



MACHINE LEARNING TOOLBOX

Welcome to the Machine Learning Toolbox!

Supervised learning

- caret R package
- Automates *supervised learning* (a.k.a. *predictive modeling*)
- Target variable



Supervised learning

- Two types of predictive models
 - Classification → Qualitative
 - Regression → Quantitative
- Use *metrics* to evaluate models
 - Quantifiable
 - Objective
- *Root Mean Squared Error* (RMSE) for regression (e.g. `lm()`)

Evaluating model performance

- Common to calculate in-sample RMSE
 - Too optimistic
 - Leads to overfitting
- Better to calculate out-of-sample error (a la caret)
 - Simulates real-world usage
 - Helps avoid overfitting

In-sample error

```
> # Fit a model to the mtcars data
> data(mtcars)
> model <- lm(mpg ~ hp, mtcars[1:20, ])

> # Predict in-sample
> predicted <- predict(model, mtcars[1:20, ], type = "response")

> # Calculate RMSE
> actual <- mtcars[1:20, "mpg"]
> sqrt(mean((predicted - actual)^2))
[1] 3.172132
```



The Machine Learning Toolbox

Let's practice!



MACHINE LEARNING TOOLBOX

Out-of-sample error measures

Out-of-sample error

- Want models that don't overfit and generalize well
- Do the models perform well on new data?
- Test models on new data, or a *test set*
 - Key insight of machine learning
 - In-sample validation almost guarantees overfitting
- Primary goal of `caret` and this course: don't overfit

Example: out-of-sample RMSE

```
> # Fit a model to the mtcars data
> data(mtcars)
> model <- lm(mpg ~ hp, mtcars[1:20, ])

> # Predict out-of-sample
> predicted <- predict(model, mtcars[21:32, ], type = "response")

> # Evaluate error
> actual <- mtcars[21:32, "mpg"]
> sqrt(mean((predicted - actual)^2))
[1] 5.507236
```

Alternatives:

```
createResamples()
createFolds()
```

Compare to in-sample RMSE

```
> # Fit a model to the full dataset
> model2 <- lm(mpg ~ hp, mtcars)

> # Predict in-sample
> predicted2 <- predict(model, mtcars, type = "response")

> # Evaluate error
> actual2 <- mtcars[, "mpg"]
> sqrt(mean((predicted2 - actual2)^2))
[1] 3.74
```

Compare to out-of-sample RMSE of 5.5



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Cross-validation

Cross-validation

Full dataset

Rows are
randomly
assigned



Fold 1

Fold 2

Fold 3

Fold 4

Fold 5

Fold 6

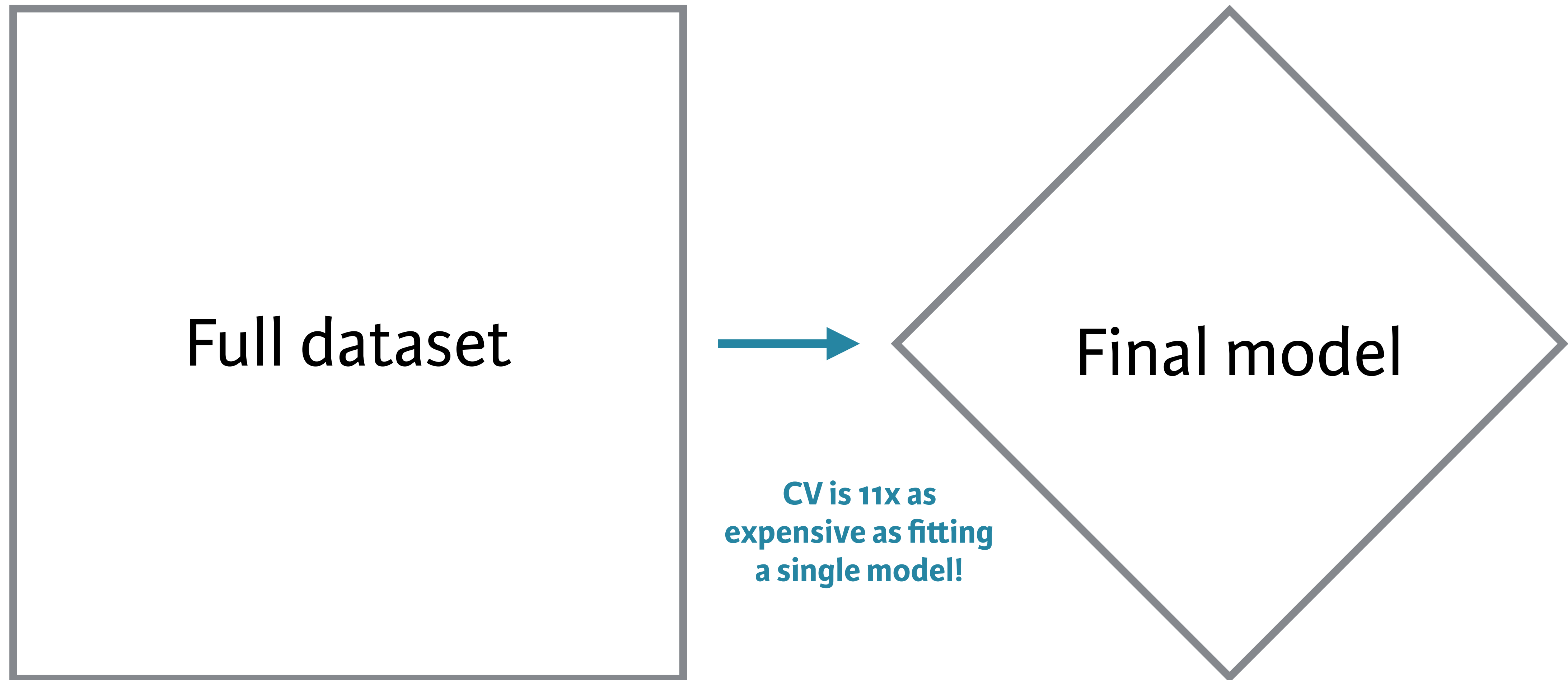
Fold 7

Fold 8

Fold 9

Fold 10

Fit final model on full dataset



Cross-validation

```
> # Set seed for reproducibility
> library(caret)
> data(mtcars)
> set.seed(42)

> # Fit linear regression model
> model <- train(mpg ~ hp, mtcars,
  method = "lm",
  trControl = trainControl(
    method = "cv", number = 10,
    verboseIter = TRUE
  )
)
+ Fold01: parameter=none
+ Fold02: parameter=none
  ...
- Fold10: parameter=none
Aggregating results
Fitting final model on full training set
```




MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Logistic regression on Sonar

Classification models

- Categorical (i.e. qualitative) target variable
- Example: will a loan default?
- Still a form of supervised learning
- Use a train/test split to evaluate performance
- Use the Sonar dataset
- Goal: distinguish rocks from mines

Example: Sonar data

```
> # Load the Sonar dataset  
> library(mlbench)  
> data(Sonar)
```

```
> # Look at the data
```

```
> Sonar[1:6, c(1:5, 61)]
```

	V1	V2	V3	V4	V5	Class
1	0.0200	0.0371	0.0428	0.0207	0.0954	R
2	0.0453	0.0523	0.0843	0.0689	0.1183	R
3	0.0262	0.0582	0.1099	0.1083	0.0974	R
4	0.0100	0.0171	0.0623	0.0205	0.0205	R
5	0.0762	0.0666	0.0481	0.0394	0.0590	R
6	0.0286	0.0453	0.0277	0.0174	0.0384	R

Splitting the data

- Randomly split data into training and test sets
- Use a 60/40 split, instead of 80/20
- Sonar dataset is small, so 60/40 gives a larger, more reliable test set

Splitting the data

```
# Randomly order the dataset
> rows <- sample(nrow(Sonar))
> Sonar <- Sonar[rows, ]

# Find row to split on
> split <- round(nrow(Sonar) * .60)
> train <- Sonar[1:split, ]
> test <- Sonar[(split + 1):nrow(Sonar), ]

# Confirm test set size
> nrow(train) / nrow(Sonar)
[1] 0.6009615
```



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Confusion matrix

Confusion matrix

Reference

Prediction

	Yes	No
Yes	True positive	False positive
No	False negative	True negative

Confusion matrix

```
# Fit a model
> model <- glm(Class ~ ., family = binomial(link = "logit"),
train)
> p <- predict(model, test, type = "response")
> summary(p)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
0.00000 0.00000 0.9885 0.5296 1.00000 1.00000

# Turn probabilities into classes and look at their frequencies
> p_class <- ifelse(p > .50, "M", "R")
> table(p_class)
p_class
 M  R
44 39
```

Confusion matrix

- Make a 2-way frequency table
- Compare predicted vs. actual classes

```
# Make simple 2-way frequency table  
> table(p_class, test[["Class"]])  
p_class  M  R  
      M 13 31  
      R 30  9
```

Confusion matrix

```
# Use caret's helper function to calculate additional statistics  
> confusionMatrix(p_class, test[["Class"]])
```

```
      Reference  
Prediction  M   R  
      M  13  31  
      R  30   9
```

```
      Accuracy : 0.2651
```

```
      95% CI : (0.1742, 0.3734)
```

```
      No Information Rate : 0.5181
```

```
      P-Value [Acc > NIR] : 1
```

```
      Kappa : -0.4731
```

```
      McNemar's Test P-Value : 1
```

```
      Sensitivity : 0.3023
```

```
      Specificity : 0.2250
```

```
      Pos Pred Value : 0.2955
```

```
      Neg Pred Value : 0.2308
```



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Class probabilities and class predictions

Different thresholds

- Not limited to 50% threshold
 - 10% would catch more mines with less certainty
 - 90% would catch fewer mines with more certainty
- Balance true positive and false positive rates
- Cost-benefit analysis

Confusion matrix

```
# Use a larger cutoff
> p_class <- ifelse(p > .99, "M", "R")
> table(p_class)
p_class
 M  R
41 42

# Make simple 2-way frequency table
> table(p_class, test[["Class"]])
p_class  M  R
      M 13 28
      R 30 12
```

Confusion matrix with caret

```
# Use caret to produce confusion matrix  
> confusionMatrix(p_class, test[["Class"]])
```

```
      Reference  
Prediction  M   R  
      M  13  28  
      R  30  12
```

```
      Accuracy : 0.3012
```

```
      95% CI : (0.2053, 0.4118)
```

```
      No Information Rate : 0.5181
```

```
      P-Value [Acc > NIR] : 1.0000
```

```
      Kappa : -0.397
```

```
      McNemar's Test P-Value : 0.8955
```

```
      Sensitivity : 0.3023
```

```
      Specificity : 0.3000
```

```
      Pos Pred Value : 0.3171
```

```
      Neg Pred Value : 0.2857
```



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Introducing the ROC curve

The challenge

- Many possible classification thresholds
- Requires manual work to choose
- Easy to overlook a particular threshold
- Need a more systematic approach

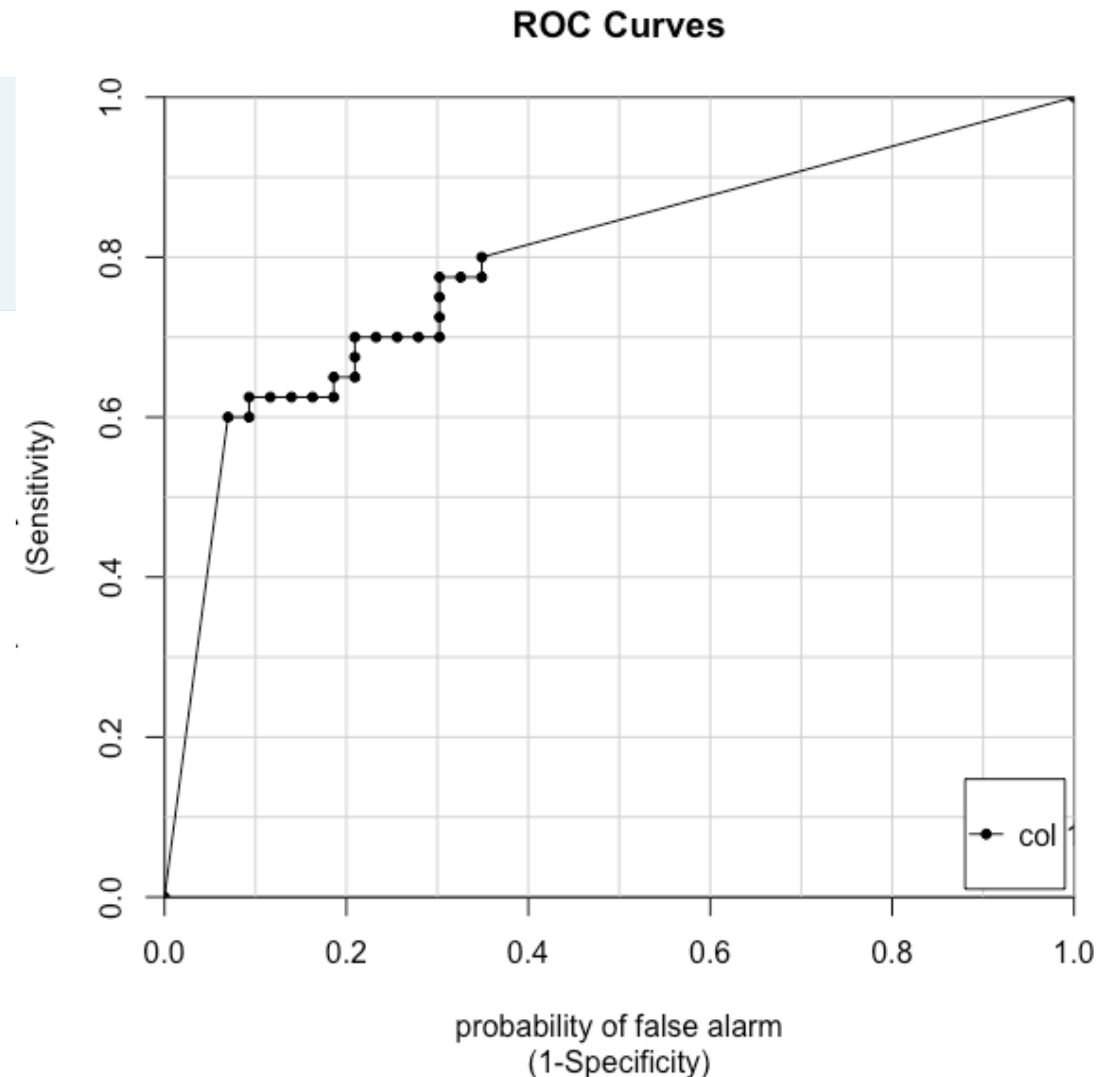
ROC curves

- Plot true/false positive rate at every possible threshold
- Visualize tradeoffs between two extremes **100% true positive rate vs. 0% false positive rate**
- Result is an ROC curve
- Developed as a method for analyzing radar signals

An example ROC curve

```
# Create ROC curve  
> library(caTools)  
> colAUC(p, test[["Class"]], plotROC = TRUE)
```

- X-axis: false positive rate
- Y-axis: true positive rate
- Each point along the curve represents a different threshold





MACHINE LEARNING TOOLBOX

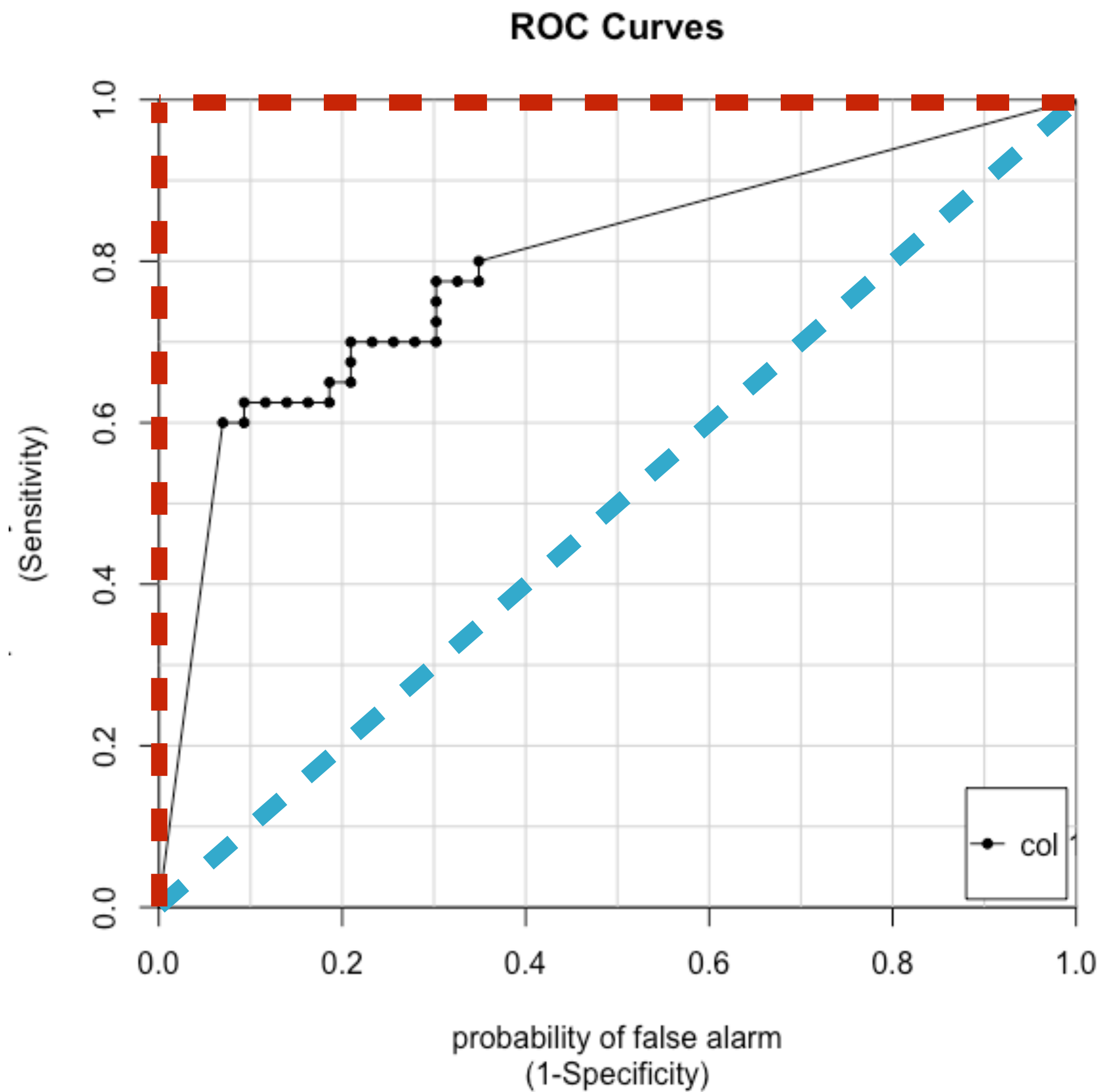
Let's practice!



MACHINE LEARNING TOOLBOX

Area under the curve (AUC)

From ROC to AUC



Defining AUC

- Single-number summary of model accuracy
- Summarizes performance across all thresholds
- Rank different models within the same dataset

Defining AUC

- Ranges from 0 to 1
 - 0.5 = random guessing
 - 1 = model always right
 - 0 = model always wrong
- Rule of thumb: AUC as a letter grade
 - 0.9 = "A"
 - 0.8 = "B"
 - ...



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Random forests and wine

Random forests

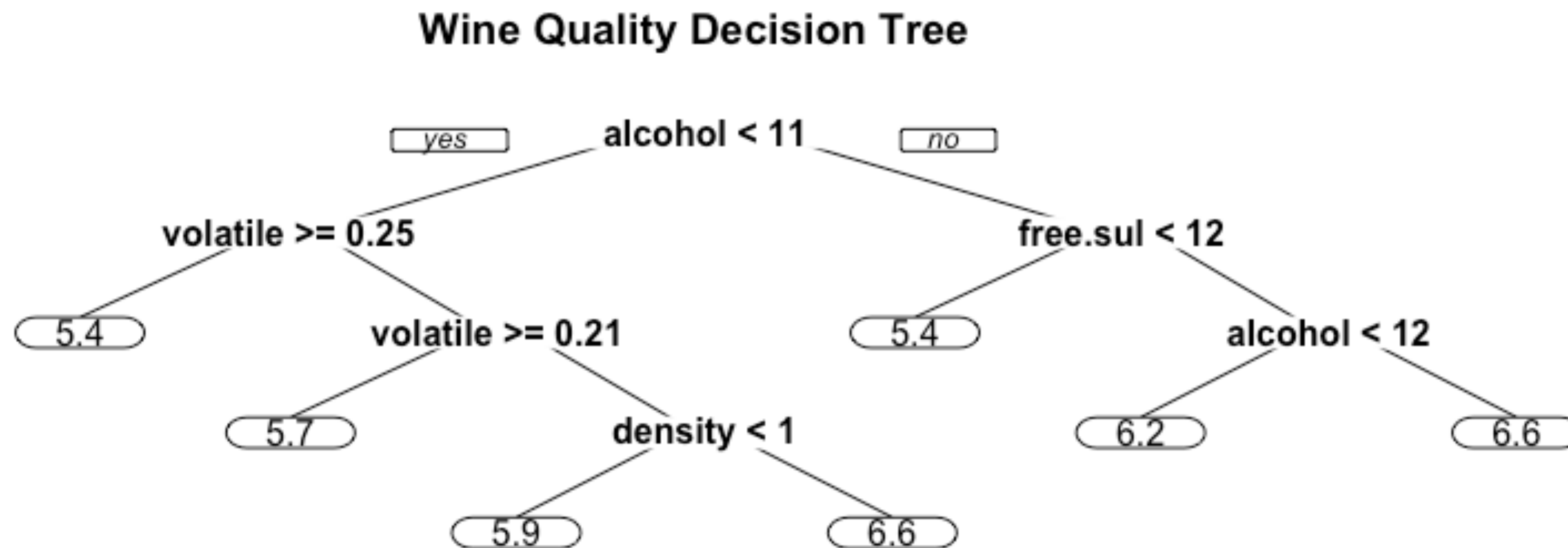
- Popular type of machine learning model
- Good for beginners
- Robust to overfitting
- Yield very accurate, non-linear models

Random forests

- Unlike linear models, they have *hyperparameters*
- Hyperparameters require manual specification
- Can impact model fit and vary from dataset-to-dataset
- Default values often OK, but occasionally need adjustment

Random forests

- Start with a simple decision tree
- Decision trees are fast, but not very accurate



Random forests

- Improve accuracy by fitting many trees
- Fit each one to a bootstrap sample of your data
- Called *bootstrap aggregation* or *bagging*
- Randomly sample columns at each split

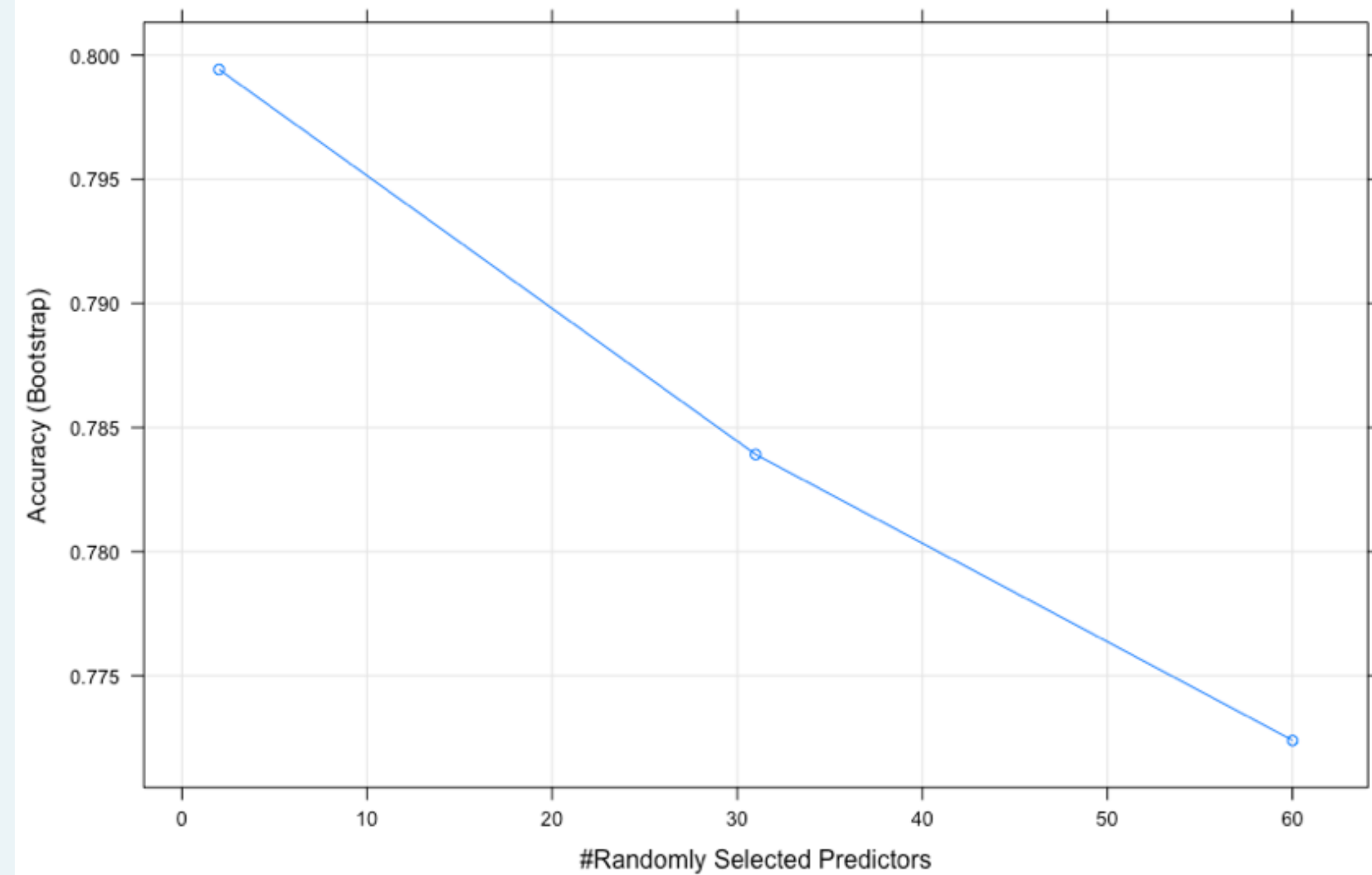
Random forests

```
# Load some data
> library(caret)
> library(mlbench)
> data(Sonar)

# Set seed
> set.seed(42)

# Fit a model
> model <- train(Class~.,
                 data = Sonar,
                 method = "ranger"
               )

# Plot the results
> plot(model)
```





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

**Explore a wider
model space**

Random forests require tuning

- *Hyperparameters* control how the model is fit
- Selected "by hand" before the model is fit
- Most important is `mtry`
 - Number of randomly selected variables used at each split
 - Lower value = more random
 - Higher value = less random
- Hard to know the best value in advance

`caret` to the rescue!

- Not only does `caret` do cross-validation...
- It also does *grid search*
- Select hyperparameters based on out-of-sample error

Example: sonar data

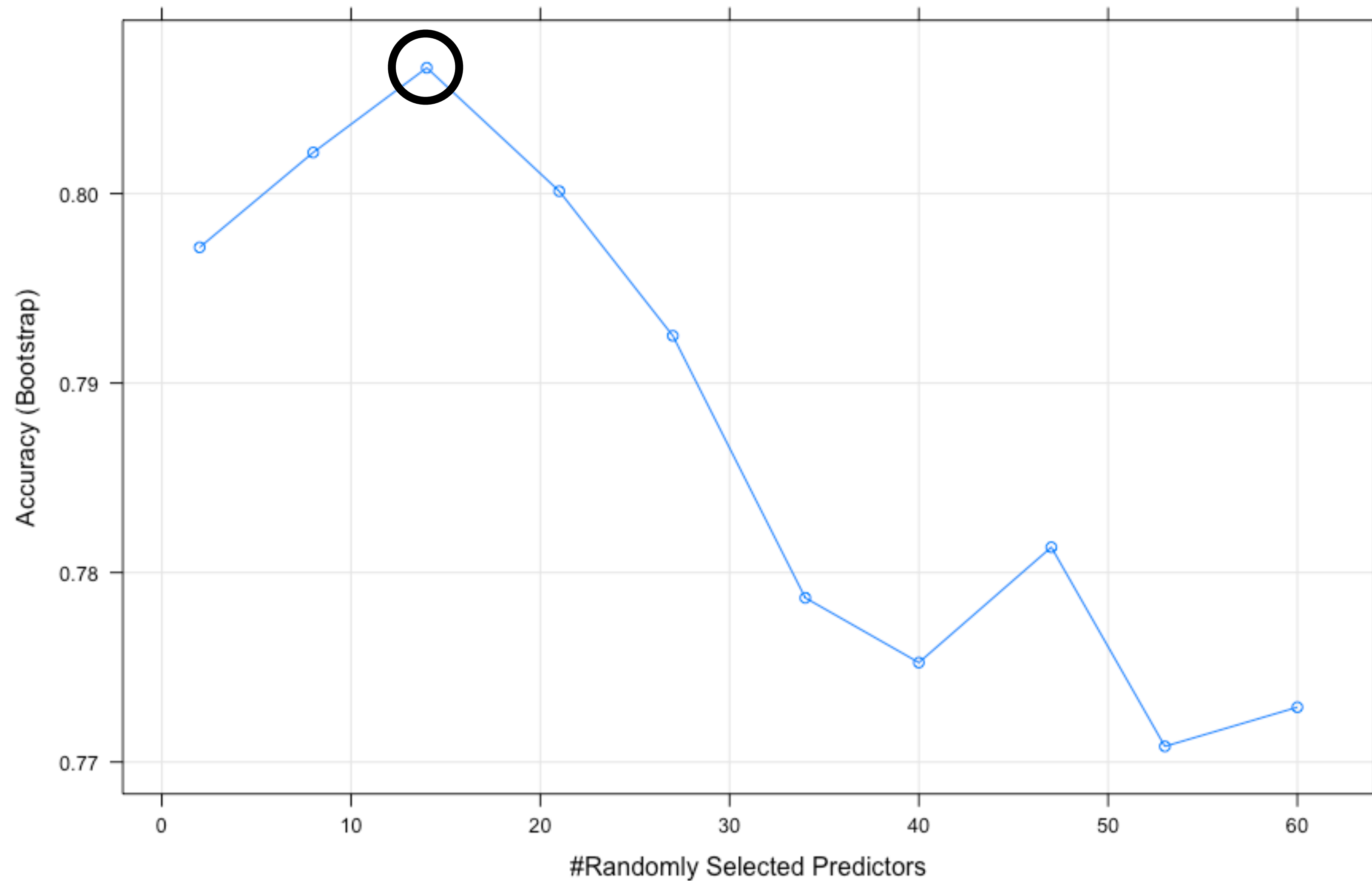
- `tuneLength` argument to `caret::train()`
- Tells `caret` how many different variations to try

```
# Load some data
> library(caret)
> library(mlbench)
> data(Sonar)

# Fit a model with a deeper tuning grid
> model <- train(Class~., data = Sonar,
                 method = "ranger", tuneLength = 10)

# Plot the results
> plot(model)
```

Plot the results





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Custom tuning grids

Pros and cons of custom tuning

- Pass custom tuning grids to `tuneGrid` argument
- Advantages
 - Most flexible method for fitting `caret` models
 - Complete control over how the model is fit
- Disadvantages
 - Requires some knowledge of the model
 - Can dramatically increase run time

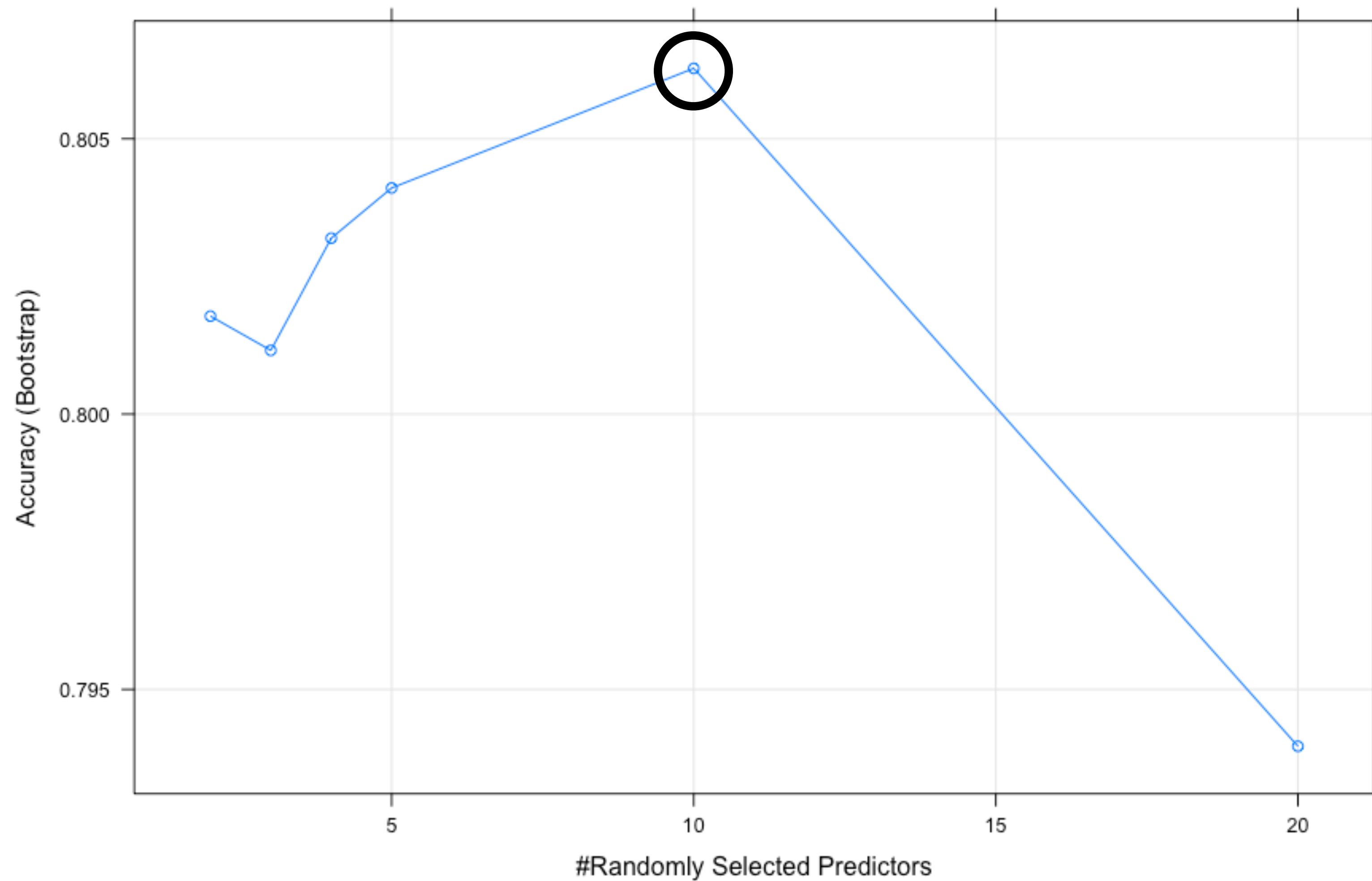
Custom tuning example

```
# Define a custom tuning grid
> myGrid <- data.frame(mtry = c(2, 3, 4, 5, 10, 20))

# Fit a model with a custom tuning grid
> set.seed(42)
> model <- train(Class ~ ., data = Sonar, method = "ranger",
                 tuneGrid = myGrid)

# Plot the results
> plot(model)
```

Custom tuning





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Introducing glmnet

Introducing `glmnet`

- Extension of `glm` models with built-in variable selection
- Helps deal with *collinearity* and small samples sizes
- Two primary forms
 - Lasso regression **Penalizes number of non-zero coefficients**
 - Ridge regression **Penalizes absolute magnitude of coefficients**
- Attempts to find a parsimonious (i.e. simple) model
- Pairs well with random forest models

Tuning `glmnet` models

- Combination of lasso and ridge regression
- Can fit a mix of the two models
- α [0, 1]: pure lasso to pure ridge
- λ (0, infinity): size of the penalty

Example: "don't overfit"

```
# Load data
> overfit <- read.csv("http://s3.amazonaws.com/assets.datacamp.com/
production/course_1048/datasets/overfit.csv")

# Make a custom trainControl
> myControl <- trainControl(
  method = "cv", number = 10,
  summaryFunction = twoClassSummary,
  classProbs = TRUE, # Super important!
  verboseIter = TRUE
)
```

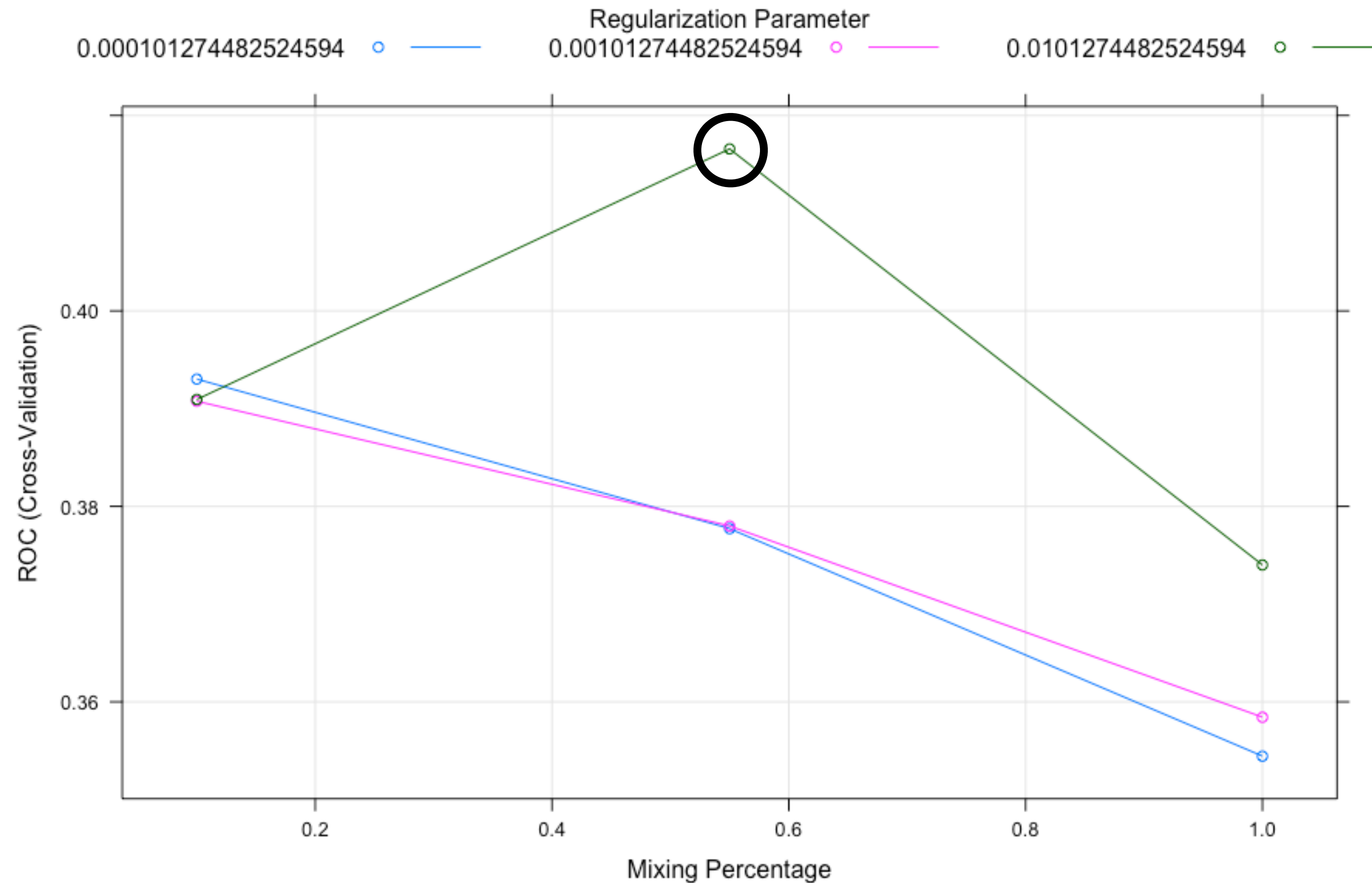
Try the defaults

```
# Fit a model
> set.seed(42)
> model <- train(y ~ ., overfit, method = "glmnet",
                 trControl = myControl)

# Plot results
> plot(model)
```

- 3 values of α
- 3 values of λ

Plot the results





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

glmnet with custom tuning grid

Custom tuning `glmnet` models

- 2 tuning parameters: α and λ
- For single α , all values of λ fit simultaneously
- Many models for the "price" of one

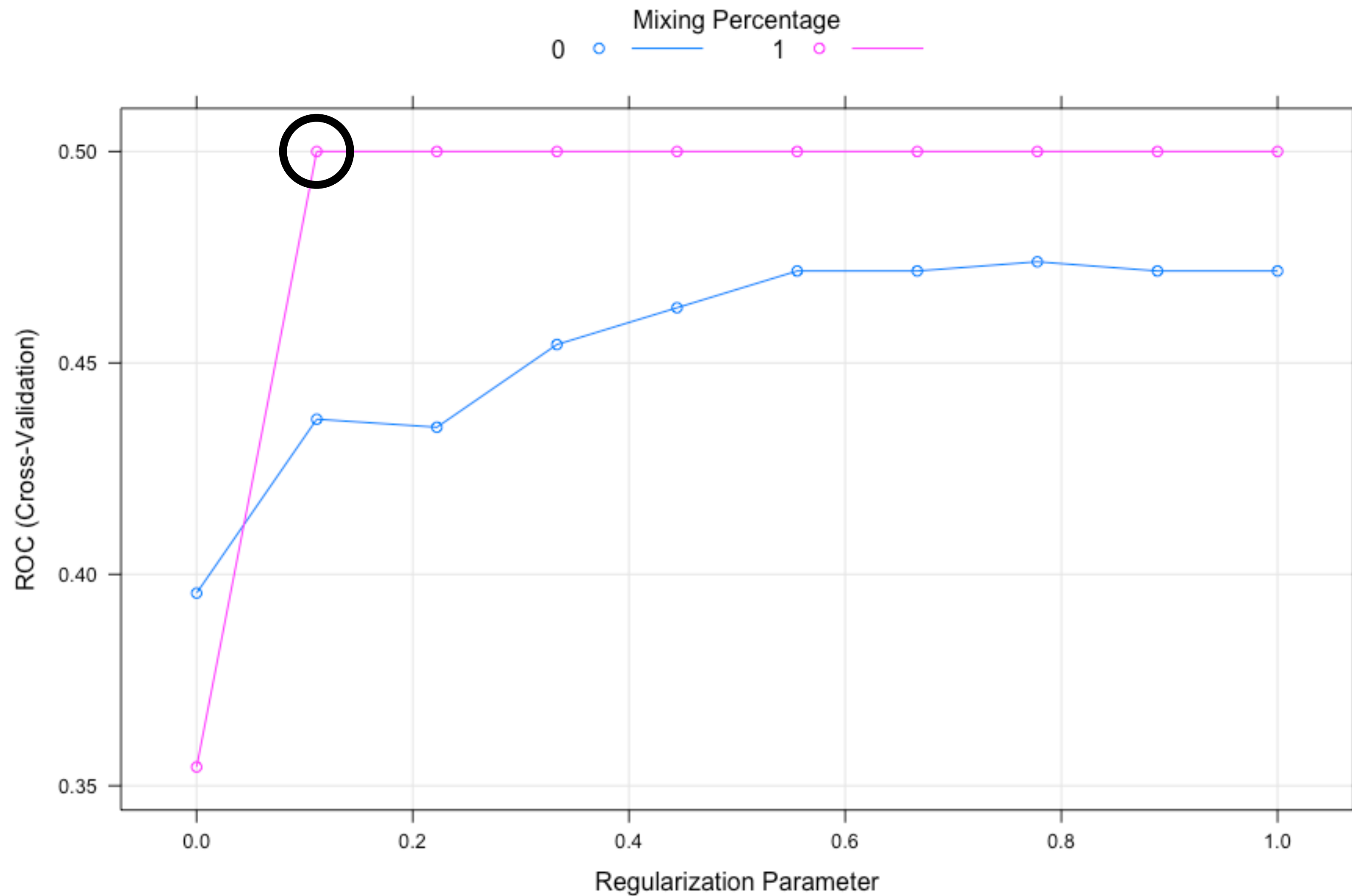
Example: glmnet tuning

```
# Make a custom tuning grid
> myGrid <- expand.grid(
  alpha = 0:1,
  lambda = seq(0.0001, 0.1, length = 10)
)

# Fit a model
> set.seed(42)
> model <- train(y ~ ., overfit, method = "glmnet",
  tuneGrid = myGrid, trControl = myControl)

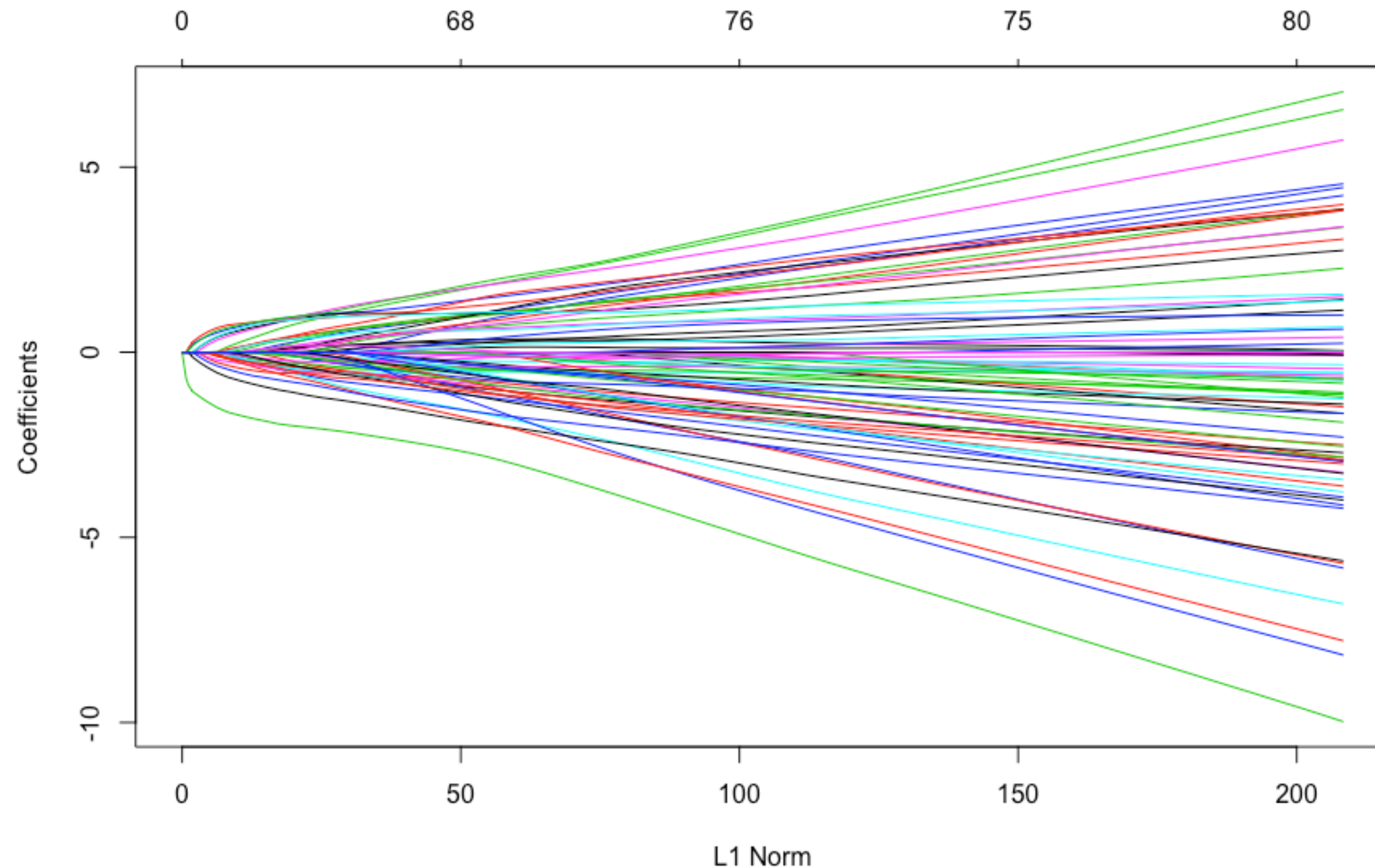
# Plot results
> plot(model)
```

Compare models visually



Full regularization path

```
> plot(model$finalModel)
```





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Median imputation

Dealing with missing values

- Most models require numbers, can't handle missing data
- Common approach: remove rows with missing data
 - Can lead to biases in data
 - Generate over-confident models
- Better strategy: median imputation!
 - Replace missing values with medians
 - Works well if data *missing at random* (MAR)

Example: mtcars

```
# Generate some data with missing values
> data(mtcars)
> set.seed(42)
> mtcars[sample(1:nrow(mtcars), 10), "hp"] <- NA

# Split target from predictors
> Y <- mtcars$mpg
> X <- mtcars[, 2:4]

# Try to fit a caret model
> library(caret)
> model <- train(x = X, y = Y)
Error in train.default(x = X, y = Y) : Stopping
```

A simple solution

```
# Now fit with median imputation
> model <- train(x = X, y = Y, preProcess = "medianImpute")
> print(model)
Random Forest
```

```
32 samples
 3 predictor
```

```
Pre-processing: median imputation (3)
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 32, 32, 32, 32, 32, 32, ...
Resampling results across tuning parameters:
```

mtry	RMSE	Rsquared
2	2.617096	0.8234652
3	2.670550	0.8164535

RMSE was used to select the optimal model using the smallest value.
The final value used for the model was mtry = 2.



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

KNN imputation

Dealing with missing values

- Median imputation is fast, but...
- Can produce incorrect results if data *missing not at random*
- k-nearest neighbors (KNN) imputation
- Imputes based on "similar" non-missing rows

Example: missing not at random

- Pretend smaller cars don't report horsepower
- Median imputation incorrect in this case **Assumes small cars have medium-large horsepower**

```
# Generate data with missing values
> data(mtcars)
> mtcars[mtcars$disp < 140, "hp"] <- NA
> Y <- mtcars$mpg
> X <- mtcars[, 2:4]

# Use median imputation
> set.seed(42)
> model <- train(x = X, y = Y, method = "glm",
                 preProcess = "medianImpute")
> print(min(model$results$RMSE))
[1] 3.612713
```

Example: missing not at random

- KNN imputation is better
- Uses cars with similar `disp` / `cyl` to impute
- Yields a more accurate (but slower) model

```
# Use KNN imputation
> set.seed(42)
> model <- train(x = X, y = Y,
                 method = "glm",
                 preProcess = "knnImpute"
               )
> print(min(model$results$RMSE))
[1] 3.558881 Compare to 3.61 for median imputation
```



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Multiple preprocessing methods

The wide world of preProcess

- You can do a lot more than median or knn imputation!
- Can chain together multiple preprocessing steps
- Common "recipe" for linear models (order matters!)
Median imputation -> center -> scale -> fit glm
- See ?preProcess for more detail

Example: preprocessing mtcars

```
# Generate some data with missing values
> data(mtcars)
> set.seed(42)
> mtcars[sample(1:nrow(mtcars), 10), "hp"] <- NA
> Y <- mtcars$mpg
> X <- mtcars[,2:4]      Missing at random

# Use linear model "recipe"
> set.seed(42)
> model <- train(
  x = X, y = Y, method = "glm",
  preProcess = c("medianImpute", "center", "scale")
)
> print(min(model$results$RMSE))
[1] 3.612713
```

Example: preprocessing mtcars

```
# PCA before modeling
> set.seed(42)
> model <- train(
  x = X, y = Y, method = "glm",
  preProcess = c("medianImpute", "center", "scale", "pca")
)
> min(model$results$RMSE)
[1] 3.402557
```

Example: preprocessing mtcars

```
# Spatial sign transform  
> set.seed(42)  
> model <- train(  
  x = X, y = Y, method = "glm",  
  preProcess = c("medianImpute", "center", "scale", "spatialSign"))  
> min(model$results$RMSE)  
[1] 4.284904
```

Preprocessing cheat sheet

- Start with median imputation **Try KNN imputation if data missing not at random**
- For linear models...
 - Center and scale
 - Try PCA and spatial sign
- Tree-based models don't need much preprocessing



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Handling low-information predictors

No (or low) variance variables

- Some variables don't contain much information
 - Constant (i.e. no variance)
 - Nearly constant (i.e. low variance)
- Easy for one fold of CV to end up with constant column
- Can cause problems for your models
- Usually remove extremely low variance variables

Example: constant column in mtcars

```
# Reproduce dataset from last video
> data(mtcars)
> set.seed(42)
> mtcars[sample(1:nrow(mtcars), 10), "hp"] <- NA
> Y <- mtcars$mpg
> X <- mtcars[, 2:4]

# Add constant-valued column to mtcars
> X$bad <- 1
```

Example: constant column in mtcars

```
# Try to fit a model with PCA + glm
> model <- train(
  x = X, y = Y, method = "glm",
  preProcess = c("medianImpute", "center", "scale", "pca")
)
```

Warning in preProcess.default(thresh = 0.95, k = 5, method =
c("medianImpute", :

These variables have zero variances: bad

Something is wrong; all the RMSE metric values are missing:

RMSE	Rsquared
Min. : NA	Min. : NA
1st Qu.: NA	1st Qu.: NA
Median : NA	Median : NA
Mean : NaN	Mean : NaN
3rd Qu.: NA	3rd Qu.: NA
Max. : NA	Max. : NA
NA's : 1	NA's : 1

caret to the rescue (again)

- "zv" removes constant columns
- "nzv" removes nearly constant columns

```
# Have caret remove those columns during modeling
> set.seed(42)
> model <- train(
  x = X, y = Y, method = "glm",
  preProcess = c("zv", "medianImpute", "center", "scale", "pca")
)
> min(model$results$RMSE)
[1] 3.402557
```



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

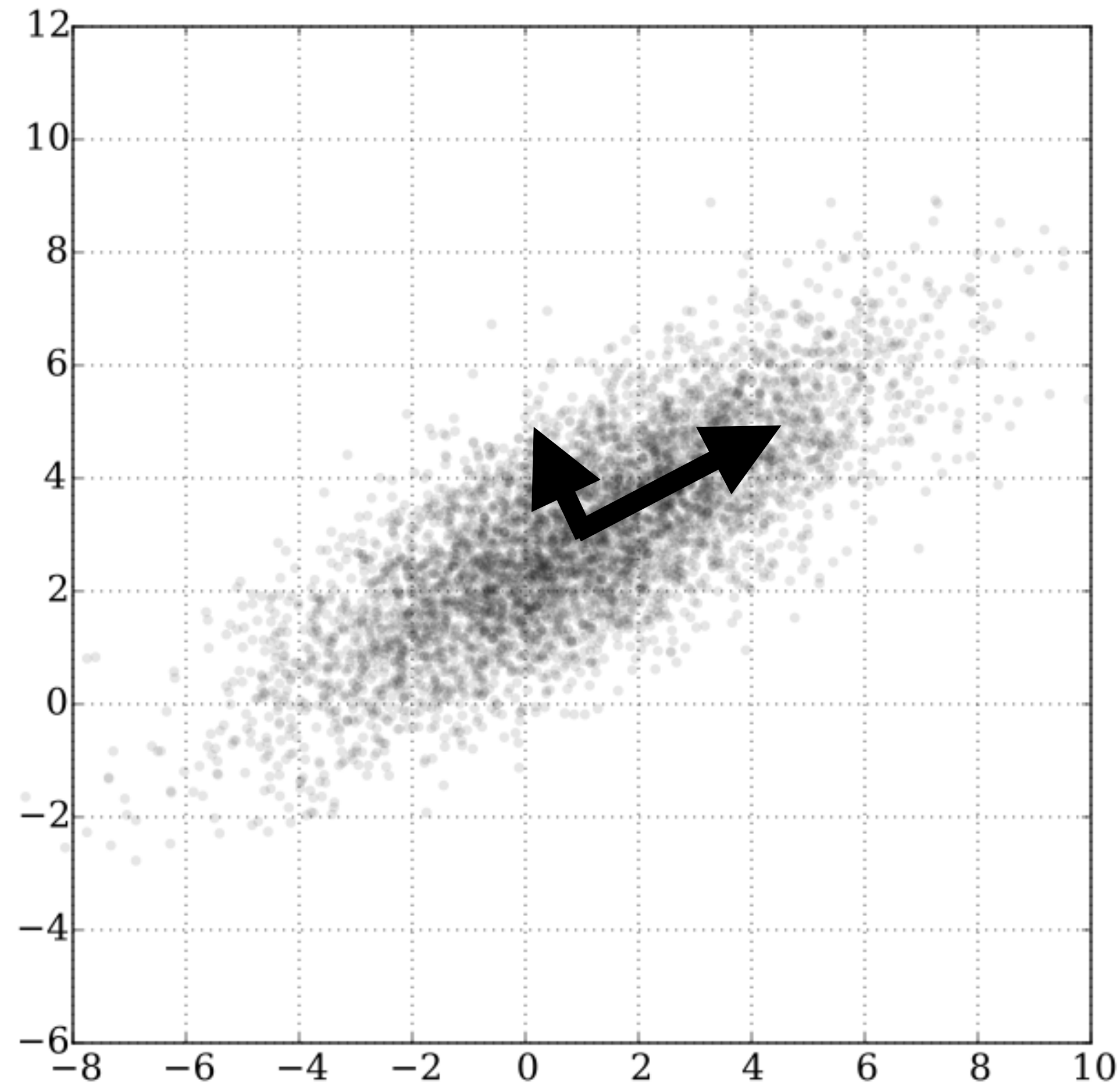
Principle components analysis (PCA)

Principle components analysis

- Combines low-variance and correlated variables
- Single set of high-variance, perpendicular predictors
- Prevents collinearity (i.e. correlation among predictors)

PCA: a visual representation

- First component has highest variance
- Second component has second highest variance
- And so on...



Example: blood-brain data

- Lots of predictors
- Many of them low-variance

```
# Load the blood brain dataset
> data(BloodBrain)
> names(bbbDescr)[nearZeroVar(bbbDescr)]
[1] "negative"      "peoe_vsa.2.1" "peoe_vsa.3.1" "a_acid"
[5] "vsa_acid"      "frac.anion7." "alert"
```

Example: blood-brain data

```
# Basic model
> set.seed(42)
> data(BloodBrain)
> model <- train(
  x = bbbDescr, y = logBBB, method = "glm",
  trControl = trainControl(method = "cv", number = 10, verbose = TRUE),
  preProcess = c("zv", "center", "scale")
)
> min(model$results$RMSE)
[1] 1.107702
```

Example: blood-brain data

```
# Remove low-variance predictors
> set.seed(42)
> data(BloodBrain)
> model <- train(
  x = bbbDescr, y = logBBB, method = "glm",
  trControl = trainControl(method = "cv", number = 10, verbose = TRUE),
  preProcess = c("nzv", "center", "scale")
)
> min(model$results$RMSE)
[1] 0.9796199
```

Example: blood-brain data

```
# Add PCA
> set.seed(42)
> data(BloodBrain)
> model <- train(
  x = bbbDescr, y = logBBB, method = "glm",
  trControl = trainControl(method = "cv", number = 10, verbose = TRUE),
  preProcess = c("zv", "center", "scale", "pca")
)
> min(model$results$RMSE)
[1] 0.9796199
```



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Reusing a `trainControl`

A real-world example

- The data: customer churn at telecom company
- Fit different models and choose the best
- Models must use the same training/test splits
- Create a shared `trainControl` object

Example: customer churn data

```
# Summarize the target variables
> library(caret)
> library(C50)
> data(churn)
> table(churnTrain$churn) / nrow(churnTrain)
```

yes	no
0.1449145	0.8550855

```
# Create train/test indexes
> set.seed(42)
> myFolds <- createFolds(churnTrain$churn, k = 5)
```

```
# Compare class distribution
> i <- myFolds$Fold1
> table(churnTrain$churn[i]) / length(i)
```

yes	no
0.1441441	0.8558559

Example: customer churn data

```
> myControl <- trainControl(  
  summaryFunction = twoClassSummary,  
  classProbs = TRUE,  
  verboseIter = TRUE,  
  savePredictions = TRUE,  
  index = myFolds  
)
```

- Use folds to create a `trainControl` object
- Exact same cross-validation folds for each model



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Reintroduce glmnet

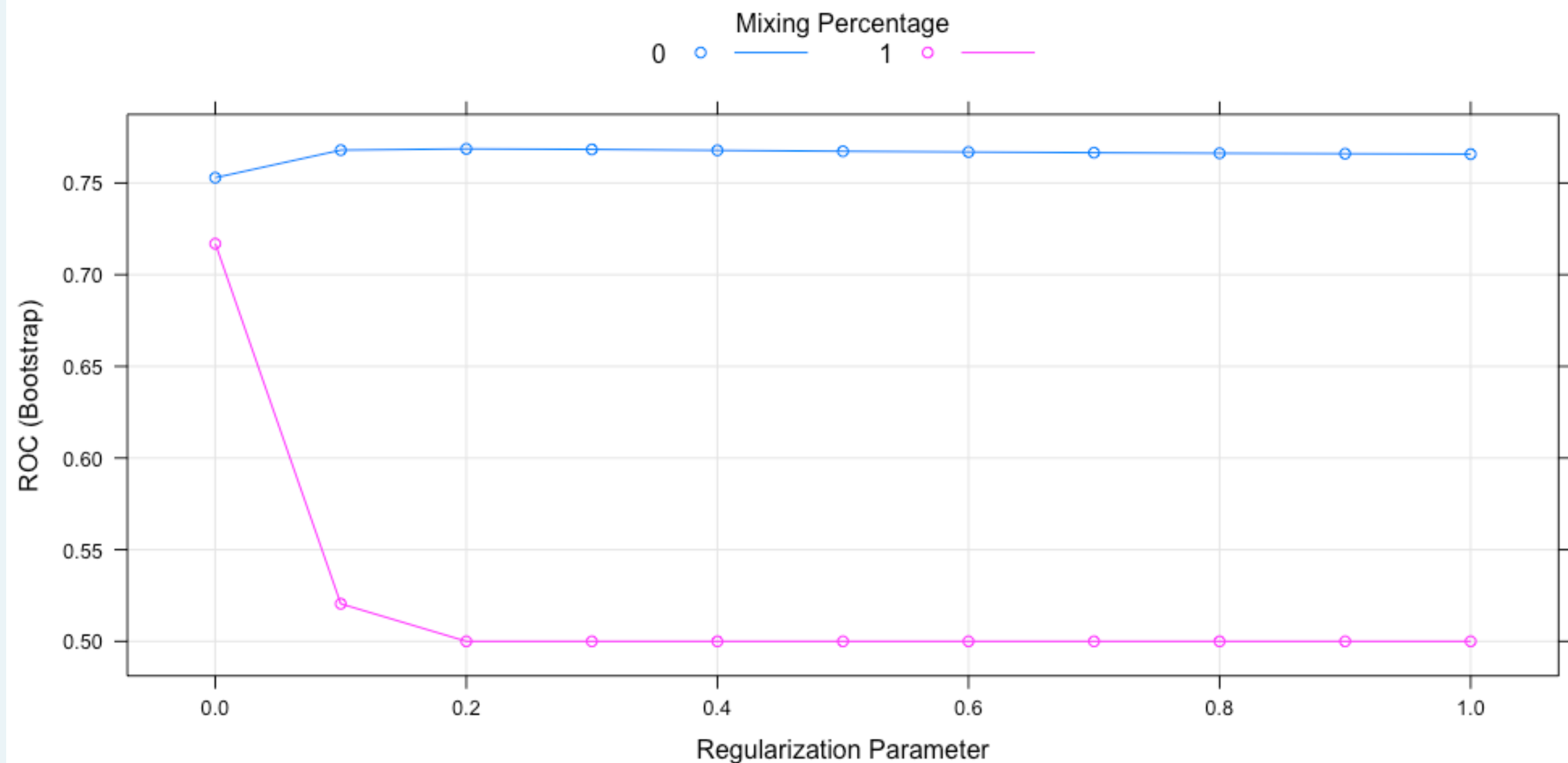
glmnet review

- Linear model with built-in variable selection
- Great baseline model
- Advantages
 - Fits quickly
 - Ignores noisy variables
 - Provides interpretable coefficients

Example: glmnet on churn data

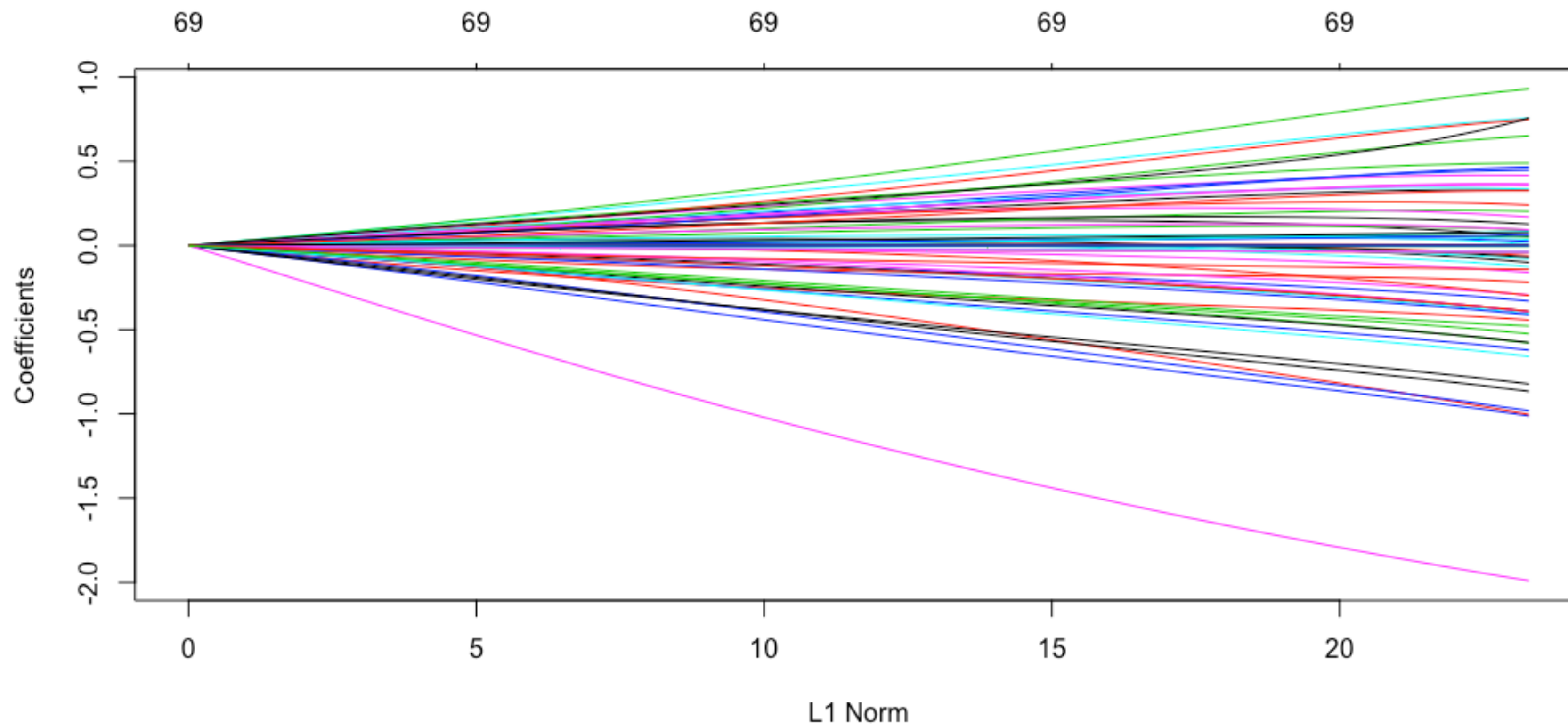
```
> # Fit the model
> set.seed(42)
> model_glmnet <- train(
  churn ~ ., churnTrain,
  metric = "ROC",
  method = "glmnet",
  tuneGrid = expand.grid(
    alpha = 0:1,
    lambda = 0:10/10
  ),
  trControl = myControl
)

> # Plot the results
> plot(model_glmnet)
```



Plot the coefficients

```
> plot(model_glmnet$finalModel)
```





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Reintroduce random forest

Random forest review

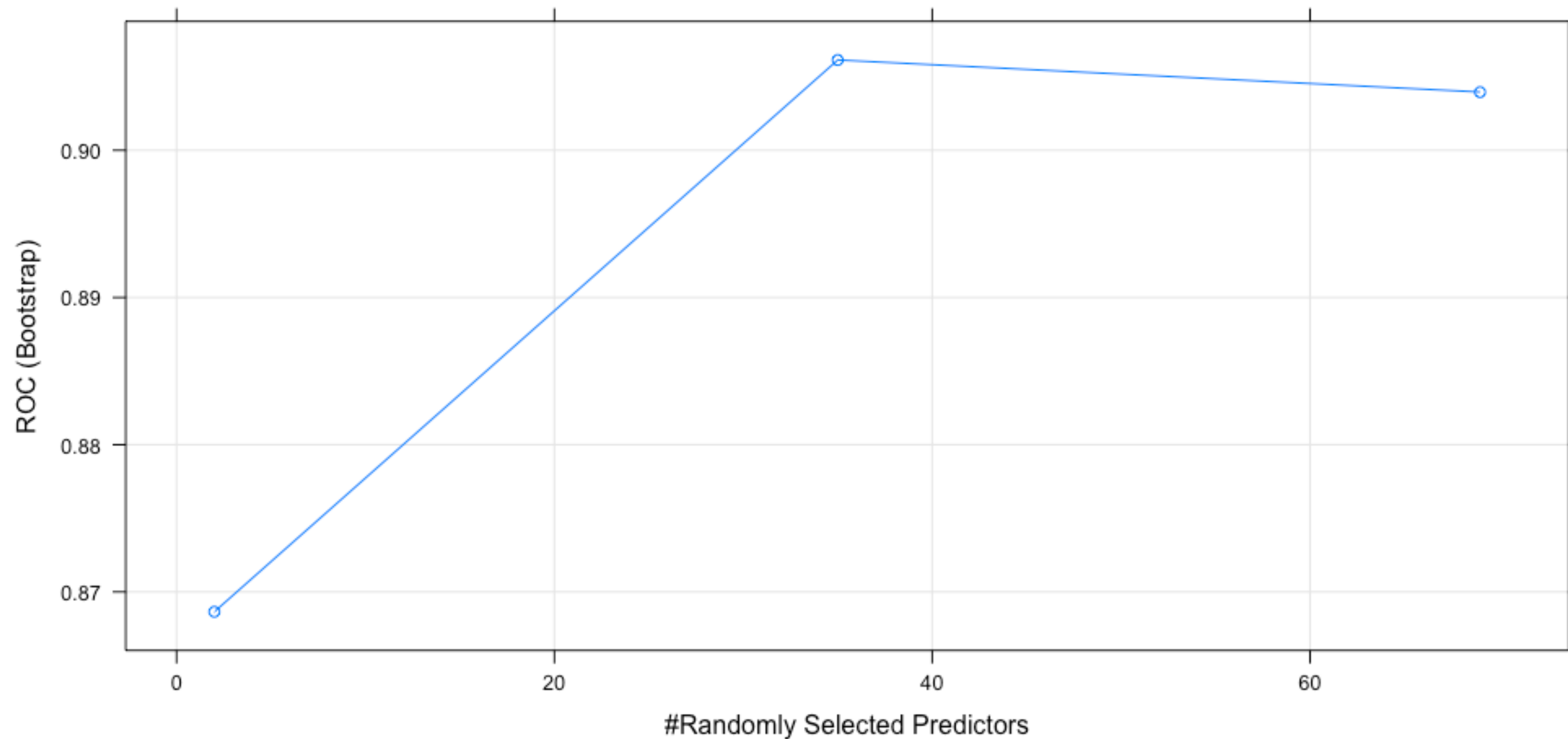
- Slower to fit than `glmnet`
- Less interpretable
- Often (but not always) more accurate than `glmnet`
- Easier to tune
- Require little preprocessing
- Capture threshold effects and variable interactions

Random forest on churn data

```
> set.seed(42)
> churnTrain$churn <- factor(churnTrain$churn, levels = c("no", "yes"))
> model_rf <- train(
  churn ~ ., churnTrain,
  metric = "ROC",
  method = "ranger",
  trControl = myControl
)
```

Random forest on churn data

```
> plot(model_rf)
```





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Comparing models

Comparing models

- Make sure they were fit on the same data!
- Selection criteria
 - Highest average AUC
 - Lowest standard deviation in AUC
- The `resamples()` function is your friend

Example: `resamples()` on churn data

```
# Make a list
> model_list <- list(
  glmnet = model_glmnet,
  rf = model_rf
)

# Collect resamples from the CV folds
> resamps <- resamples(model_list)
> resamps

Call:
resamples.default(x = model_list)

Models: glmnet, rf
Number of resamples: 5
Performance metrics: ROC, Sens, Spec
Time estimates for: everything, final model fit
```

Summarize the results

```
# Summarize the results
> summary(resamps)
Call:
summary.resamples(object = resamps)
```

```
Models: glmnet, rf
Number of resamples: 5
```

ROC

	Min.	1st Qu.	Median	Mean	3rd Qu.	Max.	NA's
glmnet	0.7526	0.7624	0.7719	0.7686	0.7722	0.7840	0
rf	0.8984	0.9028	0.9077	0.9061	0.9093	0.9125	0



MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

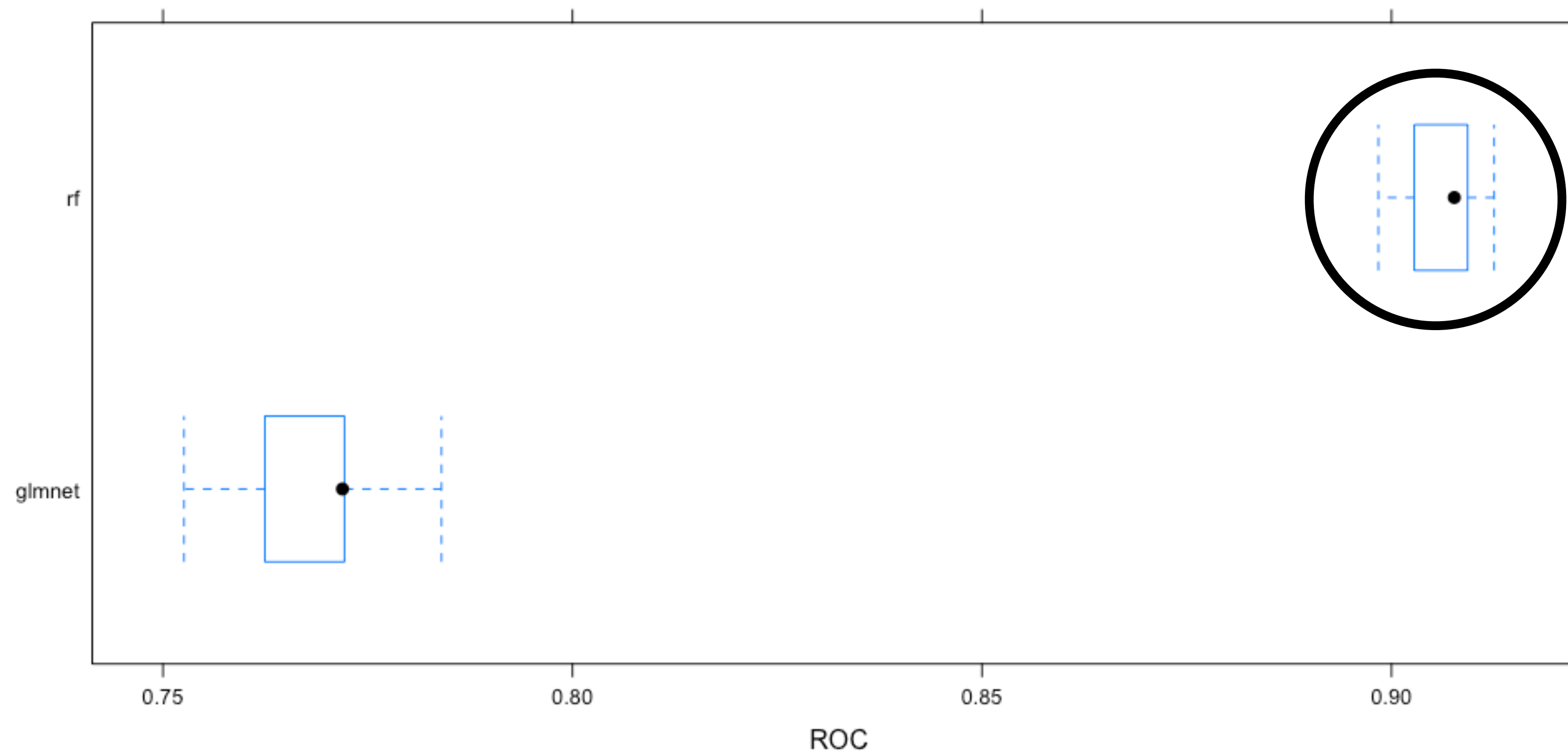
More on resamples

Comparing models

- Resamples has tons of cool methods
- One of my favorite functions (thanks Max!)
- Inspired the `caretEnsemble` package

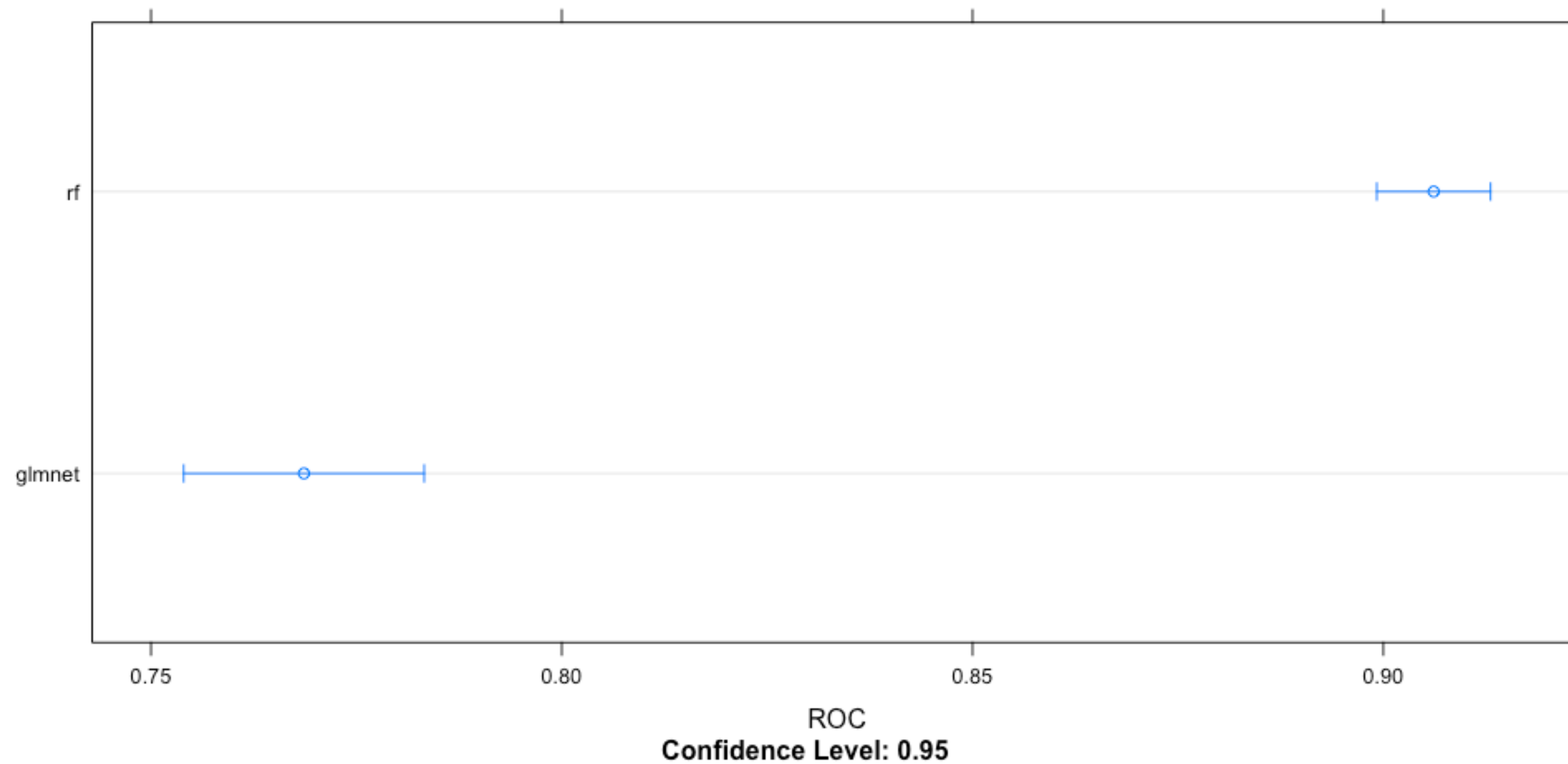
Box-and-whisker

```
> bwplot(resamps, metric = "ROC")
```



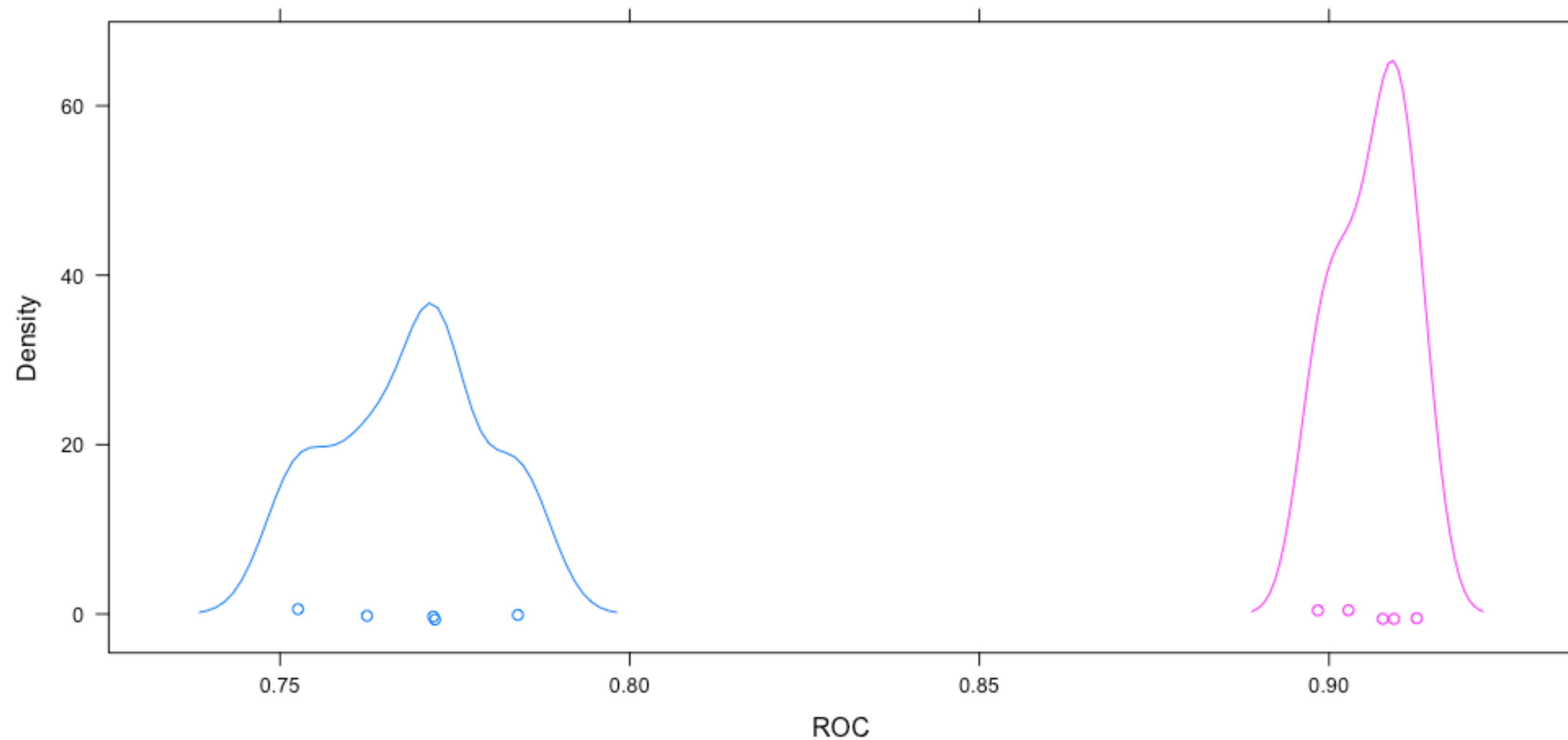
Dot plot

```
> dotplot(resamps, metric = "ROC")
```



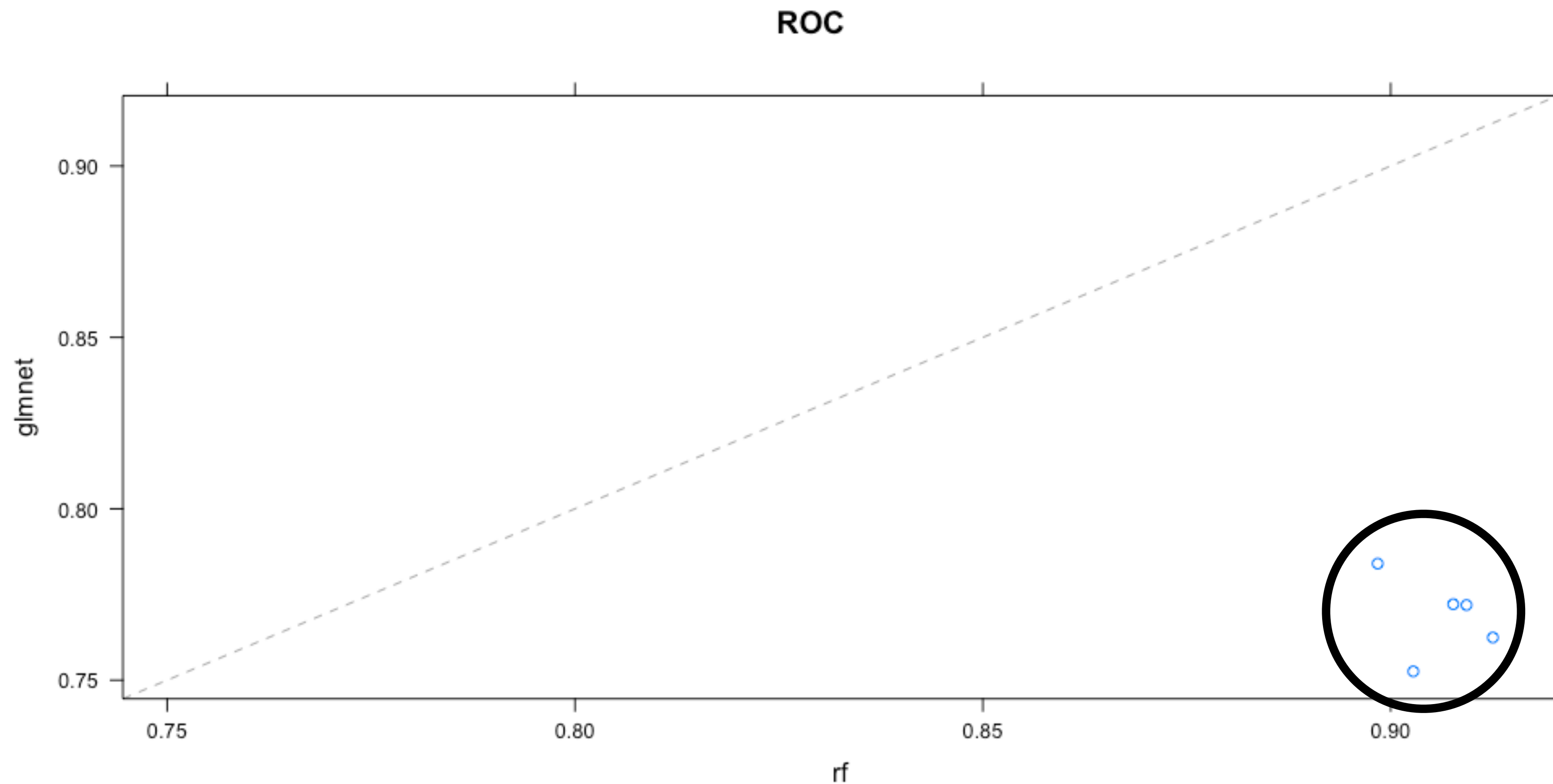
Density plot

```
> densityplot(resamps, metric = "ROC")
```



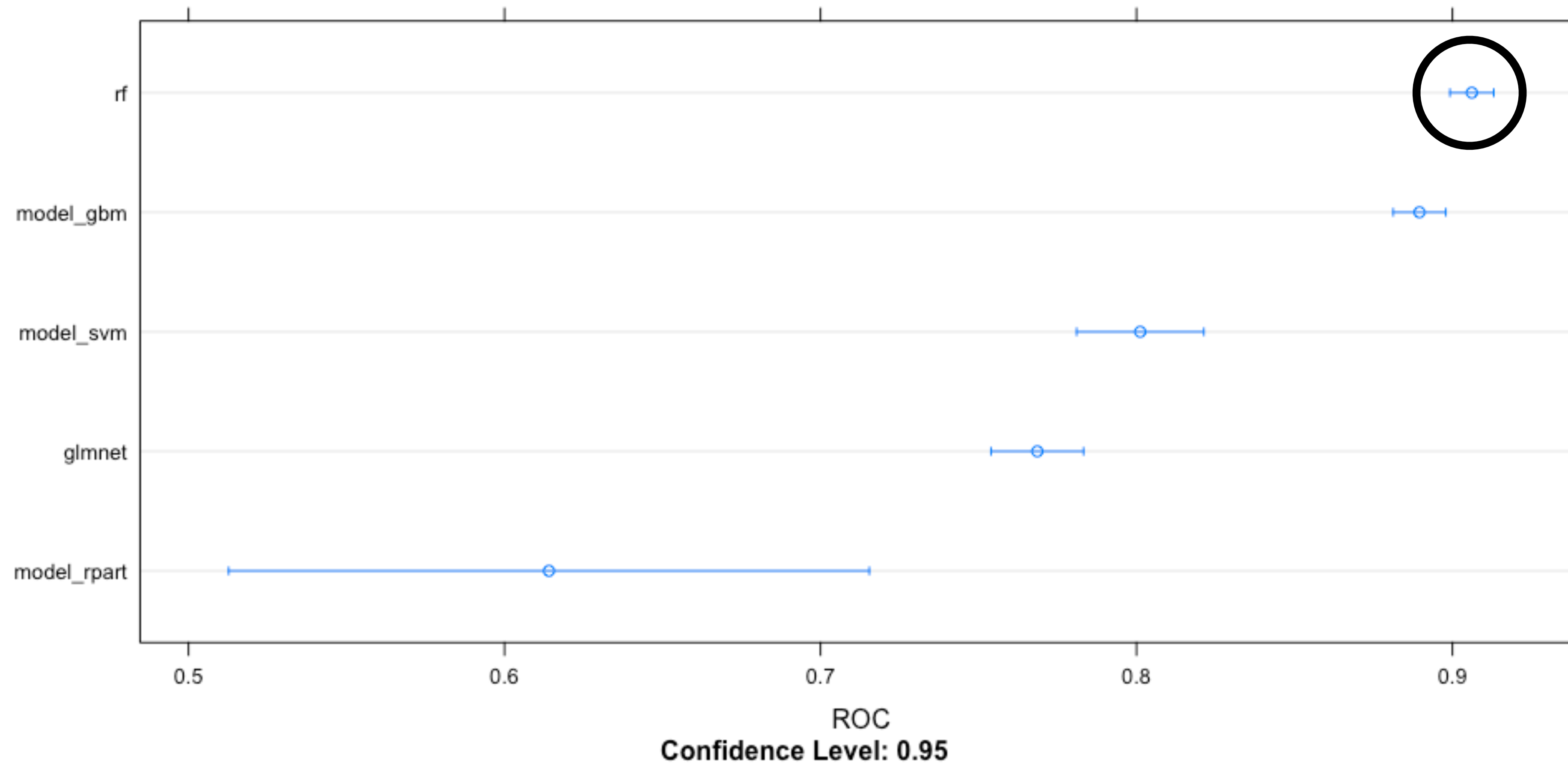
Scatter plot

```
> xyplot(resamps, metric = "ROC")
```



Another dot plot

```
> dotplot(lots_of_models, metric = "ROC")
```





MACHINE LEARNING TOOLBOX

Let's practice!



MACHINE LEARNING TOOLBOX

Summary

What you've learned

- How to use the caret package
- Model fitting and evaluation
- Parameter tuning for better results
- Data preprocessing

Goals of the `caret` package

- Simplify the predictive modeling process
- Make it easy to try many models and techniques
- Provide common interface to many useful packages



MACHINE LEARNING TOOLBOX

Go build some models!