Lec 25 - More Tidymodels

Statistical Programming

Sta 323 | Spring 2022

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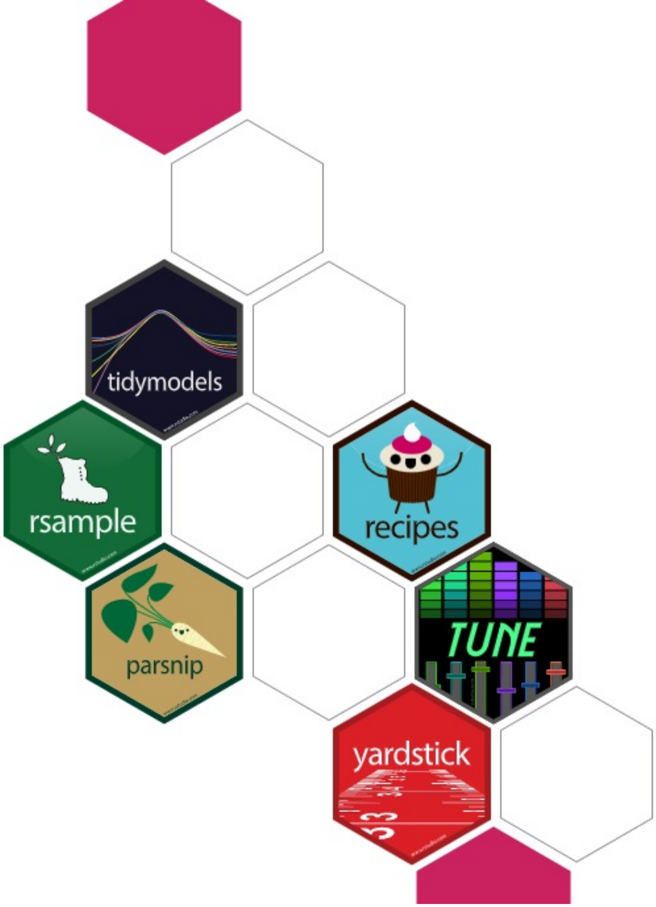

tidymodels
rsample
recipes
parsnip
TUNE
yardstick

Hotels Data

Original data from Antonio, Almeida, and Nunes (2019), Data dictionary

```
hotels = read_csv(
  'https://tidymodels.org/start/case-study/hotels.csv'
) %>%
  mutate(
    across(where(is.character), as.factor)
  )
```

```
## Rows: 50000 Columns: 23
## ── Column specification ────────────────────────────────────────
## Delimiter: ","
## chr  (11): hotel, children, meal, country, market_segmen...
## dbl  (11): lead_time, stays_in_weekend_nights, stays_in_...
## date  (1): arrival_date
##
## ℹ Use `spec()` to retrieve the full column specification for this data.
## ℹ Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

This version of the data is slightly modified from the original data - see gist for the cleanup steps

The data

```
glimpse(hotels)
```

```
## Rows: 50,000
## Columns: 23
## $ hotel                          <fct> City_Hotel, City_Ho…
## $ lead_time                      <dbl> 217, 2, 95, 143, 13…
## $ stays_in_weekend_nights        <dbl> 1, 0, 2, 2, 1, 2, 0…
## $ stays_in_week_nights           <dbl> 3, 1, 5, 6, 4, 2, 2…
## $ adults                         <dbl> 2, 2, 2, 2, 2, 2, 2…
## $ children                       <fct> none, none, none, n…
## $ meal                           <fct> BB, BB, BB, HB, HB,…
## $ country                        <fct> DEU, PRT, GBR, ROU,…
## $ market_segment                 <fct> Offline_TA/TO, Dire…
## $ distribution_channel           <fct> TA/TO, Direct, TA/T…
## $ is_repeated_guest              <dbl> 0, 0, 0, 0, 0, 0, 0…
## $ previous_cancellations         <dbl> 0, 0, 0, 0, 0, 0, 0…
## $ previous_bookings_not_canceled <dbl> 0, 0, 0, 0, 0, 0, 0…
## $ reserved_room_type             <fct> A, D, A, A, F, A, C…
## $ assigned_room_type             <fct> A, K, A, A, F, A, C…
## $ booking_changes                <dbl> 0, 0, 2, 0, 0, 0, 0…
## $ deposit_type                   <fct> No_Deposit, No_Depo…
## $ days_in_waiting_list           <dbl> 0, 0, 0, 0, 0, 0, 0…
## $ customer_type                  <fct> Transient-Party, Tr…
## $ average_daily_rate             <dbl> 80.75, 170.00, 8.00…
```

The model

Our goal is to develop a predictive model that is able to predict whether a booking will include children or not based on the other characteristics of the booking.

```
hotels %>%
  count(children) %>%
  mutate(prop = n/sum(n))
```

```
## # A tibble: 2 × 3
##   children     n   prop
##   <fct>    <int>  <dbl>
## 1 children  4038 0.0808
## 2 none     45962 0.919
```

Clustering the test/train split

```r
set.seed(123)

splits = initial_split(hotels, strata = children)

hotel_train = training(splits)
hotel_test = testing(splits)
```

```r
dim(hotel_train)
```

```
## [1] 37500    23
```

```r
dim(hotel_test)
```

```
## [1] 12500    23
```

```r
hotel_train %>%
  count(children) %>%
  mutate(prop = n/sum(n))
```

```
## # A tibble: 2 × 3
##   children     n   prop
##   <fct>    <int>  <dbl>
## 1 children  3027 0.0807
## 2 none     34473 0.919
```

```r
hotel_test %>%
  count(children) %>%
  mutate(prop = n/sum(n))
```

```
## # A tibble: 2 × 3
##   children     n   prop
##   <fct>    <int>  <dbl>
## 1 children  1011 0.0809
## 2 none     11489 0.919
```

Logistic Regression model

```
show_engines("logistic_reg")
```

```
## # A tibble: 7 × 2
##   engine    mode
##   <chr>     <chr>
## 1 glm       classification
## 2 glmnet    classification
## 3 LiblineaR classification
## 4 spark     classification
## 5 keras     classification
## 6 stan      classification
## 7 brulee    classification
```

```
lr_model = logistic_reg() %>%
  set_engine("glm")

lr_model %>%
  translate()
```

```
## Logistic Regression Model Specification (classification)
##
## Computational engine: glm
##
## Model fit template:
```

Recipe

```r
holidays = c("AllSouls", "AshWednesday", "ChristmasEve", "Easter",
             "ChristmasDay", "GoodFriday", "NewYearsDay", "PalmSunday")

lr_recipe = recipe(children ~ ., data = hotel_train) %>%
  step_date(arrival_date) %>%
  step_holiday(arrival_date, holidays = holidays) %>%
  step_rm(arrival_date) %>%
  step_rm(country) %>%
  step_dummy(all_nominal_predictors()) %>%
  step_zv(all_predictors())

lr_recipe
```

```
## Recipe
##
## Inputs:
##
##       role #variables
##    outcome          1
##  predictor         22
##
## Operations:
##
## Date features from arrival_date
```

```r
lr_recipe %>%
  prep() %>%
  bake(new_data = hotel_train)
```

```
## # A tibble: 37,500 × 76
##    lead_time stays_in_weekend_nights stays_in_week_n… adults
##        <dbl>                   <dbl>            <dbl>  <dbl>
##  1         2                       0                1      2
##  2        95                       2                5      2
##  3        67                       2                2      2
##  4        47                       0                2      2
##  5        56                       0                3      0
##  6         6                       2                2      2
##  7       130                       1                2      2
##  8        27                       0                1      1
##  9        46                       0                2      2
## 10       423                       1                1      2
## # … with 37,490 more rows, and 72 more variables:
## #   is_repeated_guest <dbl>, previous_cancellations <dbl>,
## #   previous_bookings_not_canceled <dbl>,
## #   booking_changes <dbl>, days_in_waiting_list <dbl>,
## #   average_daily_rate <dbl>,
## #   total_of_special_requests <dbl>, children <fct>,
## #   arrival_date_year <dbl>, arrival_date_AllSouls <dbl>, …
```

Workflow

```r
lr_work = workflow() %>%
  add_model(lr_model) %>%
  add_recipe(lr_recipe)
```

Fit

```r
lr_fit = lr_work %>%
  fit(data = hotel_train)
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or 1
## occurred
```

```r
lr_fit
```

```
## ══ Workflow [trained] ══════════════════════════════════════════════
## Preprocessor: Recipe
## Model: logistic_reg()
##
## ── Preprocessor ────────────────────────────────────────────────────
## 6 Recipe Steps
##
## • step_date()
## • step_holiday()
## • step_rm()
## • step_rm()
## • step_dummy()
## • step_zv()
##
## ── Model ───────────────────────────────────────────────────────────
##
```

Logistic regression predictions

```r
lr_perf = lr_fit %>%
  augment(new_data = hotel_train) %>%
  select(children, starts_with(".pred"))

lr_perf
```

```
## # A tibble: 37,500 × 4
##    children .pred_class .pred_children .pred_none
##    <fct>    <fct>                <dbl>      <dbl>
##  1 none     none                0.0861     0.914
##  2 none     none                0.0178     0.982
##  3 none     none                0.0101     0.990
##  4 children children            0.931      0.0693
##  5 children none                0.473      0.527
##  6 children none                0.144      0.856
##  7 none     none                0.0710     0.929
##  8 none     none                0.0596     0.940
##  9 none     none                0.0252     0.975
## 10 none     none                0.0735     0.926
## # … with 37,490 more rows
```

Performance metrics (within-sample)

```r
lr_perf %>%
  conf_mat(children, .pred_class)
```

```
##            Truth
## Prediction children  none
##   children     1075   420
##   none         1952 34053
```

```r
lr_perf %>%
  precision(children, .pred_class)
```

```
## # A tibble: 1 × 3
##   .metric   .estimator .estimate
##   <chr>     <chr>          <dbl>
## 1 precision binary         0.719
```

```r
lr_perf %>%
  roc_auc(children, .pred_children)
```

```
## # A tibble: 1 × 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 roc_auc binary         0.881
```

```r
lr_perf %>%
  yardstick::roc_curve(
    children,
    .pred_children
  ) %>%
  autoplot()
```

Performance metrics (out-of-sample)

```r
lr_test_perf = lr_fit %>%
  augment(new_data = hotel_test) %>%
  select(children, starts_with(".pred"))

lr_test_perf %>%
  conf_mat(children, .pred_class)
```

```
##           Truth
## Prediction children  none
##   children      359   137
##   none          652 11352
```

```r
lr_test_perf %>%
  precision(children, .pred_class)
```

```
## # A tibble: 1 × 3
##   .metric   .estimator .estimate
##   <chr>     <chr>          <dbl>
## 1 precision binary         0.724
```

```r
lr_test_perf %>%
  roc_auc(children, .pred_children)
```

```r
lr_test_perf %>%
  yardstick::roc_curve(
    children,
    .pred_children
  ) %>%
  autoplot()
```

Combining ROC curves

```r
lr_test_perf %>%
  yardstick::roc_curve(
    children,
    .pred_children
  )
```

```
## # A tibble: 11,521 × 3
##    .threshold specificity sensitivity
##         <dbl>       <dbl>       <dbl>
##  1 -Inf          0                 1
##  2    2.22e-16   0                 1
##  3    1.01e-11   0.0000870         1
##  4    4.96e-11   0.000174          1
##  5    1.16e- 9   0.000261          1
##  6    7.32e- 9   0.000348          1
##  7    8.80e- 9   0.000435          1
##  8    9.29e- 9   0.000522          1
##  9    9.67e- 9   0.000609          1
## 10    1.08e- 8   0.000696          1
## # … with 11,511 more rows
```

```r
lr_roc_train = lr_perf %>%
  yardstick::roc_curve(children, .pred_children)
```

```r
bind_rows(
  lr_roc_train,
  lr_roc_test
) %>%
  ggplot(aes(x = 1 - specificity, y = sensitivity
    geom_path(lwd = 1.5, alpha = 0.8) +
    geom_abline(lty = 3) +
    coord_equal()
```

Lasso

Lasso Model

For this we will be using the `glmnet` package which supports fitting lasso, ridge and elastic net models.

The mixture argument determines the type of model fit with: `1` -> Lasso, `0` -> Ridge, other -> elastic net.

```
lasso_model = logistic_reg(penalty = tune(), mixture = 1) %>%
  set_engine("glmnet")

lasso_model %>%
  translate()
```

```
## Logistic Regression Model Specification (classification)
##
## Main Arguments:
##   penalty = tune()
##   mixture = 1
##
## Computational engine: glmnet
##
## Model fit template:
## glmnet::glmnet(x = missing_arg(), y = missing_arg(), weights = missing_arg(),
```

Lasso Recipe

Lasso (and Ridge) models are sensitive to the scale of the model features, and so a standard approach is to normalize all features before fitting the model.

```
lasso_recipe = lr_recipe %>%
  step_normalize(all_predictors())
```

```
lasso_recipe %>%
  prep() %>%
  bake(new_data = hotel_train)
```

```
## # A tibble: 37,500 × 76
##    lead_time stays_in_weekend_nights stays_in_week_n… adults
##        <dbl>                   <dbl>            <dbl>  <dbl>
##  1    -0.858                 -0.938            -0.767  0.337
##  2     0.160                  1.09              1.32   0.337
##  3    -0.146                  1.09             -0.245  0.337
##  4    -0.365                 -0.938            -0.245  0.337
##  5    -0.267                 -0.938             0.278 -3.59
##  6    -0.814                  1.09             -0.245  0.337
##  7     0.544                  0.0735           -0.245  0.337
##  8    -0.584                 -0.938            -0.767 -1.63
##  9    -0.376                 -0.938            -0.245  0.337
## 10     3.75                   0.0735           -0.767  0.337
```

Lasso workflow

```
lasso_work = workflow() %>%
  add_model(lasso_model) %>%
  add_recipe(lasso_recipe)
```

k-Folds for tuning

```
hotel_vf = rsample::vfold_cv(hotel_train, v=5, strata = children)
hotel_vf
```

```
## #  5-fold cross-validation using stratification
## # A tibble: 5 × 2
##   splits               id
##   <list>               <chr>
## 1 <split [30000/7500]> Fold1
## 2 <split [30000/7500]> Fold2
## 3 <split [30000/7500]> Fold3
## 4 <split [30000/7500]> Fold4
## 5 <split [30000/7500]> Fold5
```

grid search

```r
lasso_grid = lasso_work %>%
  tune_grid(
    hotel_vf,
    grid = tibble(
      penalty = 10^seq(-4, -1, length.out = 10)
    ),
    control = control_grid(save_pred = TRUE),
    metrics = metric_set(roc_auc)
  )

lasso_grid
```

```
## # Tuning results
## # 5-fold cross-validation using stratification
## # A tibble: 5 × 5
##   splits               id    .metrics .notes   .predictions
##   <list>               <chr> <list>   <list>   <list>
## 1 <split [30000/7500]> Fold1 <tibble> <tibble> <tibble>
## 2 <split [30000/7500]> Fold2 <tibble> <tibble> <tibble>
## 3 <split [30000/7500]> Fold3 <tibble> <tibble> <tibble>
## 4 <split [30000/7500]> Fold4 <tibble> <tibble> <tibble>
## 5 <split [30000/7500]> Fold5 <tibble> <tibble> <tibble>
```

Results

```
lasso_grid %>%
  collect_metrics()
```

```
## # A tibble: 10 × 7
##      penalty .metric .estimator  mean     n std_
##        <dbl> <chr>   <chr>      <dbl> <int>   <d
##   1 0.0001   roc_auc binary     0.877     5 0.00
##   2 0.000215 roc_auc binary     0.877     5 0.00
##   3 0.000464 roc_auc binary     0.877     5 0.00
##   4 0.001    roc_auc binary     0.877     5 0.00
##   5 0.00215  roc_auc binary     0.877     5 0.00
##   6 0.00464  roc_auc binary     0.870     5 0.00
##   7 0.01     roc_auc binary     0.853     5 0.00
##   8 0.0215   roc_auc binary     0.824     5 0.00
##   9 0.0464   roc_auc binary     0.797     5 0.00
## 10 0.1       roc_auc binary     0.5       5 0
```

```
lasso_grid %>%
  collect_metrics() %>%
  ggplot(aes(x = penalty, y = mean)) +
    geom_point() +
    geom_line() +
    ylab("Area under the ROC Curve") +
    scale_x_log10(labels = scales::label_number()
```

"Best" models

```r
lasso_grid %>%
  show_best("roc_auc", n=10)
```

```
## # A tibble: 10 × 7
##     penalty .metric .estimator  mean     n std_err .config
##       <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
##  1 0.001    roc_auc binary     0.877     5 0.00304 Preproce…
##  2 0.00215  roc_auc binary     0.877     5 0.00263 Preproce…
##  3 0.000464 roc_auc binary     0.877     5 0.00314 Preproce…
##  4 0.000215 roc_auc binary     0.877     5 0.00316 Preproce…
##  5 0.0001   roc_auc binary     0.877     5 0.00318 Preproce…
##  6 0.00464  roc_auc binary     0.870     5 0.00253 Preproce…
##  7 0.01     roc_auc binary     0.853     5 0.00249 Preproce…
##  8 0.0215   roc_auc binary     0.824     5 0.00424 Preproce…
##  9 0.0464   roc_auc binary     0.797     5 0.00400 Preproce…
## 10 0.1      roc_auc binary     0.5       5 0       Preproce…
```

"Best" model

```
lasso_best = lasso_grid %>%
  collect_metrics() %>%
  mutate(mean = round(mean, 2)) %>%
  arrange(desc(mean), desc(penalty)) %>%
  slice(1)

lasso_best
```

```
## # A tibble: 1 × 7
##   penalty .metric .estimator  mean     n std_err .config
##     <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
## 1 0.00215 roc_auc binary      0.88     5 0.00263 Preprocess…
```

Extracting predictions

Since we used `control_grid(save_pred = TRUE)` with `tune_grid()` we can recover the predictions for the out-of-sample values for each fold:

```
lasso_train_perf = lasso_grid %>%
  collect_predictions(parameters = lasso_best)
lasso_train_perf
```

```
## # A tibble: 37,500 × 7
##    id    .pred_children .pred_none  .row penalty children
##    <chr>          <dbl>      <dbl> <int>   <dbl> <fct>
##  1 Fold1         0.366       0.634     5 0.00215 children
##  2 Fold1         0.144       0.856     6 0.00215 children
##  3 Fold1         0.0542      0.946    19 0.00215 none
##  4 Fold1         0.0266      0.973    21 0.00215 none
##  5 Fold1         0.106       0.894    22 0.00215 children
##  6 Fold1         0.0286      0.971    23 0.00215 none
##  7 Fold1         0.0205      0.980    30 0.00215 none
##  8 Fold1         0.0192      0.981    31 0.00215 none
##  9 Fold1         0.0431      0.957    32 0.00215 none
## 10 Fold1         0.0532      0.947    35 0.00215 none
## # … with 37,490 more rows, and 1 more variable:
## #   .config <chr>
```

Re-fitting

Typically with a tuned model we will refit using the complete test data and the "best" parameter value(s),

```
lasso_work_tuned = update_model(
  lasso_work,
  logistic_reg(
    mixture = 1,
    penalty = lasso_best$penalty
  ) %>%
    set_engine("glmnet")
)

lasso_fit = lasso_work_tuned %>%
  fit(data=hotel_train)
```

Test Performance (out-of-sample)

```r
lasso_test_perf = lasso_fit %>%
  augment(new_data = hotel_test) %>%
  select(children, starts_with(".pred"))

lasso_test_perf %>%
  conf_mat(children, .pred_class)
```

```
##             Truth
## Prediction children  none
##   children      330   109
##   none          681 11380
```

```r
lasso_test_perf %>%
  precision(children, .pred_class)
```

```
## # A tibble: 1 × 3
##   .metric   .estimator .estimate
##   <chr>     <chr>          <dbl>
## 1 precision binary         0.752
```

```r
lasso_test_perf %>%
  roc_auc(children, .pred_children)
```

```r
lasso_roc = lasso_test_perf %>%
  yardstick::roc_curve(
    children,
    .pred_children
  ) %>%
  mutate(name = "lasso - test")
lasso_roc %>%
  autoplot()
```

Comparing models

Random Forest

Random forest models

```r
show_engines("rand_forest")
```

```
## # A tibble: 6 × 2
##   engine       mode
##   <chr>        <chr>
## 1 ranger       classification
## 2 ranger       regression
## 3 randomForest classification
## 4 randomForest regression
## 5 spark        classification
## 6 spark        regression
```

```r
rf_model = rand_forest(mtry = tune(), min_n = tune(), trees = 100) %>%
  set_engine("ranger", num.threads = 8) %>%
  set_mode("classification")
```

Recipe & workflow

We skip dummy coding in the recipe as it is not needed by ranger,

```
rf_recipe = recipe(children ~ ., data = hotel_train) %>%
  step_date(arrival_date) %>%
  step_holiday(arrival_date, holidays = holidays) %>%
  step_rm(arrival_date) %>%
  step_rm(country)
```

```
rf_work = workflow() %>%
  add_model(rf_model) %>%
  add_recipe(rf_recipe)
```

Tuning

```r
rf_work %>%
  parameters()
```

```
## Warning: `parameters.workflow()` was deprecated
## Please use `hardhat::extract_parameter_set_dial

## Collection of 2 parameters for tuning
##
##  identifier  type    object
##        mtry  mtry nparam[?]
##       min_n min_n nparam[+]
##
## Model parameters needing finalization:
##    # Randomly Selected Predictors ('mtry')
##
## See `?dials::finalize` or `?dials::update.param
```

```r
rf_grid = rf_work %>%
  tune_grid(
    hotel_vf,
    grid = 10,
    control = control_grid(save_pred = TRUE),
    metrics = metric_set(roc_auc)
  )
```

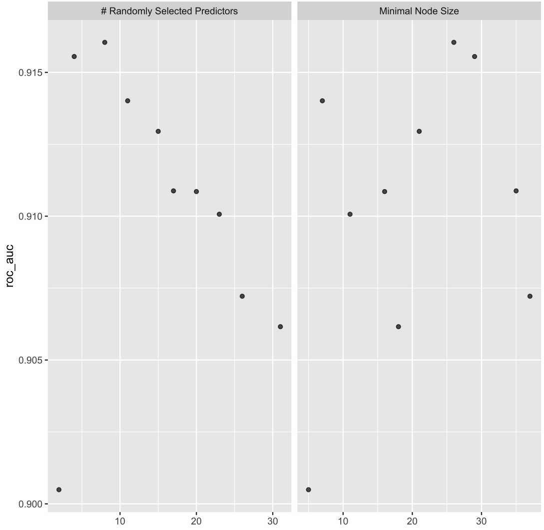
```
## i Creating pre-processing data to finalize unknown p
```

"Best" parameters

```r
rf_grid %>%
  show_best(metric = "roc_auc")
```

```
## # A tibble: 5 × 8
##    mtry min_n .metric .estimator  mean     n st
##   <int> <int> <chr>   <chr>      <dbl> <int>
## 1     8    26 roc_auc binary     0.916     5 0.
## 2     4    29 roc_auc binary     0.916     5 0.
## 3    11     7 roc_auc binary     0.914     5 0.
## 4    15    21 roc_auc binary     0.913     5 0.
## 5    17    35 roc_auc binary     0.911     5 0.
```

```r
autoplot(rf_grid)
```



Refitting

```
(rf_best = rf_grid %>%
  select_best(metric = "roc_auc"))
```

```
## # A tibble: 1 × 3
##    mtry min_n .config
##   <int> <int> <chr>
## 1     8    26 Preprocessor1_Model06
```

```
rf_work_tuned = update_model(
  rf_work,
  rand_forest(
    trees=100,
    mtry = rf_best$mtry,
    min_n = rf_best$min_n
  ) %>%
    set_engine("ranger", num.threads = 8) %>%
    set_mode("classification")
)

rf_fit = rf_work_tuned %>%
  fit(data=hotel_train)
```

Test Performance (out-of-sample)

```r
rf_test_perf = rf_fit %>%
  augment(new_data = hotel_test) %>%
  select(children, starts_with(".pred"))

rf_test_perf %>%
  conf_mat(children, .pred_class)
```

```
##             Truth
## Prediction children  none
##   children      402    69
##   none          609 11420
```

```r
rf_test_perf %>%
  precision(children, .pred_class)
```

```
## # A tibble: 1 × 3
##   .metric   .estimator .estimate
##   <chr>     <chr>          <dbl>
## 1 precision binary         0.854
```

```r
rf_test_perf %>%
  roc_auc(children, .pred_children)
```

```r
rf_roc = rf_test_perf %>%
  yardstick::roc_curve(
    children,
    .pred_children
  ) %>%
  mutate(name = "RF - test")
rf_roc %>%
  autoplot()
```

Comparing models