HYPERPARAMETER TUNING IN R

Hyperparameter tuning in caret

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Voter dataset from US 2016 election

- Split intro training and test set

```
library(tidyverse)
glimpse(voters_train_data)

Observations: 6,692
Variables: 42
$ turnout16_2016       <chr> "Did not vote", "Did not vote", "Did not vote", "Di
$ RIGGED_SYSTEM_1_2016 <int> 2, 2, 3, 2, 2, 3, 3, 1, 2, 3, 4, 4, 4, 3, 1, 2, 2,
$ RIGGED_SYSTEM_2_2016 <int> 3, 3, 2, 2, 3, 3, 2, 2, 1, 2, 4, 2, 3, 2, 3, 4, 3,
$ RIGGED_SYSTEM_3_2016 <int> 1, 1, 3, 1, 1, 1, 2, 1, 1, 2, 1, 2, 1, 2, 1, 1, 1,
$ RIGGED_SYSTEM_4_2016 <int> 2, 1, 2, 2, 2, 2, 2, 2, 1, 3, 3, 1, 3, 3, 1, 3, 3,
$ RIGGED_SYSTEM_5_2016 <int> 1, 2, 2, 2, 2, 3, 1, 1, 2, 3, 2, 2, 1, 3, 1, 1, 2,
$ RIGGED_SYSTEM_6_2016 <int> 1, 1, 2, 1, 2, 2, 2, 1, 2, 2, 1, 3, 1, 3, 1, 1, 1,
$ track_2016           <int> 2, 2, 2, 1, 2, 2, 2, 2, 2, 1, 2, 1, 2, 1, 1, 2, 2,
$ persfinretro_2016    <int> 2, 2, 2, 2, 1, 2, 2, 2, 3, 2, 3, 2, 2, 2, 2, 3, 3,
$ econtrend_2016       <int> 2, 2, 2, 3, 1, 2, 2, 2, 3, 2, 4, 1, 1, 2, 2, 2, 3,
$ Americatrend_2016    <int> 2, 3, 1, 1, 3, 3, 2, 2, 1, 2, 3, 1, 1, 2, 3, 3, 3,
$ futuretrend_2016     <int> 3, 3, 3, 4, 4, 3, 2, 2, 3, 2, 4, 1, 1, 3, 3, 3, 3,
$ wealth_2016          <int> 2, 2, 1, 2, 2, 8, 2, 8, 8, 2, 2, 2, 2, 2, 1, 2, 2,
...
```

Let's train another model with caret

- Stochastic Gradient Boosting

```
library(caret)
library(tictoc)

fitControl <- trainControl(method = "repeatedcv",
                           number = 3,
                           repeats = 5)
tic()
set.seed(42)
gbm_model_voters <- train(turnout16_2016 ~ .,
                   data = voters_train_data,
                   method = "gbm",
                   trControl = fitControl,
                   verbose = FALSE)
toc()

32.934 sec elapsed
```

Let's train another model with caret

```
gbm_model_voters

Stochastic Gradient Boosting

...

Resampling results across tuning parameters:

  interaction.depth  n.trees  Accuracy   Kappa
  1                   50      0.9604603  -0.0001774346
 ...

Tuning parameter 'shrinkage' was held constant at a value of 0.1
Tuning parameter 'n.minobsinnode' was held constant at a value of 10

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were n.trees = 50, interaction.depth = 1, sh
```

Cartesian grid search with caret

- Define a **Cartesian grid** of hyperparameters:

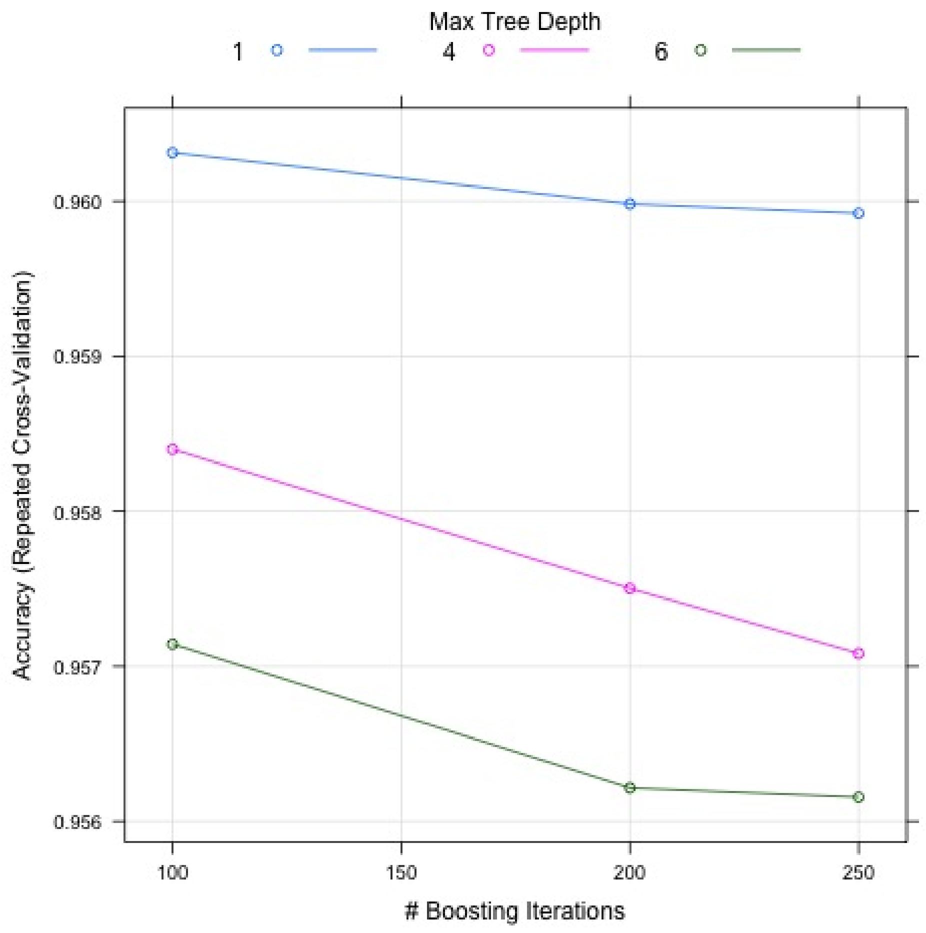
```
man_grid <-  expand.grid(n.trees = c(100, 200, 250),
                         interaction.depth = c(1, 4, 6),
                         shrinkage = 0.1,
                         n.minobsinnode = 10)

fitControl <- trainControl(method = "repeatedcv",
                           number = 3,
                           repeats = 5)
tic()
set.seed(42)
gbm_model_voters_grid <- train(turnout16_2016 ~ .,
                   data = voters_train_data,
                   method = "gbm",
                   trControl = fitControl,
                   verbose = FALSE,
                   tuneGrid = man_grid)
toc()

85.745 sec elapsed
```

Cartesian grid search with caret

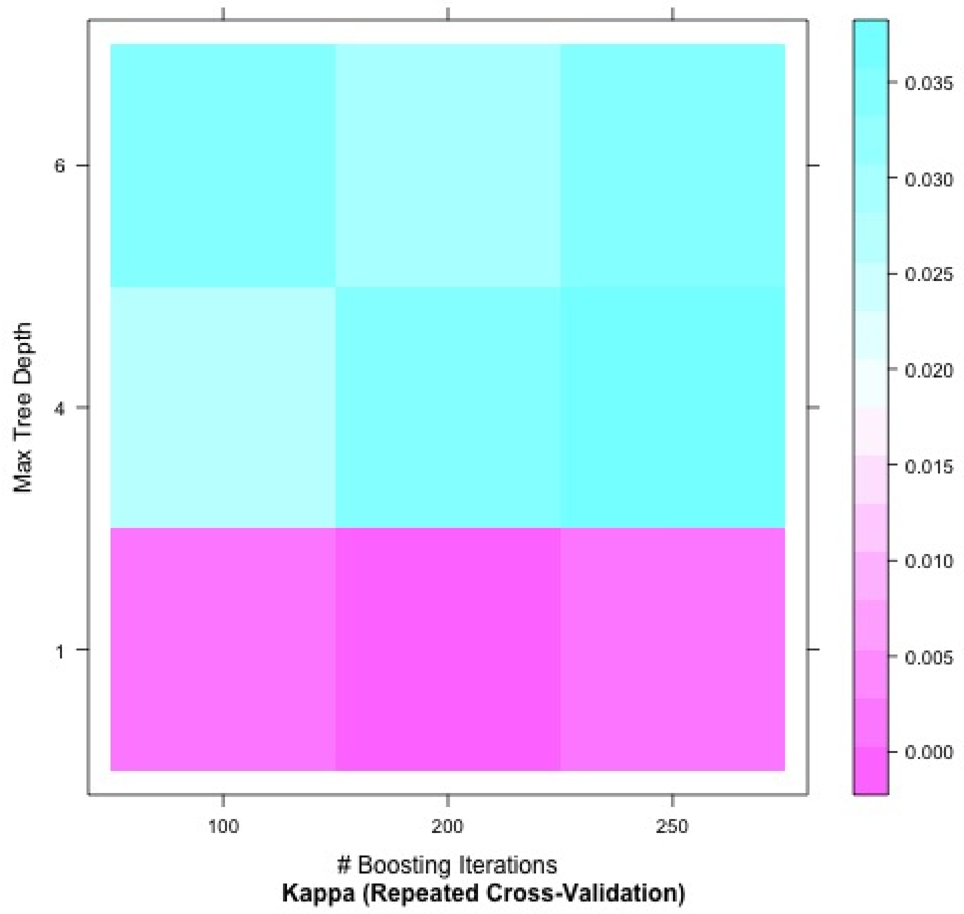
```
gbm_model_voters_grid

Stochastic Gradient Boosting

...

Resampling results across tuning parameters:

  interaction.depth  n.trees  Accuracy   Kappa
  1                  100      0.9603108  0.000912769
 ...

Tuning parameter 'shrinkage' was held constant at a value of 0.1
Tuning parameter 'n.minobsinnode' was held constant at a value of 10

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were n.trees = 100,
interaction.depth = 1, shrinkage = 0.1 and n.minobsinnode = 10.
```

Plot hyperparameter models

```
plot(gbm_model_voters_grid)
```




```
plot(gbm_model_voters_grid,
     metric = "Kappa",
     plotType = "level")
```



HYPERPARAMETER TUNING IN R

Test it out for yourself!

HYPERPARAMETER TUNING IN R

Hyperparameter tuning with Grid vs. Random Search

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Grid search continued

```
man_grid <-  expand.grid(n.trees = c(100, 200, 250),
                         interaction.depth = c(1, 4, 6),
                         shrinkage = 0.1,
                         n.minobsinnode = 10)

fitControl <- trainControl(method = "repeatedcv",
                           number = 3,
                           repeats = 5,
                           search = "grid")

tic()
set.seed(42)
gbm_model_voters_grid <- train(turnout16_2016 ~ .,
                   data = voters_train_data,
                   method = "gbm",
                   trControl = fitControl,
                   verbose= FALSE,
                   tuneGrid = man_grid)
toc()

85.745 sec elapsed
```

Grid Search with hyperparameter ranges

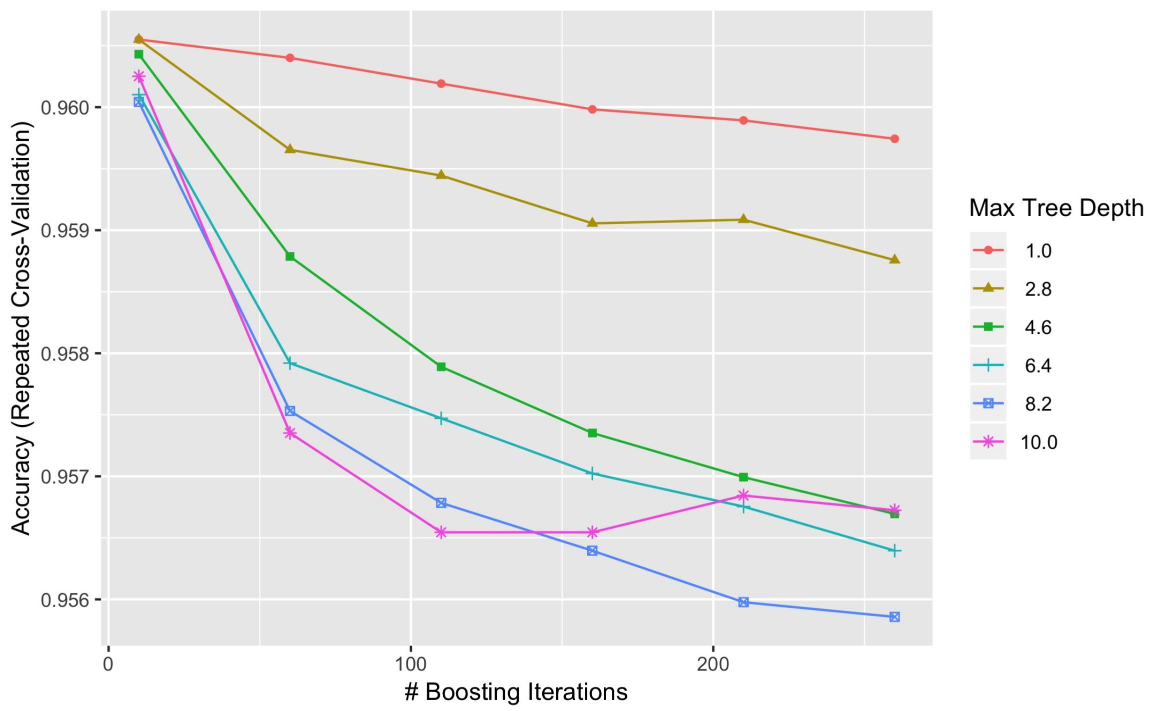
```
big_grid <-  expand.grid(n.trees = seq(from = 10, to = 300, by = 50),
                         interaction.depth = seq(from = 1, to = 10,
                                                 length.out = 6),
                         shrinkage = 0.1,
                         n.minobsinnode = 10)

big_grid
   n.trees interaction.depth shrinkage n.minobsinnode
1       10               1.0       0.1             10
2       60               1.0       0.1             10
3      110               1.0       0.1             10
4      160               1.0       0.1             10
5      210               1.0       0.1             10
6      260               1.0       0.1             10
7       10               2.8       0.1             10
8       60               2.8       0.1             10
9      110               2.8       0.1             10
10     160               2.8       0.1             10
11     210               2.8       0.1             10
12     260               2.8       0.1             10
13      10               4.6       0.1             10
...
36     260              10.0       0.1             10
```

Grid Search with many hyperparameter options

```
big_grid <-  expand.grid(n.trees = seq(from = 10, to = 300, by = 50),
                         interaction.depth = seq(from = 1, to = 10,
                                                 length.out = 6),
                         shrinkage = 0.1,
                         n.minobsinnode = 10)

fitControl <- trainControl(method = "repeatedcv",
                           number = 3,
                           repeats = 5,
                           search = "grid")

tic()
set.seed(42)
gbm_model_voters_big_grid <- train(turnout16_2016 ~ .,
                   data = voters_train_data,
                   method = "gbm",
                   trControl = fitControl,
                   verbose = FALSE,
                   tuneGrid = big_grid)
toc()

240.698 sec elapsed
```

Cartesian grid vs random search

```
ggplot(gbm_model_voters_big_grid)
```



- Grid search can get **slow** and **computationally expensive** very quickly!
- Therefore, in reality, we often use **random search**.

Random Search in caret

- Define *random* search in `trainControl` function

```
library(caret)
fitControl <- trainControl(method = "repeatedcv",
                           number = 3,
                           repeats = 5,
                           search = "random")
```

- Set *tuneLength*

```
tic()
set.seed(42)
gbm_model_voters_random <- train(turnout16_2016 ~ .,
                       data = voters_train_data,
                       method = "gbm",
                       trControl = fitControl,
                       verbose = FALSE,
                       tuneLength = 5)
toc()

46.432 sec elapsed
```

Random Search in caret

```
gbm_model_voters_random

Stochastic Gradient Boosting

...

Resampling results across tuning parameters:

  shrinkage   interaction.depth  n.minobsinnode  n.trees  Accuracy   Kappa
  0.08841129   4                  6              4396     0.9670737  -0.00853312
  0.09255042   2                  7               540     0.9630635  -0.01329168
  0.14484962   3                 21              3154     0.9570179  -0.01397025
  0.34935098  10                 10              2566     0.9610734  -0.01572681
  0.43341085   1                 13              2094     0.9460727  -0.02479105

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were n.trees = 4396,
interaction.depth = 4, shrinkage = 0.08841129 and n.minobsinnode = 6.
```

- *Beware*: in `caret` random search can **NOT** be combined with grid search!

HYPERPARAMETER TUNING IN R

Let's get coding!

HYPERPARAMETER TUNING IN R

Adaptive Resampling

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What is Adaptive Resampling?

Grid Search

- **All** hyperparameter combinations are computed.

Random Search

- Random **subsets** of hyperparameter combinations are computed.

=> Evaluation of best combination is done **at the end**.

Adaptive Resampling

- Hyperparameter combinations are **resampled** with values near combinations that performed well.
- Adaptive Resampling is, therefore, **faster and more efficient**!

"Futility Analysis in the Cross-Validation of Machine Learning Models." Max Kuhn; ARXIV 2014

Adaptive Resampling in caret

`trainControl`: `method = "adaptive_cv"` + `search = "random"` + `adaptive =`

- *min*: minimum number of resamples per hyperparameter
- *alpha*: confidence level for removing hyperparameters
- *method*: "gls" for linear model or "BT" for Bradley-Terry
- *complete*: if TRUE generates full resampling set

```
fitControl <- trainControl(method = "adaptive_cv",
                           adaptive = list(min = 2, alpha = 0.05,
                                           method = "gls", complete = TRUE),
                           search = "random")
```

Adaptive Resampling in caret

- trainControl() + `tuneLength = x`

```
fitControl <- trainControl(method = "adaptive_cv",
                            number = 3,
                            repeats = 3,
                            adaptive = list(min = 2,
                                            alpha = 0.05,
                                            method = "gls",
                                            complete = TRUE),
                            search = "random")

tic()
set.seed(42)
gbm_model_voters_adaptive <- train(turnout16_2016 ~ .,
                                   data = voters_train_data,
                                   method = "gbm",
                                   trControl = fitControl,
                                   verbose = FALSE,
                                   tuneLength = 7)

toc()
1239.837 sec elapsed
```

Adaptive Resampling

```
gbm_model_voters_adaptive

...

Resampling results across tuning parameters:

  shrinkage   interaction.depth  n.minobsinnode  n.trees  Accuracy   Kappa
  0.07137493   5                  6              4152     0.9564654  0.02856571
  0.08408739   5                 14               674     0.9547185  0.02098853
  0.28552325   8                 15              3209     0.9568141  0.03024238
  0.33663932  10                 13              2595     0.9571130  0.04250979
  0.54251480   3                 24              3683     0.9482171  0.03568586
  0.56406870   7                 25              4685     0.9549898  0.05284333
  0.58695763   8                 24              1431     0.9520286  0.02742592

Accuracy was used to select the optimal model using the largest value.

The final values used for the model were n.trees = 2595,
interaction.depth = 10, shrinkage = 0.3366393 and n.minobsinnode = 13.
```

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Let's get coding!