HIGHER DIMENSIONAL DATA



IDEA 2: HAND-CRAFTED RULES




Hand-crafted rule-based data separation
Following
3200
3000
2800
2600
2400
10
20
30
40
Tweets/day

BUT THIS IS NOT LEARNING

- often we have no idea about the relationships
- too many predictors
- too diverse a problem
- simply unknown

STEPWISE SUPERVISED ML

- clarify what `outcome` and `features` are
- determine which classification algorithm to use
- train the model

CLASSES OF SUPERVISED LEARNING

- classification (e.g. death/alive, fake/real)
- regression (e.g. income, number of deaths)

CORE AIM OF SUPERVISED LEARNING

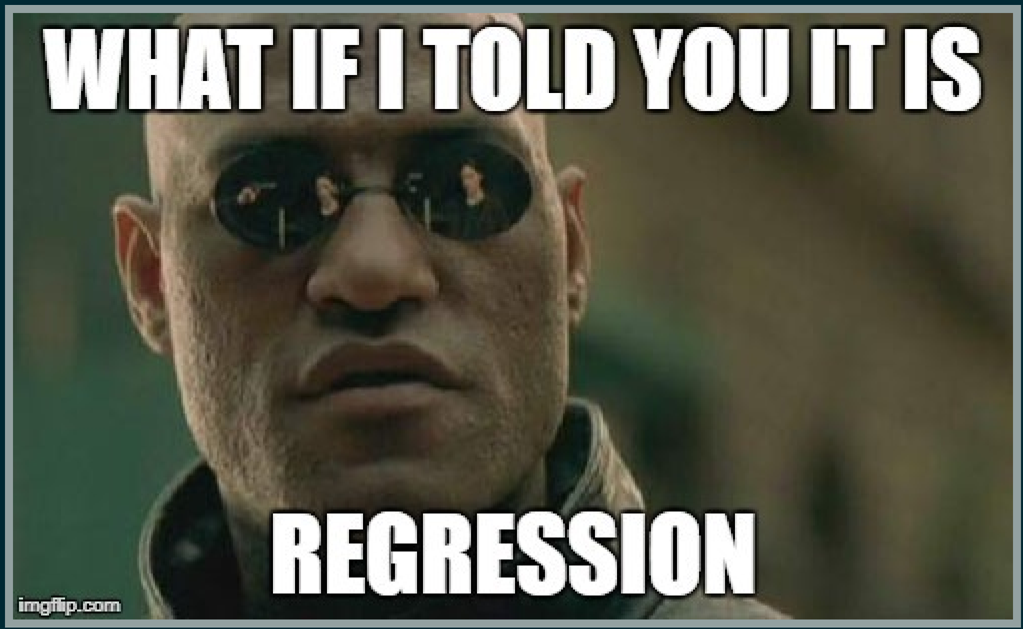
Learning from data to **make predictions** about the future.

`CARET` IN PRACTICE

```
my_first_model = glm(account ~ .
                     , data = data2
                     , family = 'binomial'
                     )
```

We have trained a model.

= you have taught an algorithm to learn to predict real vs bot accounts based on followers and tweet frequency


WHAT IF I TOLD YOU IT IS
REGRESSION
imgflip.com

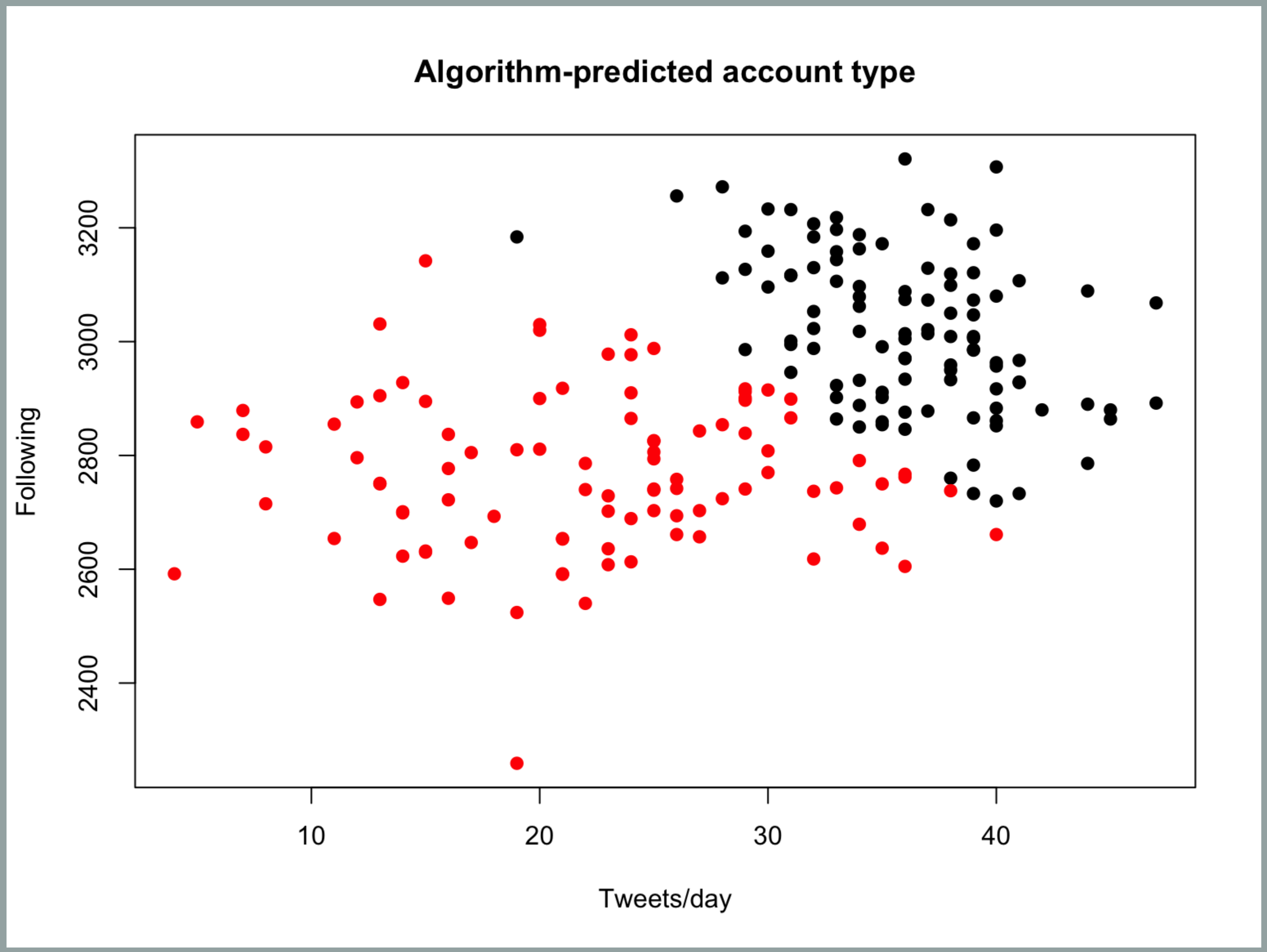
EXPLANATORY VS PREDICTIVE MODELLING

- this is where you would stop in explanatory modelling
- e.g. interpreting the coefficients
- predictive modelling focuses on the use of that model

PUTTING YOUR MODEL TO USE

```
data2$model_predictions = predict(my_first_model, data2, type = 'response
data2$model_1 = ifelse(data2$model_predictions >= .5, 'real', 'bot')
```

	bot	real
bot	90	10
real	14	86



Algorithm-predicted account type
Following
3200
3000
2800
2600
2400
10
20
30
40
Tweets/day

THE KEY CHALLENGE?

Think about what we did

PROBLEM OF INDUCTIVE BIAS

- remember: we learn from the data
- but what we really want to know is: how does it work on “unseen” data
- this is needed to estimate how good real predictions would be

How to solve this?

SPLITTING THE DATA

- split the data (e.g. 80%/20%, 60%/40%)
- use one part as TRAINING SET
- use the other as TEST SET

ENTER: `CARET`

```
library(caret)
```

- excellent package for ML in R
- well-documented website
- common interface for 200+ models

CARET: DATA PARTITIONING

```
set.seed(1)
in_training = createDataPartition(y = data3$account
                                  , p = .8
                                  , list = FALSE
                                  )
```

CREATING A TRAINING AND TEST SET

```
training_data = data3[ in_training,]
test_data = data3[-in_training,]
```

SUPERVISED ML STEPS REVISED

- define outcome
- define features
- build model on the TRAINING SET
- evaluate model on the TEST SET

BUILDING AN SVM MODEL

```
my_second_model = train(account ~ .
                        , data = training_data
                        , method = "svmLinear"
                        )
```

FIT/TEST THE SVM:

```
model_predictions = predict(my_second_model, test_data)
```

	bot	real
bot	19	1
real	4	16

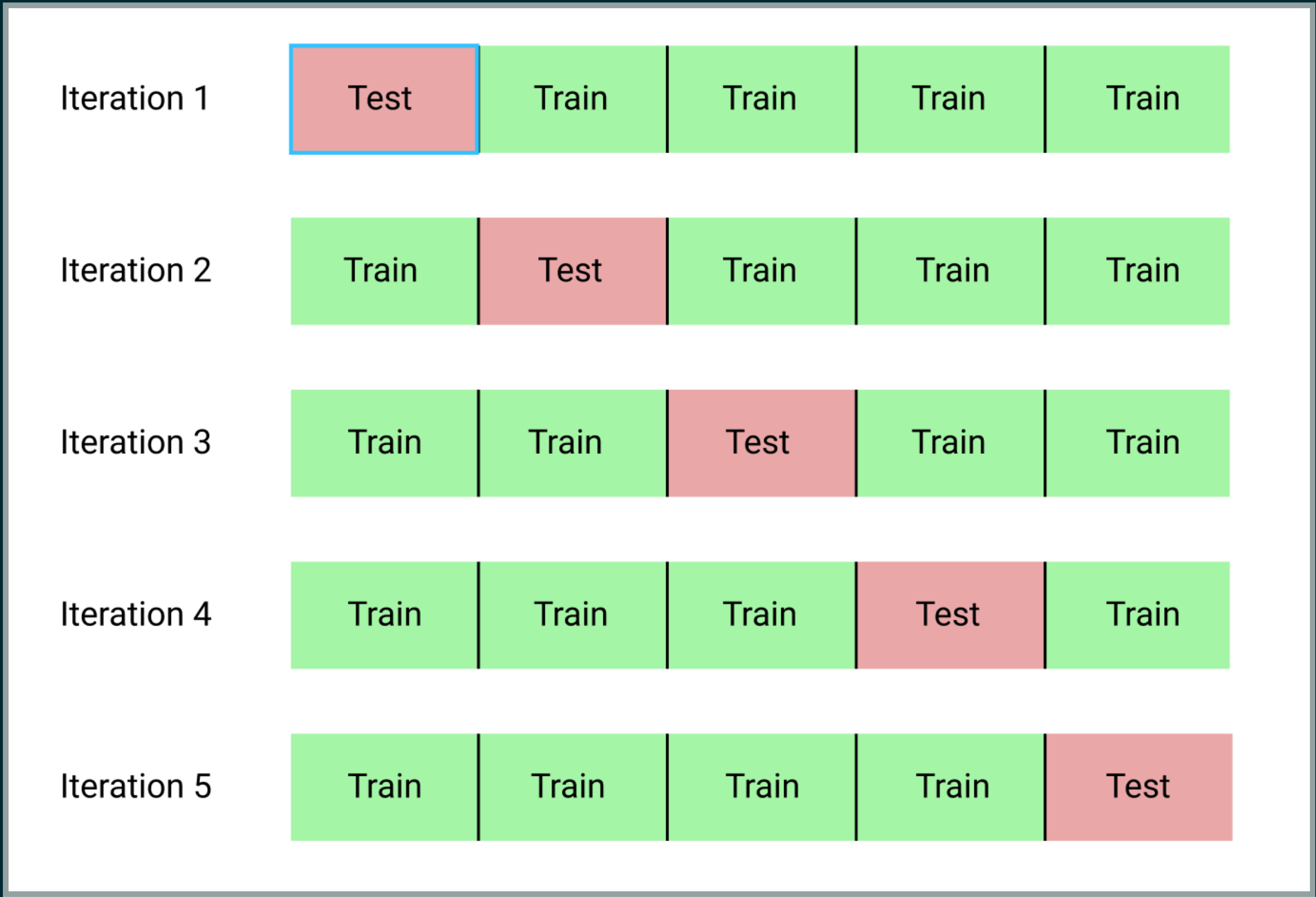
BUT!

- our model might be really dependent on the training data
- we want to be more careful

Can we do some kind of safeguarding in the training data?

CROSS-VALIDATION

K-fold cross-validation


Iteration 1
Test
Train
Train
Train
Train
Iteration 2
Train
Test
Train
Train
Train
Iteration 3
Train
Train
Test
Train
Train
Iteration 4
Train
Train
Train
Test
Train
Iteration 5
Train
Train
Train
Train
Test

img source

SPECIFYING CV IN `CARET`

```
training_controls = trainControl(method="cv"
                                 , number = 4
                                 , classProbs = TRUE
                                 )

my_third_model = train(account ~ .
                       , data = training_data
                       , trControl = training_controls
                       , method = "svmLinear"
                       )
```

```
my_third_model
```

```
## Support Vector Machines with Linear Kernel
##
## 160 samples
##   2 predictor
##   2 classes: 'bot', 'real'
##
## No pre-processing
## Resampling: Cross-Validated (4 fold)
## Summary of sample sizes: 120, 120, 120, 120
## Resampling results:
##
##   Accuracy  Kappa
##   0.85      0.7
##
## Tuning parameter 'C' was held constant at a value of 1
```

ASSESS THE CVED MODEL

```
model_predictions = predict(my_third_model, test_data)
```

	bot	real
bot	19	1
real	4	16

PERFORMANCE METRICS

SUPPOSE WE HAVE TWO MODELS

```
svm_model = train(account ~ .
                  , data = training_data
                  , trControl = training_controls
                  , method = "svmLinear"
                  )

nb_model = train(account ~ .
                  , data = training_data
                  , trControl = training_controls
                  , method = "nb"
                  )
```

TEST SET RESULTS

SVM model

	bot	real
bot	96	104
real	102	98

NB model

	bot	real
bot	124	76
real	140	60

THE CONFUSION MATRIX

	Bot	**Real**
Bot	True positives	False negatives
Real	False positives	True negatives

FALSE (TRUE) POSITIVES (NEGATIVES)

- true positives (TP): correctly identified bots
- true negatives (TN): correctly identified real accounts
- false positives (FP): false accusations
- false negatives (FN): missed bots

MOST INTUITIVE: ACCURACY

$$acc = \frac{(TP+TN)}{N}$$

$$acc_{svm} = \frac{(111+86)}{400} = 0.49$$

$$acc_{nb} = \frac{(124+60)}{400} = 0.47$$

Any problems with that?

ACCURACY

Model 1

	Bot	**Real**
Bot	100	100
Real	5	195

Model 2

	Bot	**Real**
Bot	150	50
Real	55	145

PROBLEM WITH ACCURACY

- same accuracy, different confusion matrix
- relies on thresholding idea
- not suitable for comparing models (don’t be fooled by the literature!!)

Needed: more nuanced metrics

BEYOND ACCURACY

```
##         prediction
## reality Bot Real Sum
##    Bot  100  100 200
##    Real   5  195 200
##    Sum  105  295 400
```

```
##         prediction
## reality Bot Real Sum
##    Bot  150   50 200
##    Real  55  145 200
##    Sum  205  195 400
```

PRECISION

i.e. –> how often the prediction is correct when prediction class *X*

Note: we have two classes, so we get *two* precision values

Formally:

- $Pr_{bot} = \frac{TP}{(TP+FP)}$
- $Pr_{real} = \frac{TN}{(TN+FN)}$

PRECISION

```
##          prediction
## reality Bot Real Sum
##     Bot  100  100 200
##     Real   5  195 200
##     Sum  105  295 400
```

- $Pr_{bot} = \frac{100}{105} = 0.95$
- $Pr_{real} = \frac{195}{295} = 0.64$

COMPARING THE MODELS

	Model 1	Model 2
acc	0.74	0.74
Pr_{bot}	0.95	0.73
Pr_{real}	0.64	0.74

RECALL

i.e. –> how many of class *X* is detected

Note: we have two classes, so we get *two* recall values

Also called sensitivity and specificity!

Formally:

- $R_{bot} = \frac{TP}{(TP+FN)}$
- $R_{real} = \frac{TN}{(TN+FP)}$

RECALL

```
##          prediction
## reality Bot Real Sum
##     Bot  100  100 200
##     Real   5  195 200
##     Sum  105  295 400
```

- $R_{bot} = \frac{100}{200} = 0.50$
- $R_{real} = \frac{195}{200} = 0.98$

COMPARING THE MODELS

	Model 1	Model 2
acc	0.74	0.74
Pr_{bot}	0.95	0.73
Pr_{real}	0.64	0.74
R_{bot}	0.50	0.75
R_{real}	0.98	0.73

COMBINING PR AND R

The *F1* measure.

Note: we combine Pr and R for each class, so we get *two* F1 measures.

Formally:

- $F1_{bot} = 2 * \frac{Pr_{bot} * R_{bot}}{Pr_{bot} + R_{bot}}$
- $F1_{real} = 2 * \frac{Pr_{real} * R_{real}}{Pr_{real} + R_{real}}$

F1 MEASURE

```
##         prediction
## reality Bot Real Sum
##     Bot  100  100 200
##     Real   5  195 200
##     Sum  105  295 400
```

- $F1_{bot} = 2 * \frac{0.95*0.50}{0.95+0.50} = 2 * \frac{0.475}{1.45} = 0.66$
- $F1_{real} = 2 * \frac{0.64*0.98}{0.64+0.98} = 2 * \frac{0.63}{1.62} = 0.77$

COMPARING THE MODELS

	Model 1	Model 2
acc	0.74	0.74
Pr_{bot}	0.95	0.73
Pr_{real}	0.64	0.74
R_{bot}	0.50	0.75
R_{real}	0.98	0.73
$F1_{bot}$	0.66	...
$F1_{real}$	0.77	...

IN CARET

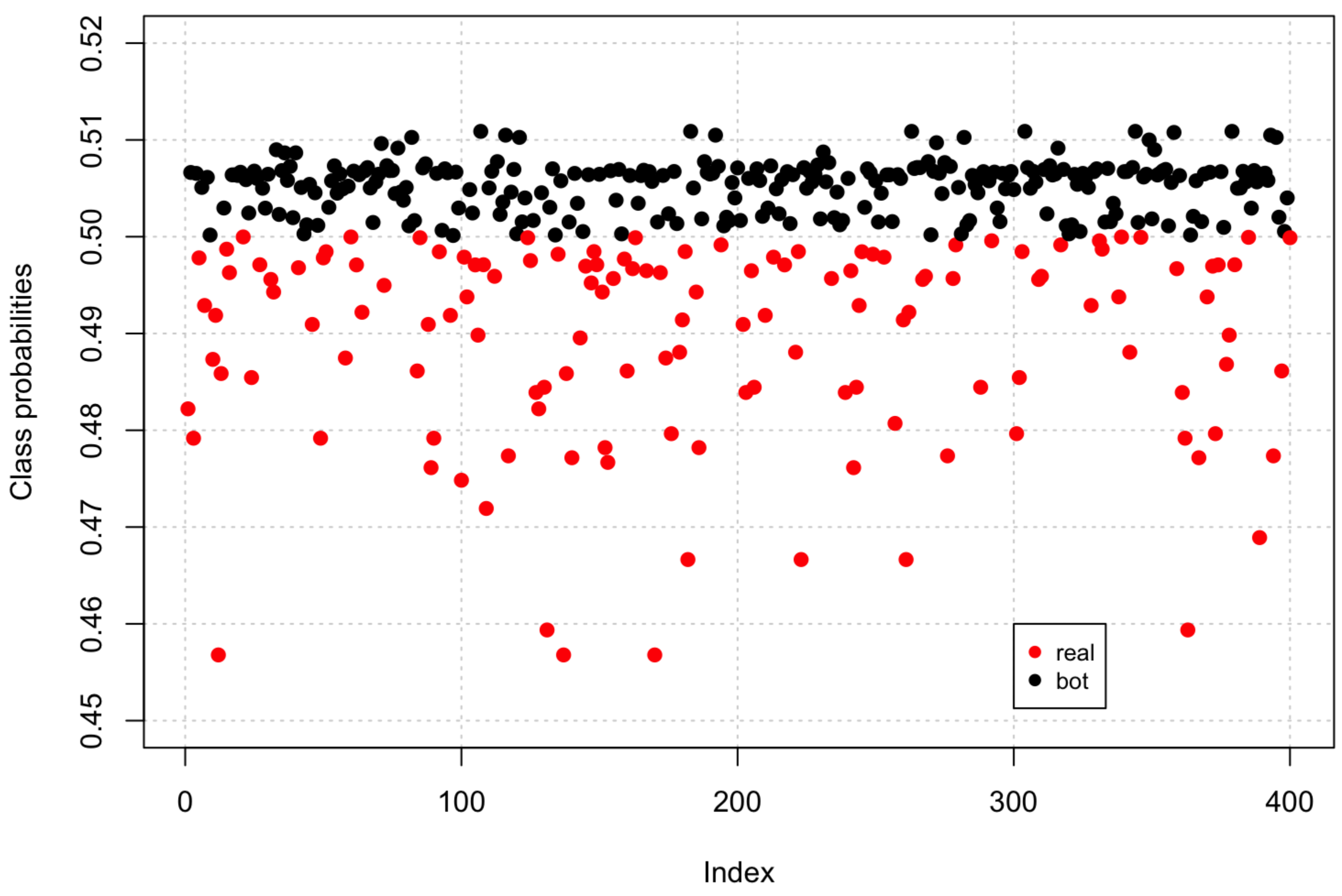
```r
confusionMatrix(nb_pred, as.factor(test_data$account))
```

```
## Confusion Matrix and Statistics
##
##            Reference
## Prediction bot real
##       bot  124  140
##       real  76   60
##
##                Accuracy : 0.46
##                  95% CI : (0.4104, 0.5102)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.9506
##
##                   Kappa : -0.08
##  Mcnemar's Test P-Value : 1.814e-05
##
##             Sensitivity : 0.6200
##             Specificity : 0.3000
##          Pos Pred Value : 0.4697
```

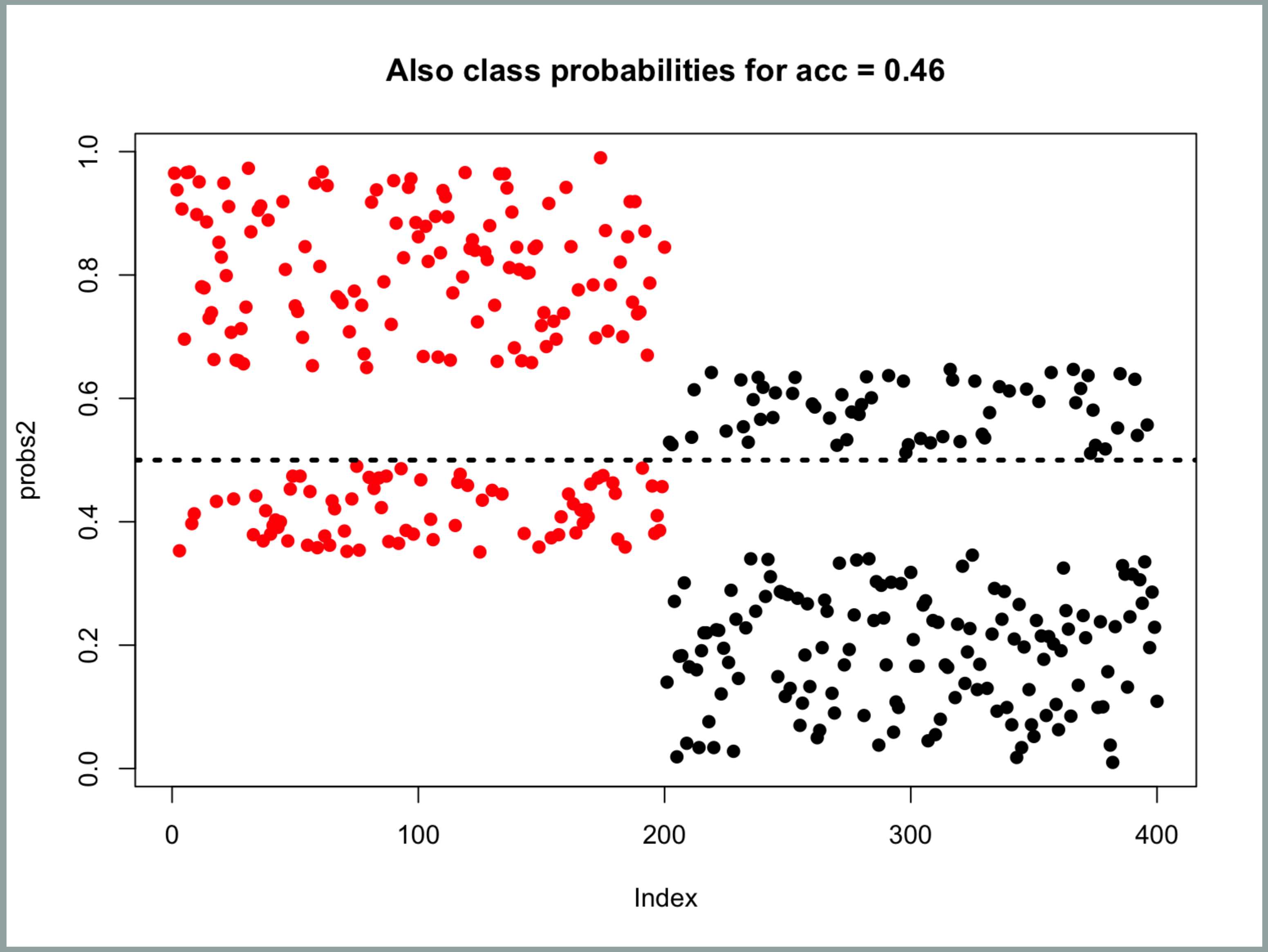
THERE'S MORE

What's behind the model's predictions?

CLASS PROBABILITIES



THE THRESHOLD PROBLEM



ISSUE!

- classification threshold little informative
- obscures certainty in judgment

Needed: a representation across all possible values

THE AREA UNDER THE CURVE (AUC)

- plot all observed values (here: class probs)
- y-axis: sensitivity
- x-axis: 1-specificity

AUC STEP-WISE

```
#for each class probability:
threshold_1 = probs[1]
threshold_1
```

```
## [1] 0.4822156
```

```
pred_threshold_1 = ifelse(probs >= threshold_1, 'bot', 'real')
```

	bot	real
bot	183	17
real	188	12

SENSITIVITY AND 1-SPECIFICITY

	bot	**real**
bot	183	17
real	188	12

$$Sens. = 183/200 = 0.92$$

$$Spec. = 12/200 = 0.06$$

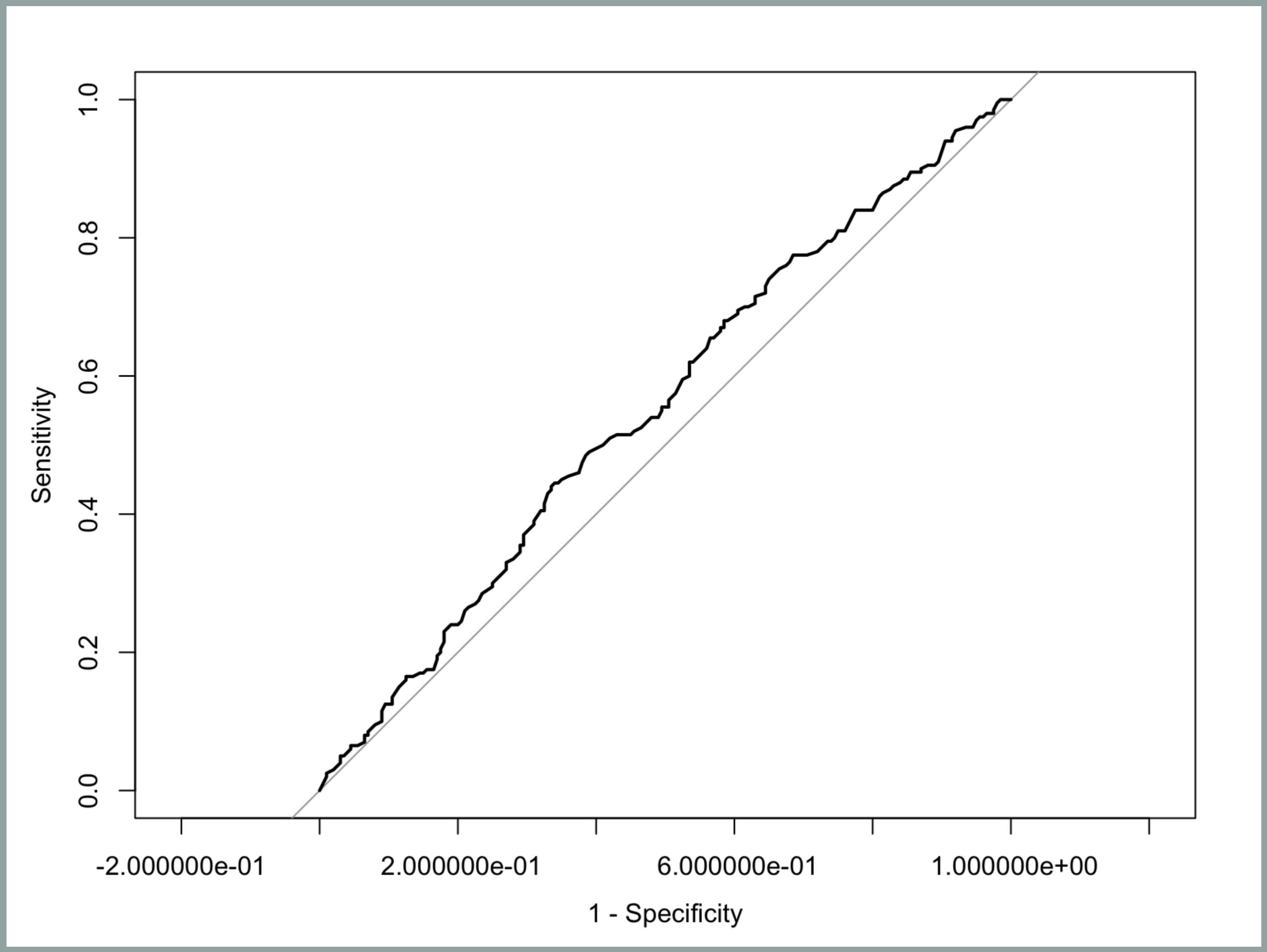
$$Sens. = 183/200 = 0.92$$

$$Spec. = 12/200 = 0.06$$

Threshold	**Sens.**	**1-Spec**
0.48	0.92	0.94

Do this for every threshold observed.

PLOT THE RESULTS:

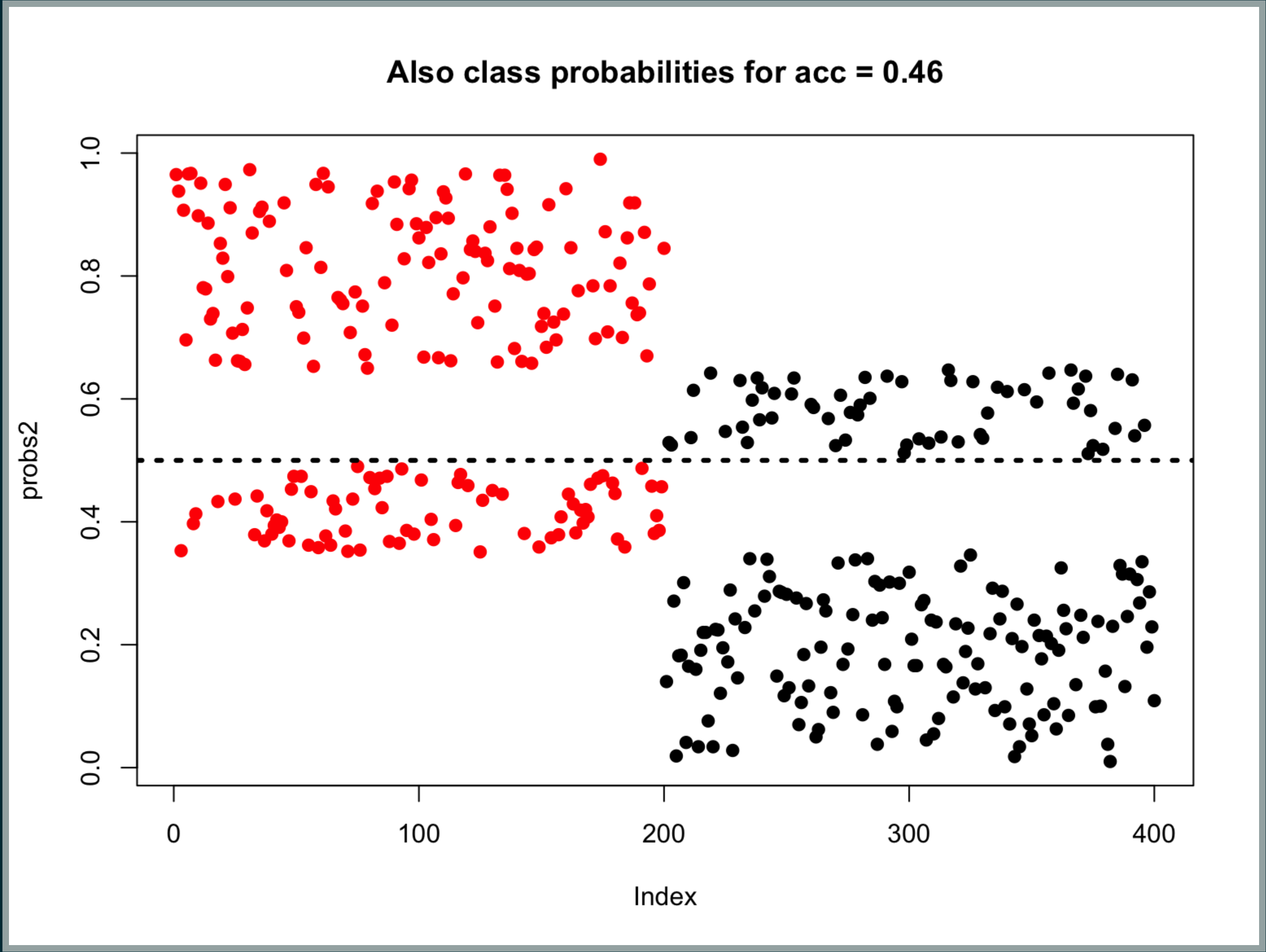


QUANTIFY THIS PLOT

```
auc1 = roc(response = test_data$account
               , predictor = probs
               , ci=T)
auc1
```

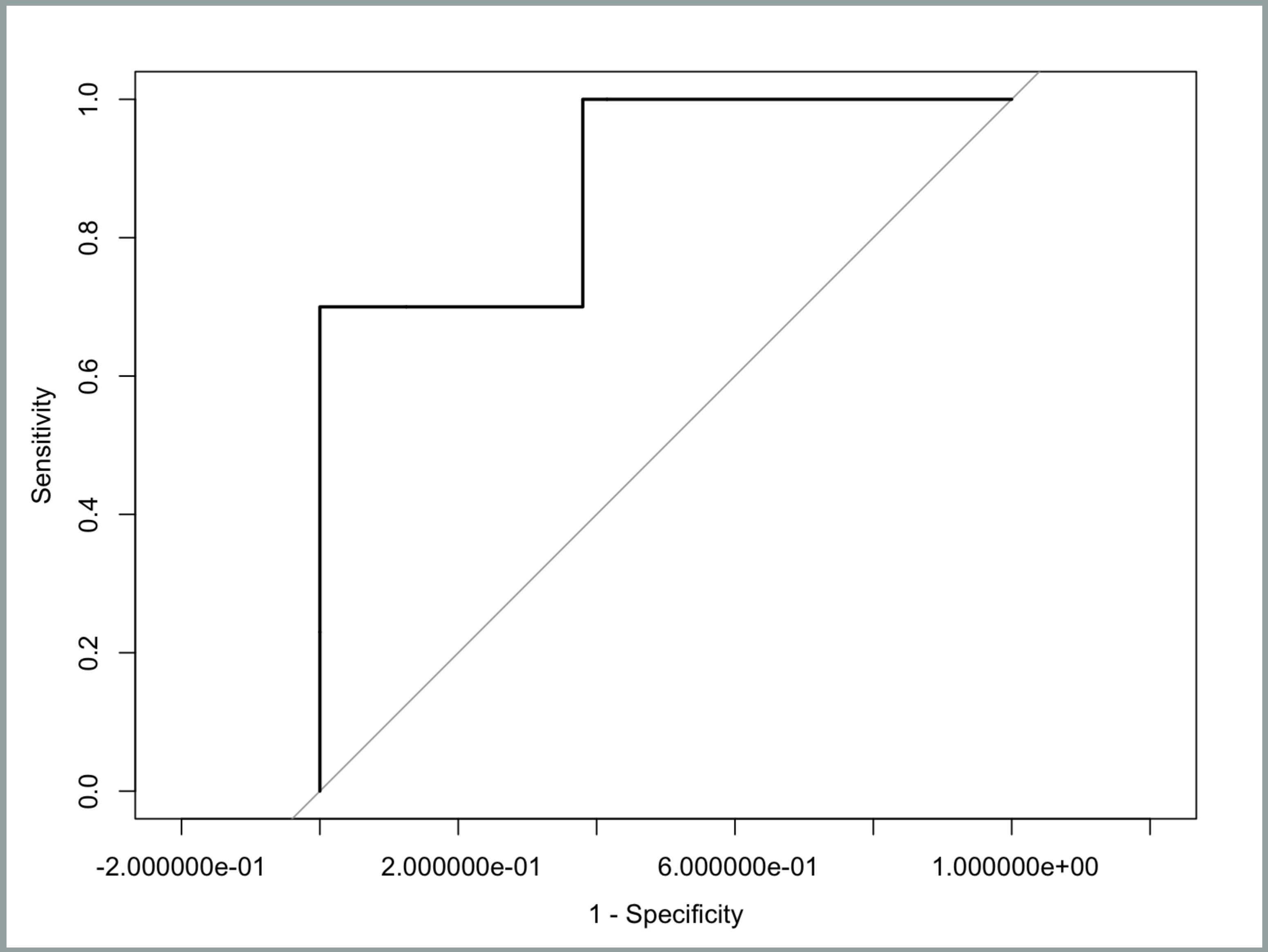
```
##
## Call:
## roc.default(response = test_data$account, predictor = probs,     ci =
##
## Data: probs in 200 controls (test_data$account bot) < 200 cases (test_
## Area under the curve: 0.5534
## 95% CI: 0.4971-0.6098 (DeLong)
```

WHAT IF WE COMPARE OUR TWO MODELS?



```r
auc2 = roc(response = test_data$account
               , predictor = probs2
               , ci=T)

plot.roc(auc2, xlim=c(1, 0), legacy.axes = T)
```



1.0
0.8
0.6
0.4
0.2
0.0
Sensitivity
-2.000000e-01
2.000000e-01
6.000000e-01
1.000000e+00
1 - Specificity

WHAT'S NEXT?

- Today's tutorial + homework: text classification, performance metrics

Next week: Machine Learning 2