Intro to tidymodels with nflfastR

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What have I done?

- Bachelor's in Kinesiology (2011) Effect of Sugar vs Sugar-Free Mouth Rinse on Performance
- Master's in Exercise Physiology (2014) Effect of Exercise on Circulating Brain Biomarkers
- PhD in Neurobiology (2018) Effect of Aging + Glutathione Deficiency on Motor and Cognitive Function

What do I do?

- RStudio, Customer Enablement Lead Help RStudio's customers utilize Open Source data science and our Professional Products
- #TidyTuesday Weekly data analysis community project (~4,000 participants in past 3 years)
- The Mock Up. blog Explanatory blogging about How to do Stuff with data + #rstats, mostly with NFL data
- espnscrapeR collect data from ESPN's public APIs, mostly for QBR and team standings
- gtExtras User-focused wrappers extensions to the gt package

Focus for Today

90 Minutes (with breaks)

Binary classification:

- Logistic Regression
- Random Forest

Slides at: cmsac-tidymodels.netlify.app/ Source code at: github.com/jthomasmock/nfl-workshop

To follow along, you can read in the subsetted data with the code below:

```
raw_url <- "https://github.com/jthomasmock/nfl-workshop/blob/master/raw_plays.rds?raw=true"
raw_plays <- readRDS(url(raw_url, method = "libcurl"))</pre>
```

Level-Setting

As much as I'd love to learn and teach all of Machine Learning/Statistics in 90 min...

It's just not possible!

Goals for today

- Make you comfortable with the **syntax** and **packages** via **tidymodels** unified interface
- So when you're learning or modeling on your own, you get to focus on the **stats** rather than re-learning different APIs over and over...

Along the way, we'll cover minimal examples and then some more quick best practices where **tidymodels** makes it easier to do more things!

tidymodels

tidymodels is a collection of packages for modeling and machine learning using tidyverse principles.

Packages

- rsample: efficient data splitting and resampling
- parsnip: tidy, unified interface to models
- recipes: tidy interface to data pre-processing tools for feature engineering
- workflows: bundles your pre-processing, modeling, and post-processing
- tune: helps optimize the hyperparameters and pre-processing steps
- yardstick: measures the performance metrics
- dials: creates and manages tuning parameters/grids
- broom: converts common R statistical objects into predictable formats
 - broom available methods

tidymodels vs broom alone

broom

broom summarizes key information about models in tidy tibble()s.

broom tidies 100+ models from popular modelling packages and almost all of the model objects in the **stats** package that comes with base R. **vignette("available-methods")** lists method availability.

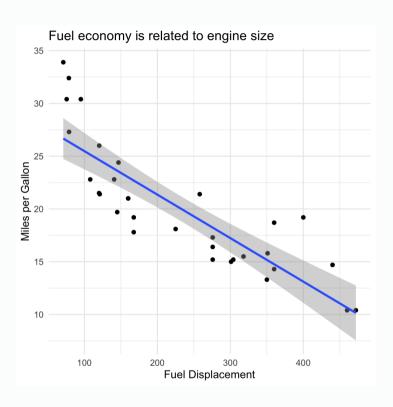
While broom is useful for summarizing the result of a single analysis in a consistent format, it is really designed for high-throughput applications, where you must combine results from multiple analyses.

I personally use **broom** for more classical statistics and **tidymodels** for machine learning. A more detailed summary of what **broom** is about can be found in the **broom** docs.

lm() example

```
library(tidyverse)

basic_plot <- mtcars %>%
   ggplot(
    aes(x = disp, y = mpg)
   ) +
   geom_point() +
   geom_smooth(method = "lm") +
   theme_minimal() +
   labs(
    x = "Fuel Displacement", y = "Miles per Gatitle = "Fuel economy is related to engine)
```



base example

```
# fit a basic linear model
basic_lm <- lm(mpg ~ disp, data = mtcars)</pre>
basic_lm
## Call:
## lm(formula = mpg ~ disp, data = mtcars)
## Coefficients:
## (Intercept)
                    disp
## 29.59985
                 -0.04122
summary(basic lm)
##
## Call:
## lm(formula = mpg ~ disp, data = mtcars)
## Residuals:
             1Q Median 3Q Max
## -4.8922 -2.2022 -0.9631 1.6272 7.2305
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 29.599855   1.229720   24.070   < 2e-16 ***
## disp
          ## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 3.251 on 30 degrees of freedom
## Multiple R-squared: 0.7183, Adjusted R-squared: 0.709
## F-statistic: 76.51 on 1 and 30 DF, p-value: 9.38e-10
```

broom example

```
broom::tidy(basic lm)
## # A tibble: 2 × 5
##
            term estimate std.error statistic p.value
           <chr> <dbl> <dbl> <dbl> <dbl>
##
## 1 (Intercept) 29.6 1.23 24.1 3.58e-21
## 2 disp -0.0412 0.00471 -8.75 9.38e-10
   broom::glance(basic_lm)
## # A tibble: 1 × 12
##
             r.squared adj.r.squared sigma statistic p.value df logLik AIC
##
                                     <dbl> <dbl > <dbl> <dbl > <db
                                                                                           0.709 3.25 76.5 9.38e-10 1 -82.1 170. 175.
## 1 0.718
## # ... with 3 more variables: deviance <dbl>, df.residual <int>, nobs <int>
```

Want more **broom**?

There's a lot more to **broom** for tidy-ier modeling - out of scope for today, but details at broom.tidymodels.org and R4DS Many Models Chapter.

Tidy Machine Learning w/ tidymodels



Core ideas for Today

A workflow for **tidy** machine learning

- Split the data
- Pre-Process and Choose a Model
- Combine into a Workflow
- Generate Predictions and Assess Model Metrics

Goal of Machine Learning

- Construct models that
- **©** generate accurate predictions
- for future, yet-to-be-seen data

Feature Engineering - Max Kuhn and Kjell Johnston and Alison Hill

Classification

Showing two examples today, comparing their outcomes, and then giving you the chance to explore on your own!

The Dataset

Filtered down from the nflfastR datasets (~2.25 GB) to only non-penalty run and pass plays for the 2017-2019 regular seasons, and on downs 1st, 2nd or 3rd. This is about 92,000 plays.

The goal: Predict if an upcoming play will be a run or a pass

glimpse(raw plays) ## Rows: 91,976 ## Columns: 20 ## \$ game id <dbl> 2017090700, 2017090700, 2017090700, 2017090... ## \$ posteam <chr> "NE", "NE", "NE", "NE", "NE", "NE", "NE", "NE", "... ## \$ play type <chr> "pass", "pass", "run", "run", "pass", "run"... ## \$ yards gained <dbl> 0, 8, 8, 3, 19, 5, 16, 0, 2, 7, 0, 3, 10, 0... ## \$ ydstogo <dbl> 10, 10, 2, 10, 7, 10, 5, 2, 2, 10, 10, 10, ... ## \$ down <dbl> 1, 2, 3, 1, 2, 1, 2, 1, 2, 1, 1, 2, 3, 1, 2... ## \$ game_seconds remaining <dbl> 3595, 3589, 3554, 3532, 3506, 3482, 3455, 3... ## \$ vardline 100 <dbl> 73, 73, 65, 57, 54, 35, 30, 2, 2, 75, 32, 3... ## \$ qtr <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 7, 7, 7, 7. ## \$ posteam score <chr> "KC", "KC", "KC", "KC", "KC", "KC", "KC", "... ## \$ defteam ## \$ defteam score <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 7, 0, 0, 0, 0... ## \$ score differential <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, -7, 7, 7, 7, 7, ... ## \$ shotgun <dbl> 0, 0, 1, 1, 1, 0, 1, 0, 0, 1, 1, 1, 1, 1, 0... ## \$ no huddle <dbl> 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0... ## \$ wp <dbl> 0.5060180, 0.4840546, 0.5100098, 0.5529816,... ## \$ goal to go <dbl> 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0... ## \$ half seconds remaining

<dbl> 1795, 1789, 1754, 1732, 1706, 1682, 1655, 1...

Data Prep

We can read in the data from a RDS file.

```
raw_plays <- readRDS(
  url("https://github.com/jthomasmock/nfl-workshop/blob/master/raw_plays.rds?raw=true", method = "l:
)</pre>
```

What is play-by-play data?

Data from ESPN

Feature Engineering

I added a few features, namely a running total of number of runs/passes pre-snap and what the previous play was.

```
all plays <- raw plays %>%
 group by(game id, posteam) %>%
 mutate(
   run = if else(play_type == "run", 1, 0),
   pass = if else(play type == "pass", 1, 0),
   total runs = if else(play type == "run", cumsum(run) - 1, cumsum(run)),
   total_pass = if_else(play_type == "pass", cumsum(pass) - 1, cumsum(pass)),
   previous play = if else(posteam == lag(posteam),
                           lag(play type), "First play of Drive"
   previous play = if else(is.na(previous play),
                            replace na("First play of Drive"), previous play
 ) %>%
 ungroup() %>%
 mutate at(vars(
   play type, shotgun, no huddle,
   posteam timeouts remaining, defteam timeouts remaining,
   previous play, goal to go
 ). as.factor) %>%
 mutate(
   down = factor(down, levels = c(1, 2, 3), ordered = TRUE),
   qtr = factor(qtr, levels = c(1, 2, 3, 4), ordered = TRUE),
   in red zone = if else(yardline 100 <= 20, 1, 0),
   in fg range = if else(yardline 100 <= 35, 1, 0),
   two min drill = if else(half seconds remaining <= 120, 1, 0)
 ) %>%
 mutate(
   in red zone = factor(if else(yardline 100 <= 20, 1, 0)),
   in fg range = factor(if else(yardline 100 <= 35, 1, 0)),
   two min drill = factor(if else(half seconds remaining <= 120, 1, 0))
 select(-run, -pass)
```

Core ideas for Today

A workflow for **tidy** machine learning

- Split the data
- Pre-Process and Choose a Model
- Combine into a Workflow
- Generate Predictions and Assess Model Metrics

Split

```
split_data <- initial_split(data, 0.75)
train_data <- training(split_data)
test_data <- testing(split_data)</pre>
```

Pre-Process & choose a model

```
model_recipe <- recipe(pred ~ predictors, data = train_data)

# Choose a model and an engine
lr_mod <- logistic_reg(mode = "classification") %>%
    set_engine("glm")
```

Combine into a workflow

```
# Combine the model and recipe to the workflow
lr_wflow <- workflow() %>%
  add_recipe(model_recipe) %>%
  add_model(lr_mod)

# Fit/train the model
model_fit <- lr_wflow %>%
  fit(data = train_data)
```

Predict and get metrics

```
# Get predictions
pred_lr <- predict(pbp_fit_lr, test_data)

# Check metrics
pred_lr %>%
  metrics(truth = pred, .pred_class) %>%
  bind_cols(select(test_data, pred)) %>%
  bind_cols(predict(fit_lr, test_data, type = "prob"))
```

Split

```
# Split
split_pbp <- initial_split(all_plays, 0.75, strata = play_type)

# Split into test/train
train_data <- training(split_pbp)
test_data <- testing(split_pbp)</pre>
```

Pre-Process & Choose a model

```
pbp_rec <- recipe(play_type ~ ., data = train_data) %>%
    step_rm(half_seconds_remaining) %>% # remove
    step_string2factor(posteam, defteam) %>% # convert to factors
    update_role(yards_gained, game_id, new_role = "ID") %>% # add as ID
    step_corr(all_numeric(), threshold = 0.7) %>% # remove auto-correlated
    step_center(all_numeric()) %>% # substract mean from numeric
    step_zv(all_predictors()) # remove zero-variance predictors

# Choose a model and an engine

lr_mod <- logistic_reg(mode = "classification") %>%
    set_engine("glm")
```

Combine into a workflow

```
# Combine the model and recipe to the workflow
lr_wflow <- workflow() %>%
  add_recipe(pbp_rec) %>%
  add_model(lr_mod)

# Fit/train the model
pbp_fit_lr <- lr_wflow %>%
  fit(data = train_data)
```

Predict and get metrics

```
# Get predictions
pbp_pred_lr <- predict(pbp_fit_lr, test_data) %>%
    bind_cols(test_data %>% select(play_type)) %>%
    bind_cols(predict(pbp_fit_lr, test_data, type = "prob"))
# Check metrics
pbp_pred_lr %>%
metrics(truth = play type, .pred class)
```

rsample



rsample

Now that we've created the dataset to use, I'll start with **tidymodels** proper.

rsample at a minimum does your train/test split, but also takes care of things like boostrapping, stratification, v-fold cross validation, validation splits, rolling origin, etc.

Data Splitting w/ rsample

Do the initial split and stratify by play type to make sure there are equal ratios of run vs pass in test and train

```
split_pbp <- initial_split(all_plays, 0.75, strata = play_type)
split_pbp

## <Analysis/Assess/Total>
## <68981/22995/91976>

# separate the training data
train_data <- training(split_pbp)

# separate the testing data
test_data <- testing(split_pbp)</pre>
```

Test vs Train

Split into train_data and test_data and then confirm the ratios.

```
train_data %>%
  count(play type) %>%
  mutate(ratio = n/sum(n))
## # A tibble: 2 × 3
## play_type n ratio
## <fct> <int> <dbl>
## 1 pass 40751 0.591
## 2 run 28230 0.409
test_data %>%
  count(play_type) %>%
  mutate(ratio = n/sum(n))
## # A tibble: 2 × 3
  play_type n ratio
  <fct> <int> <dbl>
## 1 pass 13584 0.591
## 2 run 9411 0.409
```

Model recipes



Add recipe steps with recipes

recipe steps are changes we make to the dataset, including things like centering, dummy encoding, update columns as ID only, or even custom feature engineering.

```
pbp_rec <- recipe(play_type ~ ., data = train_data) %>%
  step_rm(half_seconds_remaining) %>% # remove
  step_string2factor(posteam, defteam) %>% # convert to factors
  # ignore these vars for train/test, but include in data as ID
  update_role(yards_gained, game_id, new_role = "ID") %>%
  # removes vars that have large absolute correlations w/ other vars
  step_corr(all_numeric(), threshold = 0.7) %>%
  step_center(all_numeric()) %>% # substract mean from numeric
  step_zv(all_predictors()) # remove zero-variance predictors
```

In recipes vs dplyr/tidyr

Generally:

- In tidyverse, do reshaping or basic cleaning
- In recipes do statistical transformations or other things that are intended for modeling
 - Possible step_??? for many many things!

usemodels

Relatively early in package life cycle, but helps with boilerplate

```
usemodels::use ranger(play type ~ ., train data)
## ranger recipe <-
    recipe(formula = play type ~ ., data = train data) %>%
    step string2factor(one of(posteam, defteam))
##
## ranger spec <-
    rand_forest(mtry = tune(), min_n = tune(), trees = 1000) %>%
    set mode("classification") %>%
    set engine("ranger")
## ranger workflow <-
    workflow() %>%
    add recipe(ranger recipe) %>%
    add model(ranger spec)
## set.seed(66699)
## ranger tune <-
   tune grid(ranger workflow, resamples = stop("add your rsample object"), grid = stop("add number of candidate points"))
```

parsnip

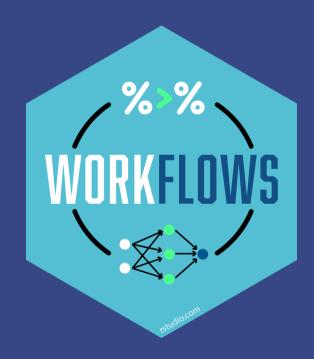


Choose a model and start your engines!

parsnip supplies a general modeling interface to the wide world of R models!

```
# Note that mode = "classification" is the default here anyway!
lr_mod <- logistic_reg(mode = "classification") %>%
  set_engine("glm")
```

workflows



Combine into a workflow

We can now combine the model and recipe into a workflow - this allows us to define exactly what model and data are going into our fit/train call.

```
lr_wflow <- workflow() %>%
  add_model(lr_mod) %>% # parsnip model
  add_recipe(pbp_rec) # recipe from recipes
```

What is a workflow?

A workflow is an object that can bundle together your pre-processing, modeling, and post-processing requests. For example, if you have a **recipe** and **parsnip** model, these can be combined into a workflow. The advantages are:

- You don't have to keep track of separate objects in your workspace.
- The recipe prepping and model fitting can be executed using a single call to fit().
- If you have custom tuning parameter settings, these can be defined using a simpler interface when combined with tune.

Steps so far

- Build a recipe for any pre-processingChoose and build a model
- Combine them into a workflow

Fit/train the model with parsnip

Now we can move forward with fitting/training the model - this is really a one-liner.

```
pbp_fit_lr <- lr_wflow %>%
  fit(data = train_data) # fit the model against the training data
```

Predict outcomes with parsnip

After the model has been trained we can compare the training data against the holdout testing data.

```
pbp_pred_lr <- predict(pbp_fit_lr, test_data) %>%
  # Add back a "truth" column for what the actual play_type was
bind_cols(test_data %>% select(play_type)) %>%
  # Get probabilities for the class for each observation
bind_cols(predict(pbp_fit_lr, test_data, type = "prob"))
```

```
## # A tibble: 22,995 × 4
##
     .pred_class play_type .pred_pass .pred_run
##
   <fct>
                <fct>
                              <dbl>
                                       <dbl>
   1 run
                pass
                              0.168 0.832
                              0.237 0.763
##
  2 run
                run
                              0.665 0.335
##
  3 pass
                run
                              0.801
                                     0.199
##
   4 pass
                run
                                     0.299
##
   5 pass
                              0.701
                pass
##
   6 run
                              0.370
                                       0.630
                run
                              0.743
                                       0.257
##
  7 pass
                run
                              0.861
                                     0.139
   8 pass
                pass
                              0.694
                                      0.306
##
   9 pass
                run
## 10 run
                              0.400
                                       0.600
                run
## # ... with 22,985 more rows
```

Predict outcomes with parsnip

pbp last lr <- last fit(lr mod, pbp rec, split = split pbp)</pre>

Note that out previous code of predict() %>% bind_cols() %>% bind_cols() is really the equivalent to the below:

```
pbp last lr %>%
  pluck(".predictions", 1)
## # A tibble: 22,995 × 6
      .pred_pass .pred_run .row .pred_class play_type .config
##
##
           <dbl>
                     <dbl> <int> <fct>
                                              <fct>
                                                        <chr>>
                     0.832
##
  1
           0.168
                                                        Preprocessor1 Model1
                               8 run
                                              pass
##
          0.237
                     0.763
                               9 run
                                              run
                                                        Preprocessor1 Model1
##
          0.665
                     0.335
                                                        Preprocessor1 Model1
                              10 pass
                                              run
                                                        Preprocessor1 Model1
##
           0.801
                     0.199
                              13 pass
                                              run
##
   5
           0.701
                     0.299
                                                        Preprocessor1 Model1
                              19 pass
                                              pass
##
  6
           0.370
                     0.630
                              27 run
                                                        Preprocessor1 Model1
                                              run
                                                        Preprocessor1_Model1
##
           0.743
                     0.257
                              37 pass
                                              run
          0.861
                                                        Preprocessor1_Model1
##
                     0.139
                              38 pass
                                              pass
                                                        Preprocessor1_Model1
##
           0.694
                     0.306
                              50 pass
                                              run
## 10
           0.400
                     0.600
                                                        Preprocessor1 Model1
                               52 run
                                              run
    ... with 22,985 more rows
```

Assessing Accuracy with yardstick



Check outcomes with yardstick

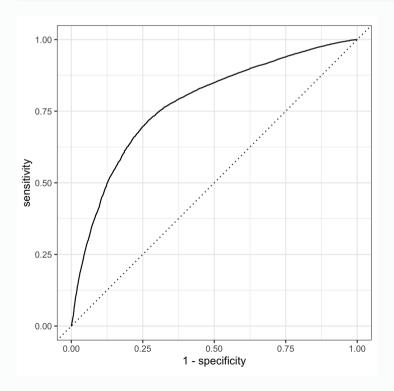
For confirming how well the model predicts, we can use **yardstick** to plot ROC curves, get AUC and collect general metrics.

```
pbp pred lr %>%
  # get Area under Curve
  roc_auc(truth = play_type,
          .pred_pass)
## # A tibble: 1 × 3
    .metric .estimator .estimate
   <chr> <chr>
                        <dbl>
## 1 roc_auc binary
                           0.776
pbp pred lr %>%
  # collect and report metrics
  metrics(truth = play_type,
          .pred_class)
## # A tibble: 2 × 3
    .metric .estimator .estimate
##
    <chr> <chr>
                          <dbl>
```

0.722

1 accuracy binary

```
pbp_pred_lr %>%
  # calculate ROC curve
roc_curve(truth = play_type, .pred_pass) %>%
autoplot()
```



Note on Checking Outcomes

You could use last_fit():

This functions is intended to be used after fitting a variety of models and the final tuning parameters (if any) have been finalized. The next step would be to fit using the entire training set and verify performance using the test data.

```
lr_last_fit <- last_fit(lr_mod, pbp_rec, split = split_pbp)
collect_metrics(lr_last_fit)</pre>
```

Split

```
# Split
split
split(all_plays, 0.75, strata = play_type)

# Split into test/train
train_data <- training(split_pbp)
test_data <- testing(split_pbp)</pre>
```

Pre-Process & Choose a model

```
pbp_rec <- recipe(play_type ~ ., data = train_data) %>%
    step_rm(half_seconds_remaining) %>% # remove
    step_string2factor(posteam, defteam) %>% # convert to factors
    update_role(yards_gained, game_id, new_role = "ID") %>% # add as ID
    step_corr(all_numeric(), threshold = 0.7) %>% # remove auto-correlated
    step_center(all_numeric()) %>% # substract mean from numeric
    step_zv(all_predictors()) # remove zero-variance predictors

# Choose a model and an engine

lr_mod <- logistic_reg(mode = "classification") %>%
    set_engine("glm")
```

Combine into a workflow

```
# Combine the model and recipe to the workflow
lr_wflow <- workflow() %>%
  add_recipe(pbp_rec) %>%
  add_model(lr_mod)

# Fit/train the model
pbp_fit_lr <- lr_wflow %>%
  fit(data = train_data)
```

Predict and get metrics

```
# Get predictions
pbp_pred_lr <- predict(pbp_fit_lr, test_data) %>%
    bind_cols(test_data %>% select(play_type)) %>%
    bind_cols(predict(pbp_fit_lr, test_data, type = "prob"))

# Check metrics
pbp_pred_lr %>%
metrics(truth = play type, .pred class)
```

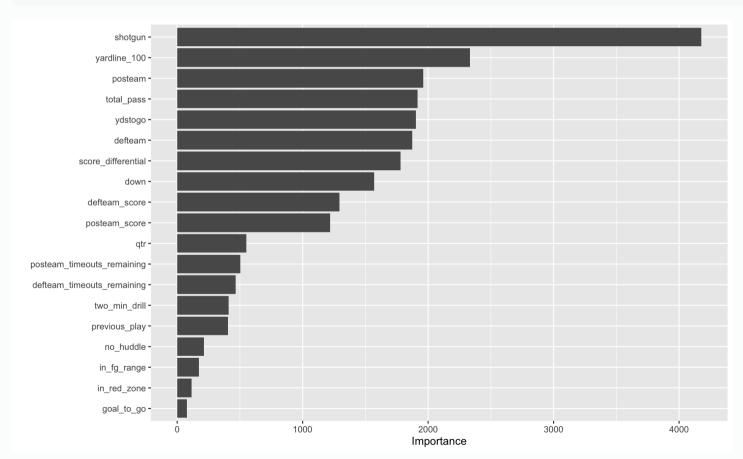
Change the model

How about a Random Forest model? Just change the model and re-run!

```
rf mod <- rand forest(trees = 100) %>%
 set engine("ranger",
            importance = "impurity", # variable importance
            num.threads = 4) %>% # Parallelize
 set_mode("classification")
rf wflow <- workflow() %>%
 add_recipe(pbp_rec) %>% # Same recipe
 add_model(rf_mod) # New model
pbp_fit_rf <- rf_wflow %>% # New workflow
 fit(data = train data) # Fit the Random Forest
# Get predictions and check metrics
pbp_pred_rf <- predict(pbp_fit_rf, test_data) %>%
 bind_cols(test_data %>% select(play_type)) %>%
 bind cols(predict(pbp fit rf, test data, type = "prob"))
```

Feature Importance

```
pbp_fit_rf %>%
  pull_workflow_fit() %>%
  vip(num_features = 20)
```



Quick Model Comparison

The random forest model slightly outperforms the logistic regression, although both are not perfect

```
pbp pred lr %>% # Logistic Regression predictions
  metrics(truth = play type, .pred class)
## # A tibble: 2 × 3
  .metric .estimator .estimate
  <chr> <chr>
                  <dbl>
## 1 accuracy binary 0.722
## 2 kap
            binary 0.416
pbp_pred_rf %>% # Random Forest predictions
  metrics(truth = play_type, .pred_class)
## # A tibble: 2 × 3
    .metric .estimator .estimate
  <chr> <chr> <chr> <dbl>
## 1 accuracy binary 0.729
## 2 kap
            binary 0.438
```

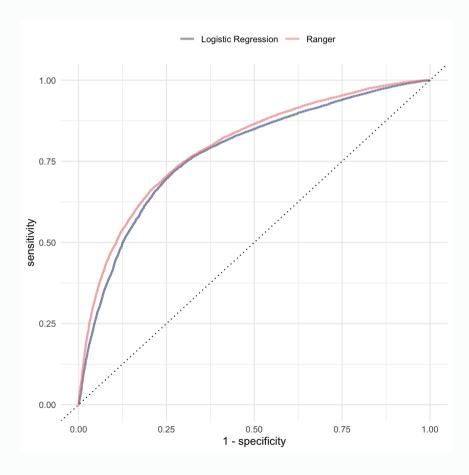
Quick Model Comparison

```
pbp pred lr %>% # Logistic Regression predictions
  conf mat(truth = play type, .pred class)
##
            Truth
## Prediction pass
                    run
##
        pass 10837
                    3649
##
              2747
        run
                    5762
pbp_pred_rf %>% # Random Forest predictions
  conf_mat(truth = play_type, .pred_class)
##
            Truth
## Prediction pass
                    run
        pass 10558
##
                    3209
              3026 6202
##
        run
```

Comparing Models Together

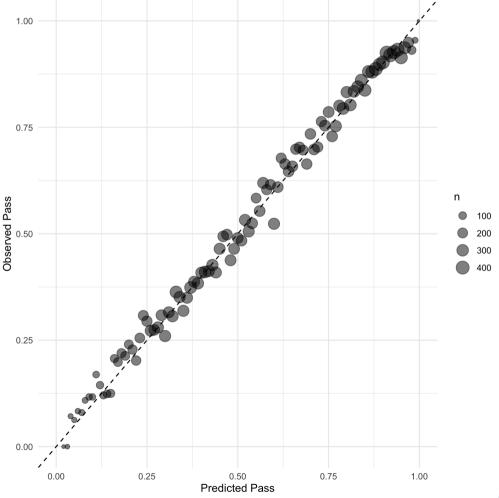
```
roc_rf <- pbp_pred_rf %>%
 roc_curve(truth = play_type, .pred_pass) %>%
 mutate(model = "Ranger")
roc lr <- pbp pred lr %>%
 roc_curve(truth = play_type, .pred_pass) %>%
 mutate(model = "Logistic Regression")
full_plot <- bind_rows(roc_rf, roc_lr) %>%
  # Note that autoplot() works here!
  ggplot(aes(x = 1 - specificity,
             y = sensitivity,
             color = model)) +
  geom_path(lwd = 1, alpha = 0.5) +
  geom_abline(lty = 3) +
  scale_color_manual(
    values = c("#374785", "#E98074")
 theme minimal() +
 theme(legend.position = "top",
        legend.title = element_blank())
```

full_plot



Calibration Plot

```
calibration_plot <- pbp_pred_rf %>%
 mutate(
    pass = if_else(play_type == "pass", 1, 0),
    pred rnd = round(.pred pass, 2)
    ) %>%
 group_by(pred_rnd) %>%
 summarize(
   mean_pred = mean(.pred_pass),
   mean_obs = mean(pass),
   n = n()
    ) %>%
 ggplot(aes(x = mean_pred, y = mean_obs)) +
 geom_abline(linetype = "dashed") +
 geom_point(aes(size = n), alpha = 0.5) +
 theme_minimal() +
 labs(
   x = "Predicted Pass",
    v = "Observed Pass"
 coord_cartesian(
   xlim = c(0,1), ylim = c(0, 1)
```



Quick Re-Cap

A workflow for tidy modeling

- Split the data
- Pre-Process and Choose a Model
- Combine into a Workflow
- Generate Predictions and Assess Model Metrics

So the unified interface hopefully makes the idea of learning and applying many algorithms easier.

tidymodels really shines when you start to go further or apply best practices like:

- Resampling, Cross Validation, Bootstrapping
- Model Tuning and Model Optimization
- Grid Search, Iterative Search

A Deeper Dive on Best Practices

Comparing Models

Previously we've just compared two models by seeing how accurate they were on our testing data, but....

The test set as the data that *should* be used to conduct a proper evaluation of model performance on the **final model(s)**. This begs the question of, "How can we tell what is best if we don't measure performance until the test set?"

However, we usually need to understand the effectiveness of the model before using the test set.

• Tidy Modeling with R

Resampling and Cross Validation

Resampling methods are empirical simulation systems that emulate the process of using some data for modeling and different data for evaluation. Most resampling methods are iterative, meaning that this process is repeated multiple times.

Cross-validation is a well established resampling method

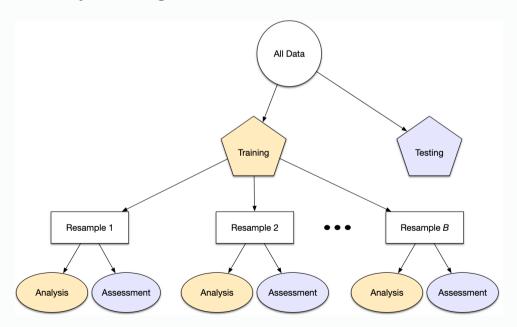
• Tidy Modeling with R

Get Started w/ Resampling and test drive on RStudio Cloud.

Resampling and Cross Validation

Resampling is only conducted on the training set. The test set is not involved. For each iteration of resampling, the data are partitioned into two subsamples:

- The model is fit with the analysis set.
- The model is evaluated with the assessment set.
- Tidy Modeling with R



Resampling and Cross-validation

```
vfold cv(train data, v = 10)
     10-fold cross-validation
## #
## # A tibble: 10 × 2
                           id
##
      splits
   t>
                           <chr>
##
   1 <split [62082/6899]> Fold01
   2 <split [62083/6898]> Fold02
##
   3 <split [62083/6898]> Fold03
##
   4 <split [62083/6898]> Fold04
##
   5 <split [62083/6898]> Fold05
##
   6 <split [62083/6898]> Fold06
   7 <split [62083/6898]> Fold07
##
##
   8 <split [62083/6898]> Fold08
   9 <split [62083/6898]> Fold09
  10 <split [62083/6898]> Fold10
```

```
vfold cv(train data, v = 10, repeats = 5)
## # 10-fold cross-validation repeated 5 times
## # A tibble: 50 × 3
      splits
                           id
                                   id2
##
   t>
                                   <chr>
                           <chr>
    1 <split [62082/6899]> Repeat1 Fold01
    2 <split [62083/6898] > Repeat1 Fold02
    3 <split [62083/6898] > Repeat1 Fold03
##
    4 <split [62083/6898]> Repeat1 Fold04
##
    5 <split [62083/6898] > Repeat1 Fold05
    6 <split [62083/6898] > Repeat1 Fold06
    7 <split [62083/6898]> Repeat1 Fold07
    8 <split [62083/6898] > Repeat1 Fold08
    9 <split [62083/6898]> Repeat1 Fold09
## 10 <split [62083/6898]> Repeat1 Fold10
## # ... with 40 more rows
```

Estimate Performance w/ Cross Validation

9 <split [62085/6898] > Repeat1 Fold09

10 <split [62085/6898]> Repeat1 Fold10

... with 40 more rows

NOTE: Fitting the model multiple times can take a while with larger models or more folds/repeats! I recommend running this as a background job in RStudio, so you don't lock up your session for the duration.

```
set.seed(20201024)
# Create 10 folds and 5 repeats
 pbp_folds <- vfold_cv(train_data, v = 10, repeats = 5)</pre>
pbp_folds
## # 10-fold cross-validation repeated 5 times
## # A tibble: 50 × 3
##
     splits
                          id id2
   <list>
                          <chr>
                                  <chr>
   1 <split [62084/6899] > Repeat1 Fold01
   2 <split [62084/6899] > Repeat1 Fold02
##
   3 <split [62084/6899] > Repeat1 Fold03
##
   4 <split [62085/6898] > Repeat1 Fold04
##
   5 <split [62085/6898] > Repeat1 Fold05
   6 <split [62085/6898] > Repeat1 Fold06
   7 <split [62085/6898]> Repeat1 Fold07
   8 <split [62085/6898] > Repeat1 Fold08
##
```

Estimate Performance w/ Cross Validation

```
keep pred <- control resamples(save pred = TRUE, verbose = TRUE)</pre>
set.seed(20201024)
# Fit resamples
rf res <- fit resamples(rf wflow, resamples = pbp_folds, control = keep_pred)</pre>
rf res
## # Resampling results
## # 10-fold cross-validation repeated 5 times
## # A tibble: 50 × 6
##
     splits
                          id id2 .metrics .notes .predictions
   st>
                          <chr> <chr> <list> <list>
                                                                         t>
##
   1 <split [62084/6899]> Repeat1 Fold01 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
   2 <split [62084/6899]> Repeat1 Fold02 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
##
   3 <split [62084/6899]> Repeat1 Fold03 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
   4 <split [62085/6898]> Repeat1 Fold04 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
   5 <split [62085/6898]> Repeat1 Fold05 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
   6 <split [62085/6898]> Repeat1 Fold06 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
   7 <split [62085/6898] > Repeat1 Fold07 <tibble [2 × 3] > <tibble [0 × 1] > <tibble [6,...
   8 <split [62085/6898]> Repeat1 Fold08 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
   9 <split [62085/6898]> Repeat1 Fold09 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
## 10 <split [62085/6898]> Repeat1 Fold10 <tibble [2 × 3]> <tibble [0 × 1]> <tibble [6,...
## # ... with 40 more rows
```

What just happened???

We just fit a model for each resample, evaluated it against a within resample assessment set, and stored it into a single **tibble**!

```
rf_res %>%
    # grab specific columns and resamples
pluck(".predictions", 10)
```

```
## # A tibble: 6,898 × 5
##
     .pred_pass .pred_run .row .pred_class play_typ
                   <dbl> <int> <fct>
##
          <dbl>
                                          <fct>
##
   1
          0.552 0.448
                             8 pass
                                          pass
          0.711 0.289
##
                            18 pass
                                          pass
          0.697 0.303
##
                            26 pass
                                          run
##
          0.977 0.0227
                            41 pass
                                          pass
##
          0.947
                 0.0530
                            48 pass
                                          pass
##
          0.295
                 0.705
                            51 run
                                          run
##
          0.437
                  0.563
                            75 run
                                          run
          0.701
##
                 0.299
                            96 pass
                                          pass
##
          0.610
                 0.390
                           111 pass
                                          run
## 10
          0.810
                  0.190
                           117 pass
                                          pass
## # ... with 6,888 more rows
```

What else can you do?

```
# Summarize all metrics
rf_res %>%
  collect_metrics(summarize = TRUE)
```

```
## # A tibble: 2 × 5
##
     .metric .estimator
                         mean
                                      std err
     <chr>
              <chr>
                         <dbl> <int>
                                         <dbl>
  1 accuracy binary
                         0.730
                                  50 0.000651
## 2 roc auc
              binary
                         0.797
                                  50 0.000631
```

```
rf_res %>%
  # combine ALL predictions
collect_predictions()
```

```
## # A tibble: 344,915 × 7
                     .pred pass .pred run .row .pred class play type
              id2
      <chr> <chr>
                          <dbl>
                                    <dbl> <int> <fct>
                                                            <fct>
   1 Repeat1 Fold01
                          0.663
                                    0.337
                                              3 pass
                                                            run
                          0.730
   2 Repeat1 Fold01
                                             22 pass
                                    0.270
                                                            pass
   3 Repeat1 Fold01
                          0.424
                                    0.576
                                             23 run
                                                            pass
   4 Repeat1 Fold01
                          0.348
                                    0.652
                                             27 run
                                                            run
   5 Repeat1 Fold01
                          0.482
                                    0.518
                                             28 run
                                                            run
   6 Repeat1 Fold01
                          0.695
                                    0.305
                                             35 pass
                                                            run
   7 Repeat1 Fold01
                          0.381
                                    0.619
                                             61 run
                                                             pass
   8 Repeat1 Fold01
                          0.166
                                    0.834
                                             69 run
                                                            run
## 9 Repeat1 Fold01
                          0.781
                                    0.219
                                             80 pass
                                                            pass
                          0.333
                                    0.667
## 10 Repeat1 Fold01
                                             84 run
                                                            run
## # ... with 344,905 more rows
```

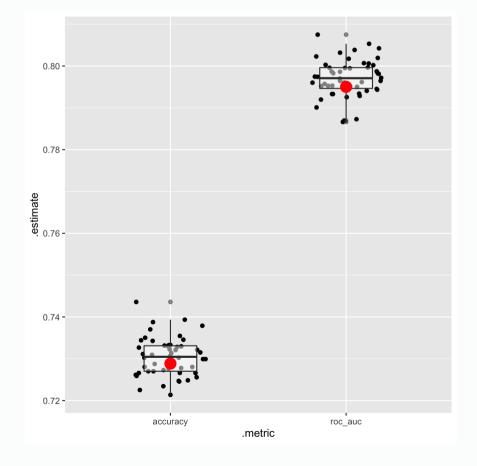
Collect metrics

First show our predicted model with compared against our test data.

```
# Naive Model on Testing Data
rf_compare_df <- bind_rows(
  accuracy(pbp_pred_rf, truth = play_type, .pred_class),
  roc_auc(pbp_pred_rf, truth = play_type, .pred_pass)
)</pre>
```

And then the what our resampled data looks like, which still would leave our test data as unseen.

```
combo_plot <- rf_res %>%
  collect_metrics(summarize = FALSE) %>%
  ggplot(aes(x = .metric, y = .estimate)) +
  geom_jitter(width = 0.2) +
  geom_boxplot(width = 0.3, alpha = 0.5) +
  geom_point(data = rf_compare_df,color = "red", size = 5)
```



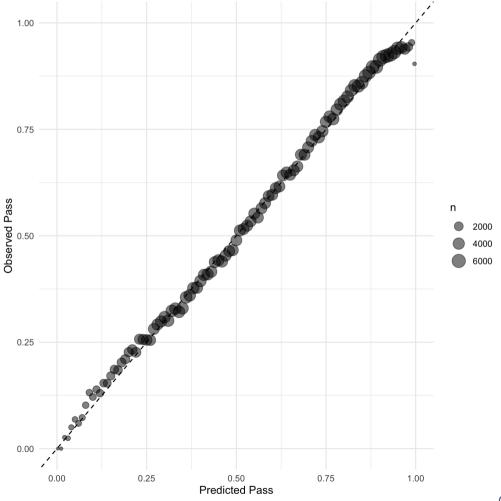
Estimate Performance w/ Cross Validation

Now, since we aren't supposed to "know" our test results... we can collect our predictions and do another calibration plot. I'm going to round to 3 decimal places and get ~100 data points to plot (instead of our actual ~345,000 points from the combined 50 runs).

```
assess res <- collect predictions(rf res)</pre>
assess res
## # A tibble: 344,915 × 7
             id2
##
      id
                    .pred pass .pred run .row .pred class play type
             <chr>
                         <dbl>
                                    <dbl> <int> <fct>
     <chr>
                                                            <fct>
   1 Repeat1 Fold01
                         0.663
                                    0.337
                                              3 pass
                                                            run
   2 Repeat1 Fold01
                    0.730
                                    0.270
                                            22 pass
                                                            pass
   3 Repeat1 Fold01
                         0.424
                                    0.576
                                            23 run
##
                                                            pass
   4 Repeat1 Fold01
##
                         0.348
                                    0.652
                                            27 run
                                                            run
##
   5 Repeat1 Fold01
                         0.482
                                    0.518
                                            28 run
                                                            run
   6 Repeat1 Fold01
                         0.695
                                    0.305
                                             35 pass
                                                            run
   7 Repeat1 Fold01
                         0.381
                                    0.619
                                             61 run
                                                            pass
##
   8 Repeat1 Fold01
                         0.166
                                    0.834
                                             69 run
                                                            run
   9 Repeat1 Fold01
                         0.781
                                    0.219
                                             80 pass
                                                            pass
  10 Repeat1 Fold01
                         0.333
                                    0.667
                                             84 run
                                                            run
  # ... with 344,905 more rows
```

Cross Validation Calibration Plot

```
res_calib_plot <- assess_res %>%
 mutate(
    pass = if_else(play_type == "pass", 1, 0),
    pred rnd = round(.pred pass, 2)
    ) %>%
 group_by(pred_rnd) %>%
 summarize(
   mean_pred = mean(.pred_pass),
   mean_obs = mean(pass),
   n = n()
    ) %>%
 ggplot(aes(x = mean_pred, y = mean_obs)) +
 geom_abline(linetype = "dashed") +
 geom_point(aes(size = n), alpha = 0.5) +
 theme_minimal() +
 labs(
   x = "Predicted Pass",
    v = "Observed Pass"
 coord_cartesian(
   xlim = c(0,1), ylim = c(0,1)
```



Model Tuning with tune



tune

We never adjusted our model! We just used naive models and evaluated their performance.

Now, their performance was pretty decent (~68-73% accuracy), but could we get better?

Get Started with Tuning and test drive on RStudio Cloud

Resample + Tune

We're going to use grid-search for our tuning process, and we also need to specify which hyperparameters of our random forest we want to tune.

Note: A hyperparameter is a parameter who value is used to control the learning process - Wikipedia)

```
tune_pbp_rf <- rand_forest(
  mtry = tune(), # add placeholder for tune
  trees = 100,
  min_n = tune() # add placeholder for tune
) %>%
  set_mode("classification") %>%
  set_engine("ranger")

tune_rf_wf <- workflow() %>%
  add_recipe(pbp_rec) %>%
  add_model(tune_pbp_rf)
```

```
tune rf wf
  = Workflow =
## Preprocessor: Recipe
## Model: rand forest()
## — Preprocessor
## 5 Recipe Steps
## • step rm()
   step string2factor()
## • step corr()
## • step center()
## • step zv()
## Random Forest Model Specification (classification)
## Main Arguments:
     mtrv = tune()
   trees = 100
    min n = tune()
## Computational engine: ranger
```

Grid Search

We'll create a grid of possible hyperparameters and then estimate how well they fit with our resamples.

Note that this took about 20 min to run!

I'm doing 15x models by 5x folds, where we train a model and predict outcomes each time! The beauty here is that you could run this as a background job.

```
set.seed(20201024)

pbp_folds <- vfold_cv(train_data, v = 5)

tic()

tune_res <- tune_grid(
    tune_rf_wf,
    resamples = pbp_folds,
    grid = 15, # 15 combos of model parameters
    control = control_grid(verbose = TRUE)
)

toc()
# 1478.385 sec elapsed</pre>
```

Grid Search

Here are the results!

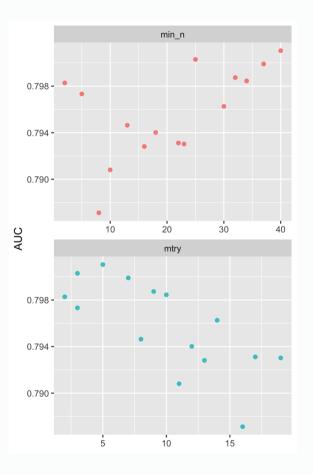
```
## # Tuning results
## # 5-fold cross-validation
## # A tibble: 5 × 4
## splits id .metrics .notes
## clist> chr> clist> clist>
## 1 <split [55186/13797]> Fold1 <tibble [30 × 6]> <tibble [0 × 1]>
## 2 <split [55186/13797]> Fold2 <tibble [30 × 6]> <tibble [0 × 1]>
## 3 <split [55186/13797]> Fold3 <tibble [30 × 6]> <tibble [0 × 1]>
## 4 <split [55187/13796]> Fold4 <tibble [30 × 6]> <tibble [0 × 1]>
## 5 <split [55187/13796]> Fold5 <tibble [30 × 6]> <tibble [0 × 1]>
```

Check it out

It's nested tibbles for the split data, the fold id, metrics, and any notes.

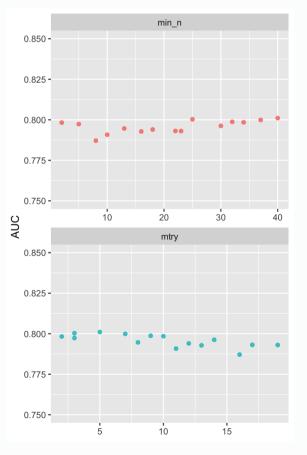
```
# Essentially the same as tune res[[".metrics"]][[1]]
tune res %>%
  pluck(".metrics", 3)
## # A tibble: 30 × 6
       mtry min_n .metric .estimator .estimate .config
##
      <int> <int> <chr>
                           <chr>
                                          <dbl> <chr>
##
##
               32 accuracy binary
                                          0.735 Model01
##
  2
               32 roc auc
                           binary
                                          0.797 Model01
##
         17
               22 accuracy binary
                                          0.729 Model02
##
               22 roc_auc
                           binary
                                          0.792 Model02
               16 accuracy binary
##
         13
                                          0.727 Model03
               16 roc auc
                           binary
                                          0.792 Model03
##
                2 accuracy binary
##
                                          0.735 Model04
##
                2 roc_auc binary
                                          0.796 Model04
##
               25 accuracy binary
                                          0.737 Model05
                           binary
                                          0.800 Model05
## 10
               25 roc auc
## # ... with 20 more rows
```

Check it out



Check it out (scaling matters!)

```
plot_tuned +
  scale_y_continuous(limits = c(0.75, 0.85))
```



Finalize

Here we are investigating which hyperparameters maximized ROC Area Under the Curve.

```
# Which 5x were best?
show best(tune res, "roc auc", n = 5)
## # A tibble: 5 × 8
##
     mtry min_n .metric .estimator
                                           n std err .config
                                 mean
                                                <dbl> <chr>
    <int> <int> <chr> <chr>
                                 <dbl> <int>
          40 roc_auc binary
                                 0.801
                                           5 0.000944 Model14
## 1
## 2
     3 25 roc_auc binary
                                 0.800 5 0.000780 Model05
     7 37 roc_auc binary
## 3
                                 0.800 5 0.000926 Model07
## 4
     9 32 roc auc binary
                                 0.799 5 0.00106 Model01
            34 roc auc binary
## 5
       10
                                 0.798
                                           5 0.000781 Model06
# Select the best
best_fit_auc <- select_best(tune_res, "roc_auc")</pre>
# Select wflow for the model with best hyperparams
rf_tuned <- finalize_workflow(
  rf wflow,
  parameters = best_fit_auc
```

Finalize

Show the outcomes!

```
set.seed(20201024)
rf_tuned_fit <- last_fit(rf_tuned, split_pbp)</pre>
rf tuned fit %>% # tuned model metrics
  collect metrics()
## # A tibble: 2 × 4
  .metric .estimator .estimate .config
##
  <chr> <chr>
                         <dbl> <chr>
## 1 accuracy binary 0.730 Preprocessor1_Model1
## 2 roc_auc binary 0.796 Preprocessor1_Model1
rf_compare_df # naive model metrics
## # A tibble: 2 × 3
   .metric .estimator .estimate
  <chr> <chr>
##
                          <dbl>
## 1 accuracy binary 0.729
## 2 roc_auc binary 0.795
```

Addendums

- Model training/fitting (or simulation) is likely to be the most time-intensive computation you do as such, it's a good idea to run them as **background jobs** in RStudio
- Also can turn on verbose reporting so you know where you're at in the Cross-validation or tuning steps
 - o control_grid(verbose = TRUE)

Going Deeper

Tidy Modeling with R - get started quickly with tidymodels

Introduction to Statistical Learning - the 2nd Edition was just released!

Hands on Machine Learning with R - get started quickly with modeling in R (mix of base R, caret, and tidymodels)

Thank you

• All y'all for listening in 😇

Learn more

- tidymodels.org has step by step guides of various complexities
- Julia Silge's (a tidymodels maintainer) blog, video series, or free interactive course
- Alison Hill's Workshop from rstudio::conf2020