Random forests and wine

MACHINE LEARNING WITH CARET IN R

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Random forests

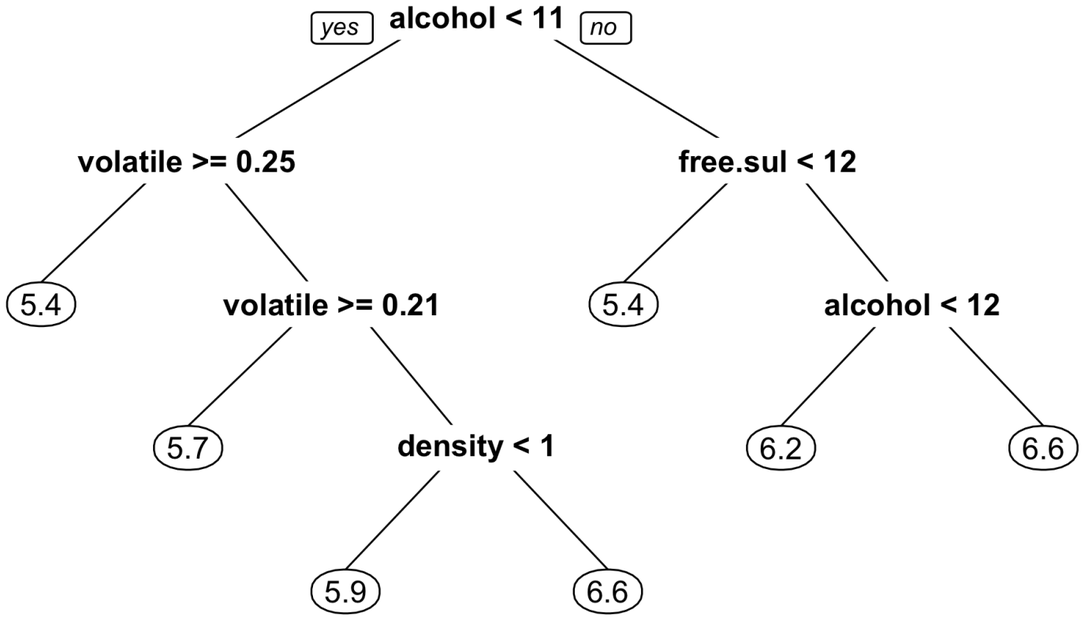
- Popular type of machine learning model
- Good for beginners
- Robust to overfitting
- Yield very accurate, non-linear models

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

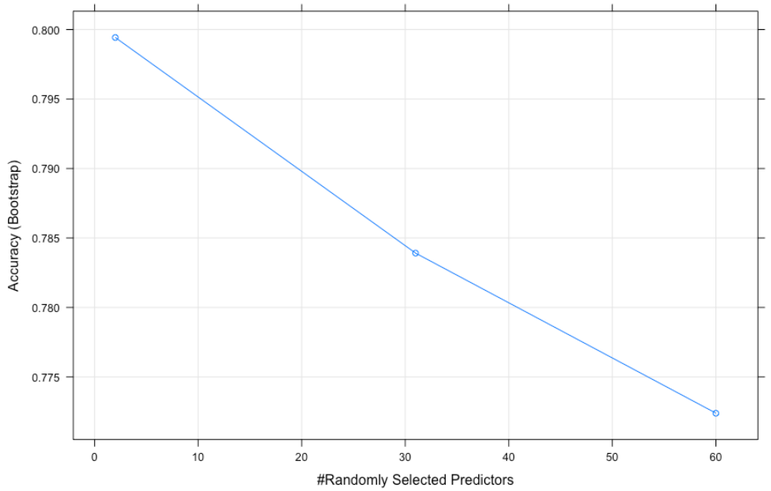


Random forests

- 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

Running a random forest

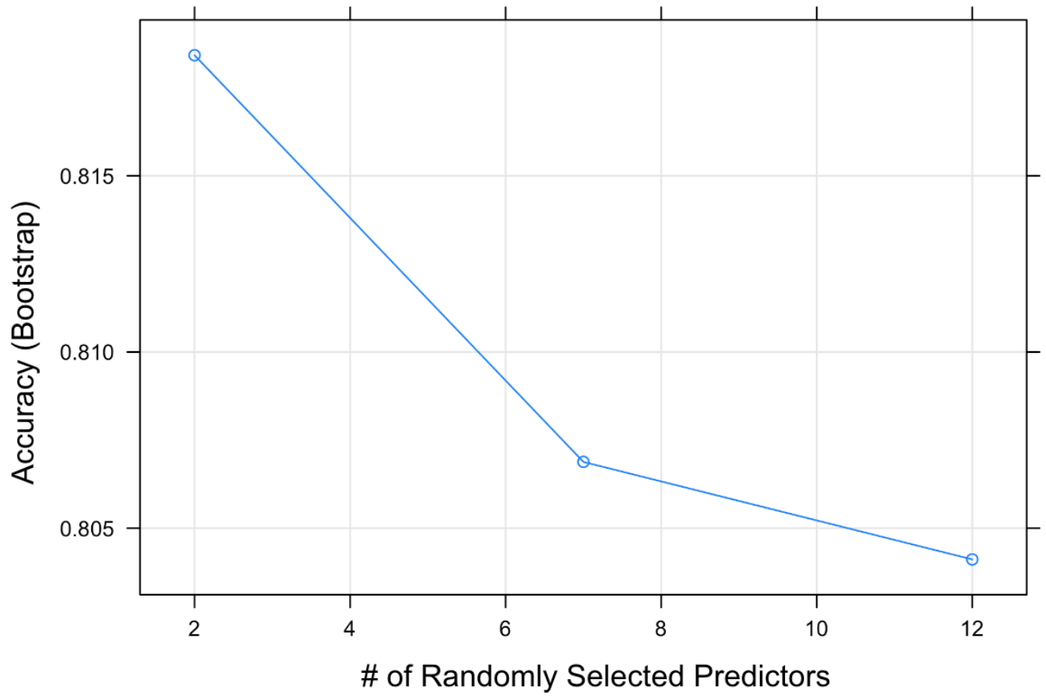
```
# Load some data
library(caret)
library(mlbench)
data(Sonar)

# Set seed
set.seed(42)
```




```
model <- train(
  Class ~ .,
  data = Sonar,
  method = "ranger"
)
```

Plotting the results

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



Let's practice!

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Explore a wider model space

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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

Example: sonar data

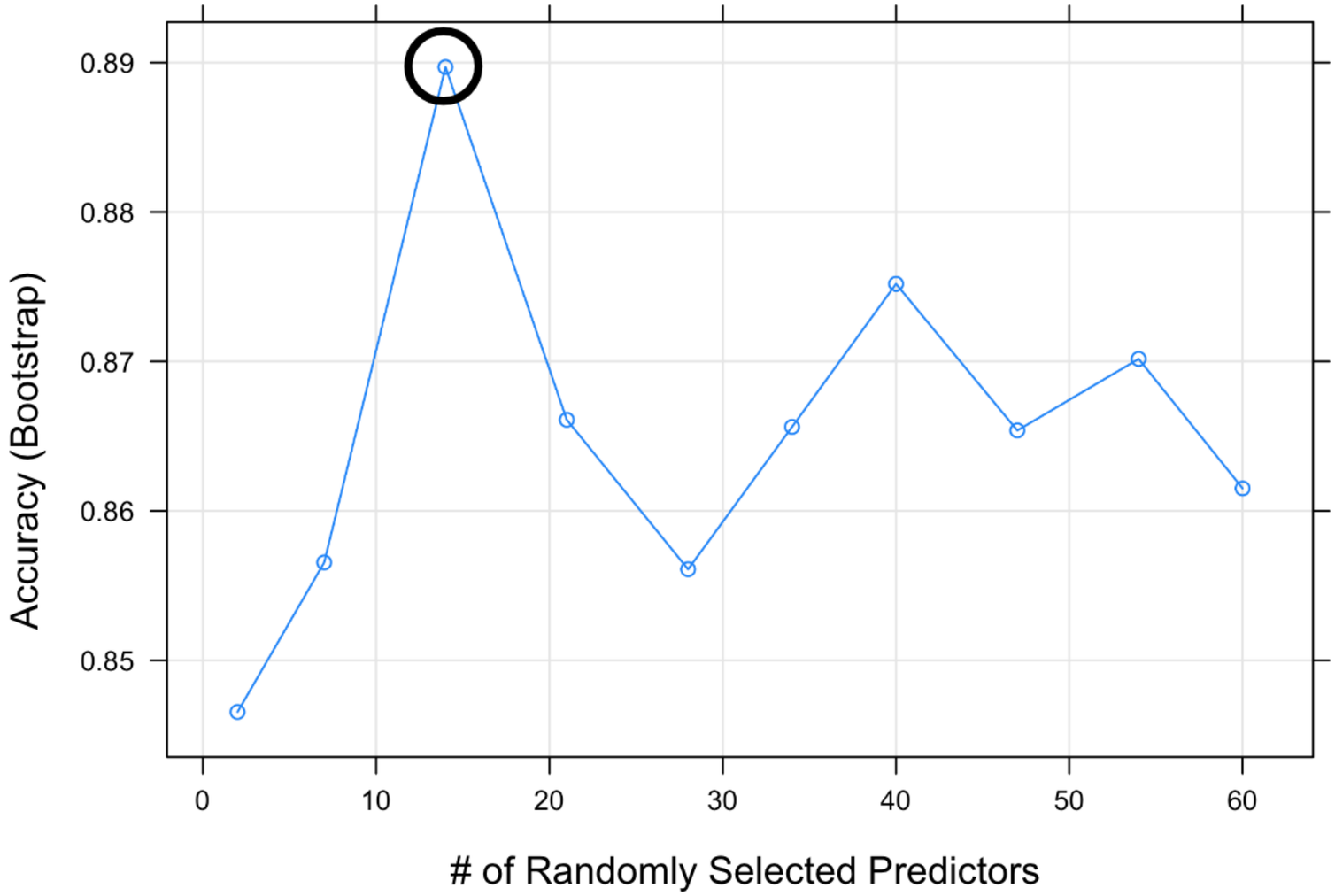
- `tuneLength` argument to `caret::train()`
- Tells `caret` how many different variations to try

```
# 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



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Custom tuning grids

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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

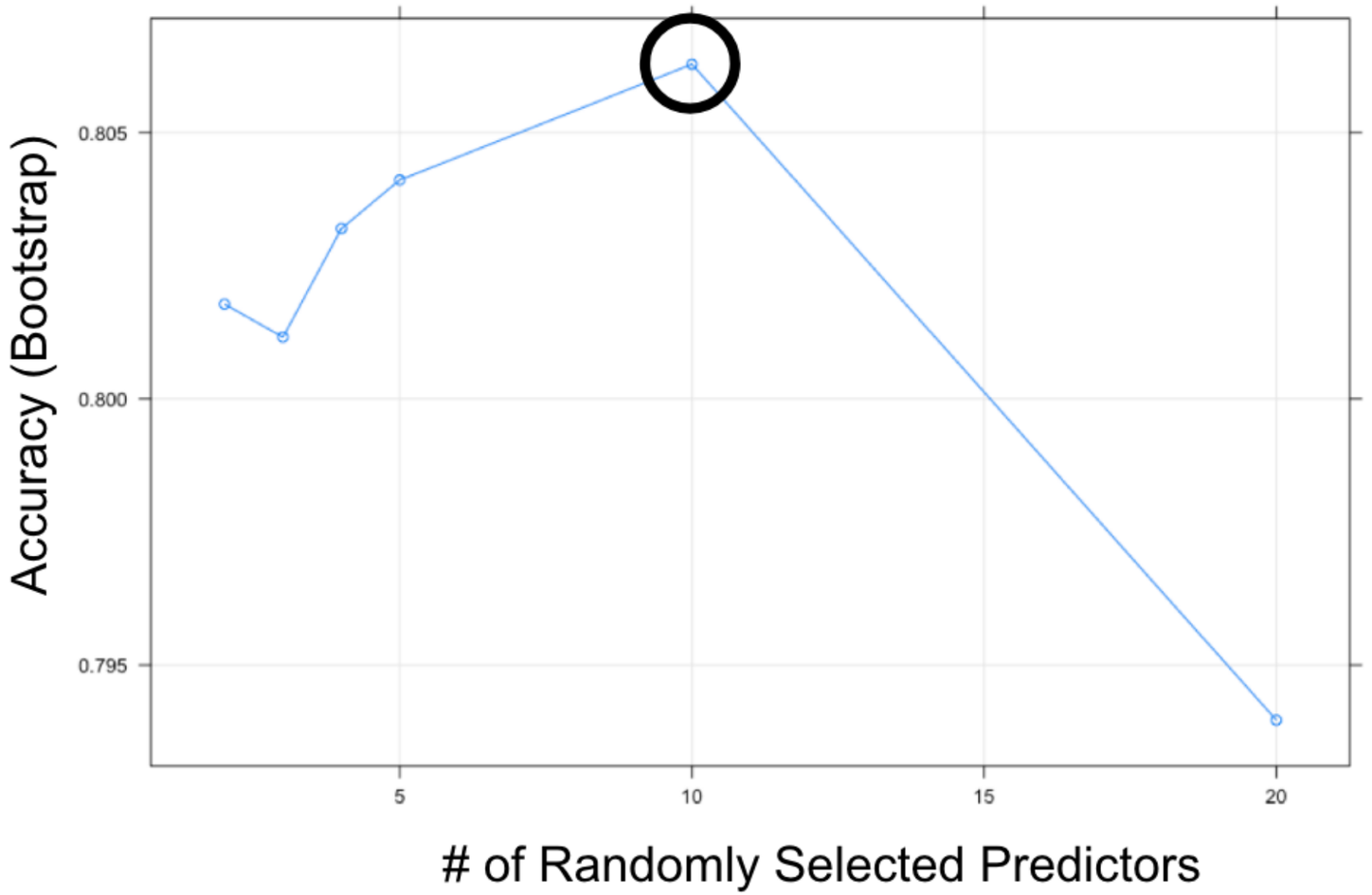
Custom tuning example

```
# 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



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Introducing glmnet

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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
- `alpha [0, 1]` : pure ridge to pure lasso
- `lambda (0, infinity)` : size of the penalty

Example: "don't overfit"

```
# Load data
overfit <- read.csv("overfit.csv")

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

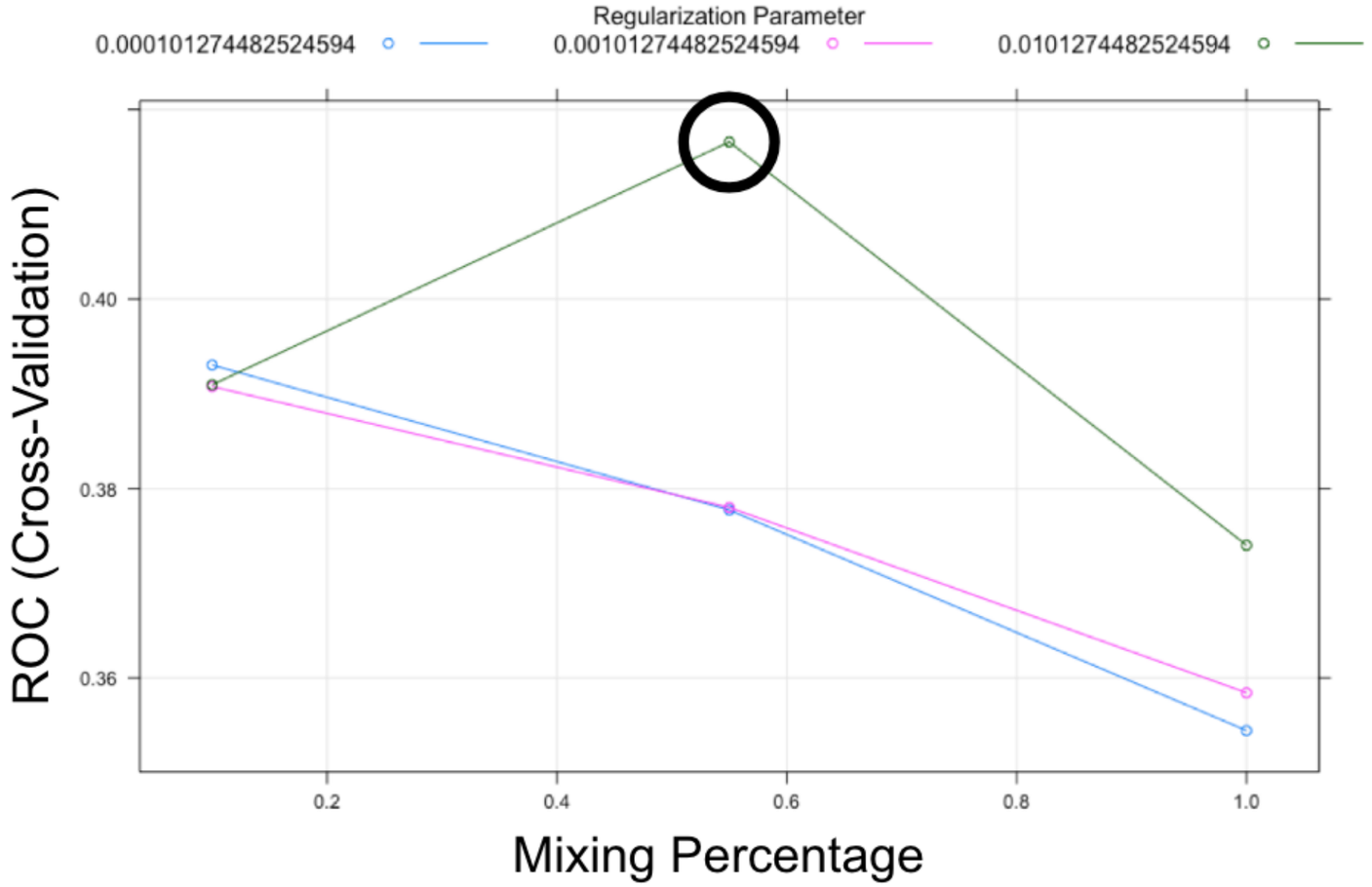
Try the defaults

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

# Plot results
plot(model)
```

- 3 values of `alpha`
- 3 values of `lambda`

Plot the results



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glmnet with custom tuning grid

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Custom tuning glmnet models

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

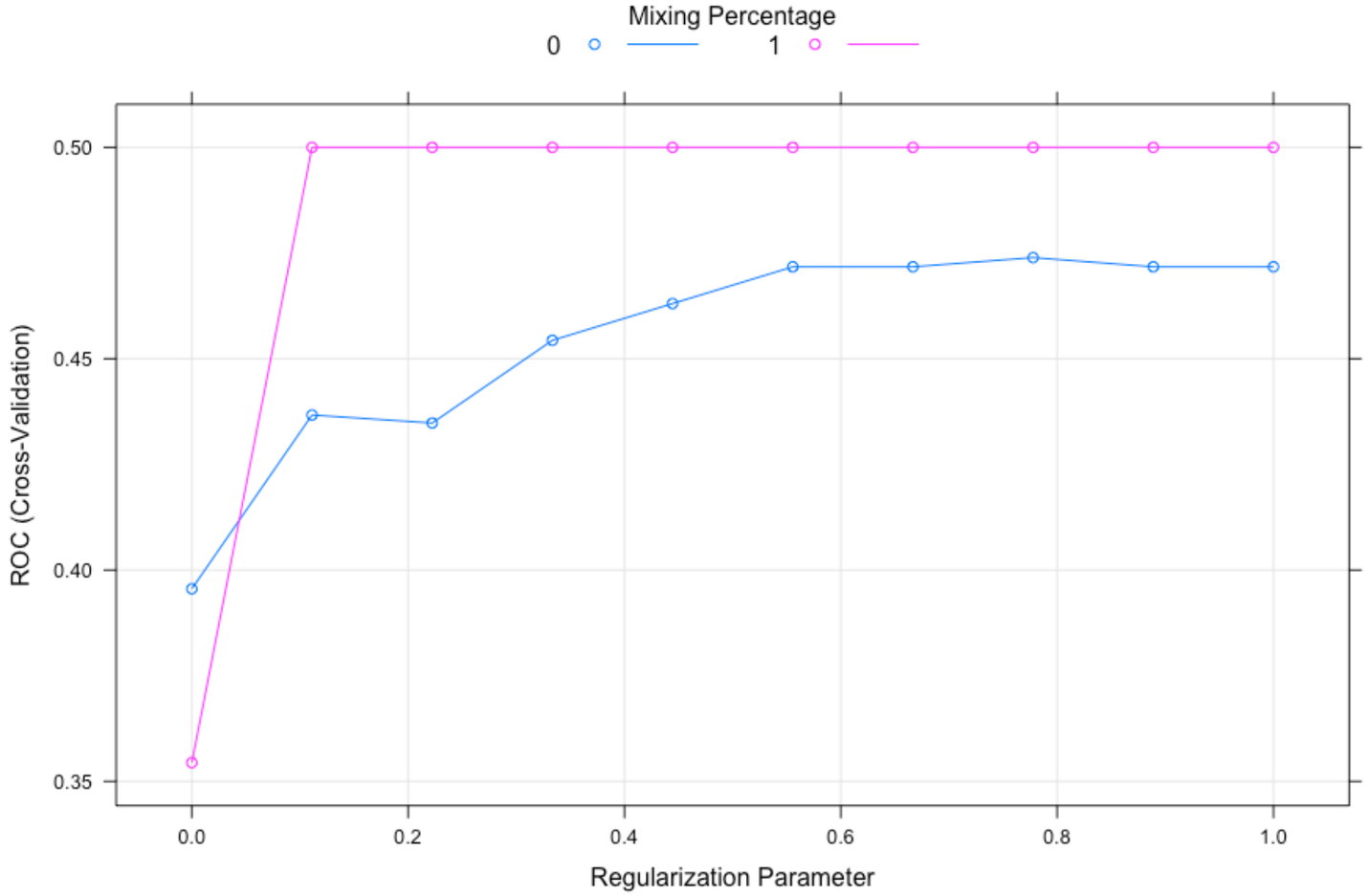
Example: glmnet tuning

```
# 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
)
```

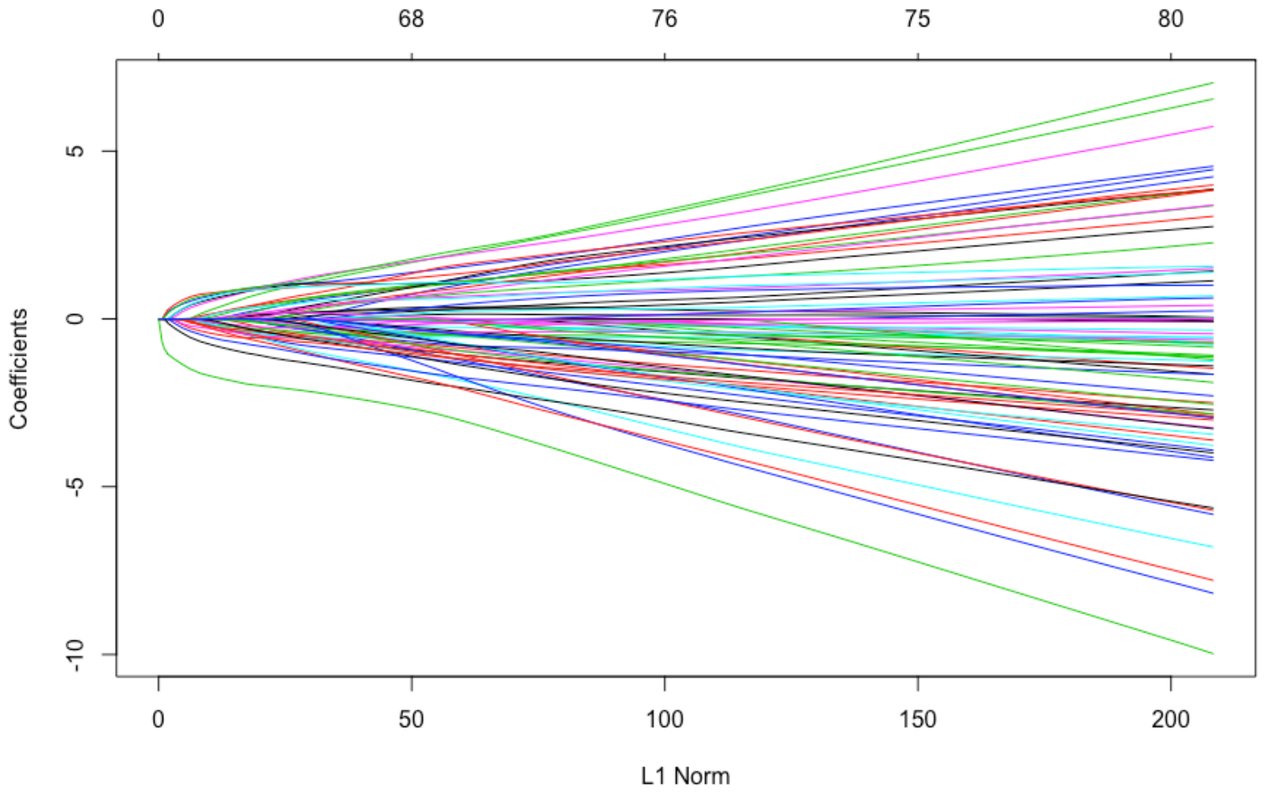
```
# Plot results
plot(model)
```

Compare models visually



Full regularization path

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



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