More Tidymodels

Lecture 23

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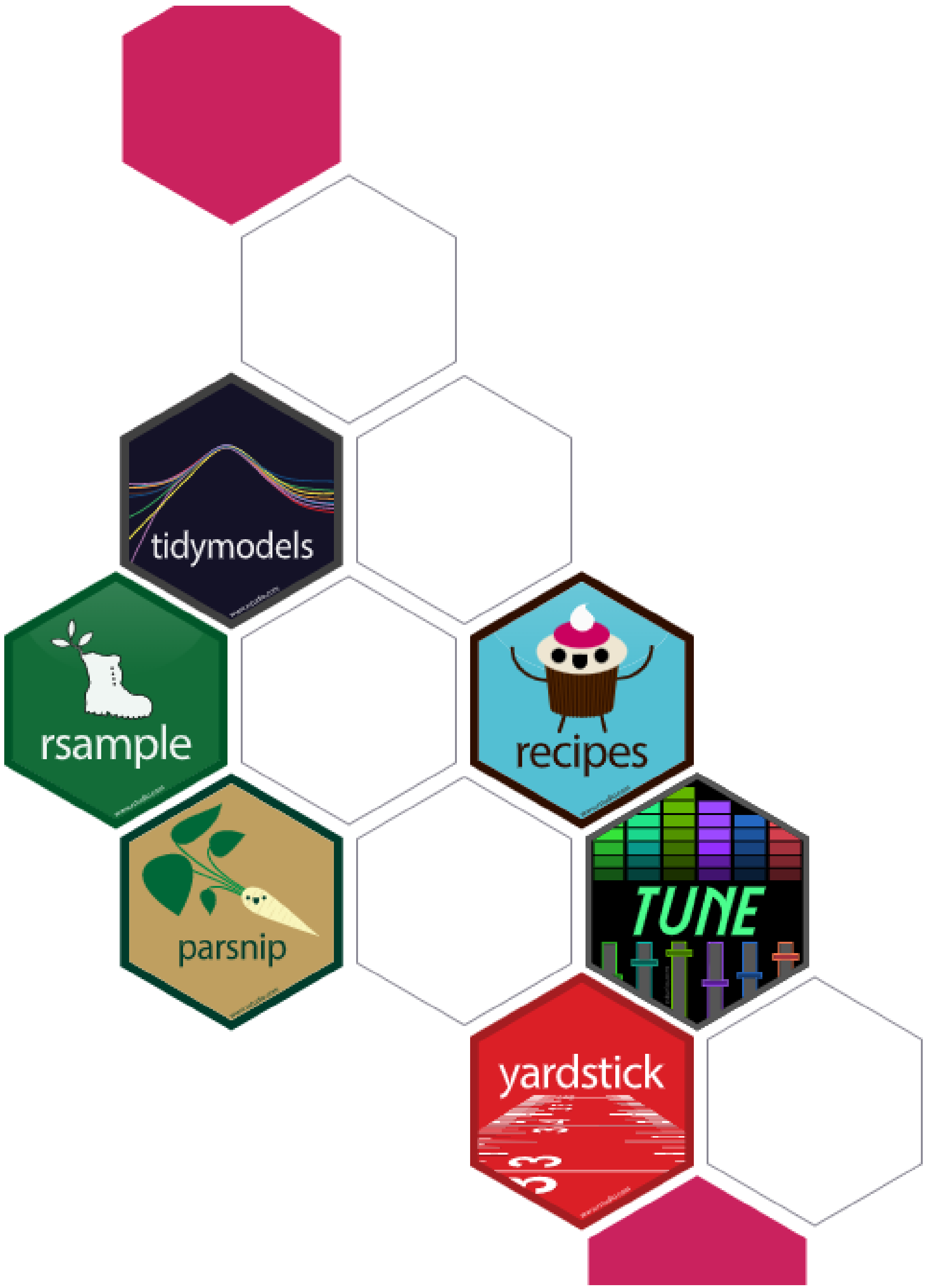

tidymodels
rsample
recipes
parsnip
TUNE
yardstick

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)
  )
```


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

The data

```r
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…
```

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.

```r
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")
translate(lr_model)
```

```
Logistic Regression Model Specification (classification)

Computational engine: glm

Model fit template:
stats::glm(formula = missing_arg(), data = missing_arg(), weights = missing_arg(),
    family = stats::binomial)
```

Recipe

```
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
Holiday features from arrival_date
Variables removed arrival_date
Variables removed country
```

```
Dummy variables from all_nominal_predictors()
Zero variance filter on all_predictors()
```

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

```
# A tibble: 37,500 × 76
   lead_time stays_…¹ stays…² adults is_re…³ previ…⁴ previ…⁵
       <dbl>    <dbl>   <dbl>  <dbl>   <dbl>   <dbl>   <dbl>
 1         2        0       1      2       0       0       0
 2        95        2       5      2       0       0       0
 3        67        2       2      2       0       0       0
 4        47        0       2      2       0       0       0
 5        56        0       3      0       0       0       0
 6         6        2       2      2       0       0       0
 7       130        1       2      2       0       0       0
 8        27        0       1      1       0       0       0
 9        46        0       2      2       0       0       0
10       423        1       1      2       0       0       0
# … with 37,490 more rows, 69 more variables:
#   booking_changes <dbl>, days_in_waiting_list <dbl>,
#   average_daily_rate <dbl>,
#   total_of_special_requests <dbl>, children <fct>,
```

Workflow

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

```
══ Workflow ════════════════════════════════════════════════
Preprocessor: Recipe
Model: logistic_reg()

── Preprocessor ────────────────────────────────────────────
6 Recipe Steps

• step_date()
• step_holiday()
• step_rm()
• step_rm()
• step_dummy()
• step_zv()

── Model ───────────────────────────────────────────────────
Logistic Regression Model Specification (classification)
```

Fit

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

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 ───────────────────────────────────────────────

Call:  stats::glm(formula = ..y ~ ., family = stats::binomial, data = data)
```

Logistic regression predictions

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

```
# 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
```

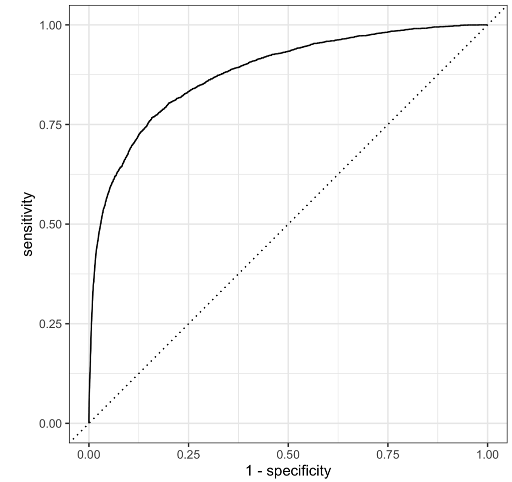
```r
lr_perf %>%
  precision(children, .pred_class)
```

```
# 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)

```
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
```

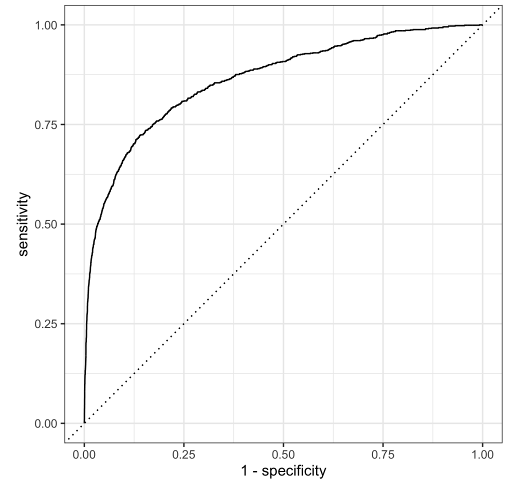
```
lr_test_perf %>%
  precision(children, .pred_class)
```

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

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

```
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.864
```

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

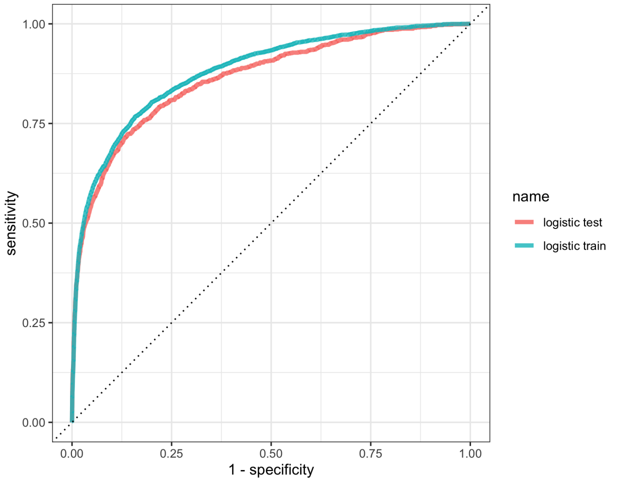


Combining ROC curves

```
lr_roc_train = lr_perf %>%
  yardstick::roc_curve(children, .pred_children)
  mutate(name="logistic train")

lr_roc_test = lr_test_perf %>%
  yardstick::roc_curve(children, .pred_children)
  mutate(name="logistic test")
```

```
bind_rows(
  lr_roc_train,
  lr_roc_test
) %>%
  ggplot(aes(x = 1 - specificity, y = sensitivit
    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(),
    alpha = 1, family = "binomial")
```

```r
lasso_model %>%
  parameters()
```

```
Collection of 1 parameters for tuning

 identifier    type    object
    penalty penalty nparam[+]
```

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_…¹ stays…² adults is_re…³ previ…⁴ previ…⁵
       <dbl>    <dbl>   <dbl>  <dbl>   <dbl>   <dbl>   <dbl>
 1    -0.858  -0.938   -0.767  0.337  -0.213 -0.0597  -0.112
 2     0.160   1.09     1.32   0.337  -0.213 -0.0597  -0.112
 3    -0.146   1.09    -0.245  0.337  -0.213 -0.0597  -0.112
 4    -0.365  -0.938   -0.245  0.337  -0.213 -0.0597  -0.112
 5    -0.267  -0.938    0.278 -3.59   -0.213 -0.0597  -0.112
 6    -0.814   1.09    -0.245  0.337  -0.213 -0.0597  -0.112
 7     0.544   0.0735  -0.245  0.337  -0.213 -0.0597  -0.112
 8    -0.584  -0.938   -0.767 -1.63   -0.213 -0.0597  -0.112
 9    -0.376  -0.938   -0.245  0.337  -0.213 -0.0597  -0.112
10     3.75    0.0735  -0.767  0.337  -0.213 -0.0597  -0.112
# … with 37,490 more rows, 69 more variables:
#   booking_changes <dbl>, days_in_waiting_list <dbl>,
#   average_daily_rate <dbl>,
```

Lasso workflow

::: {.small}

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

```
══ Workflow ════════════════════════════════════════════════
Preprocessor: Recipe
Model: logistic_reg()

── Preprocessor ────────────────────────────────────────────
7 Recipe Steps

• step_date()
• step_holiday()
• step_rm()
• step_rm()
• step_dummy()
• step_zv()
```

v-folds for hyperparameter tuning

```r
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)
    )
)
```

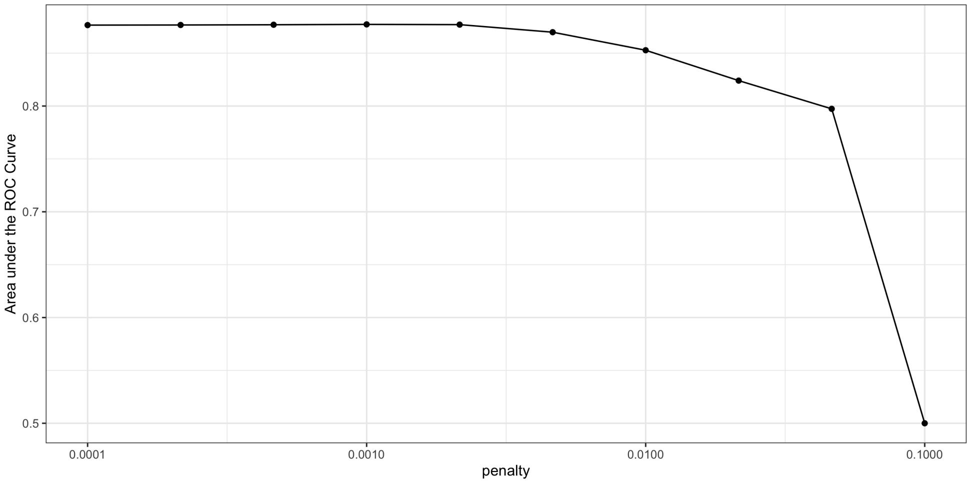
```
# Tuning results
# 5-fold cross-validation using stratification
# A tibble: 5 × 5
  splits               id    .metrics .notes   .predictions
  <list>               <chr> <list>   <list>   <list>
1 <split [30000/7500]> Fold1 <tibble> <tibble> <tibble>
2 <split [30000/7500]> Fold2 <tibble> <tibble>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

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

```
# A tibble: 10 × 7
    penalty .metric .estimator  mean     n std_err
.config
      <dbl> <chr>   <chr>      <dbl> <int>   <dbl>
<chr>
 1 0.0001   roc_auc binary     0.877     5 0.00318
Preproce…
 2 0.000215 roc_auc binary     0.877     5 0.00316
Preproce…
 3 0.000464 roc_auc binary     0.877     5 0.00314
Preproce…
 4 0.001    roc_auc binary     0.877     5 0.00304
Preproce…
 5 0.00215  roc_auc binary     0.877     5 0.00263
Preproce…
 6 0.00464  roc_auc binary     0.870     5 0.00253
Preproce…
```

```r
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

```
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

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

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

```
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.877
```

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
```

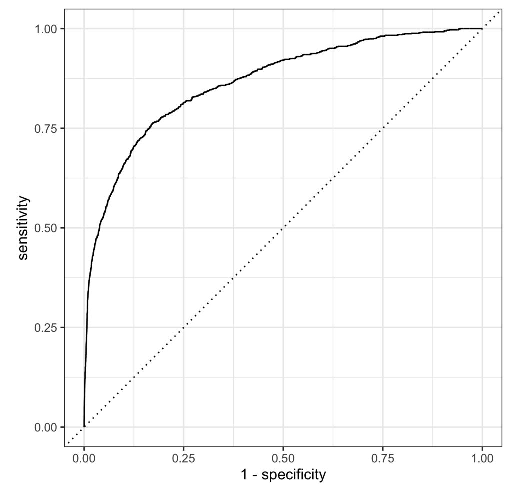
```r
lasso_test_perf %>%
  precision(children, .pred_class)
```

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

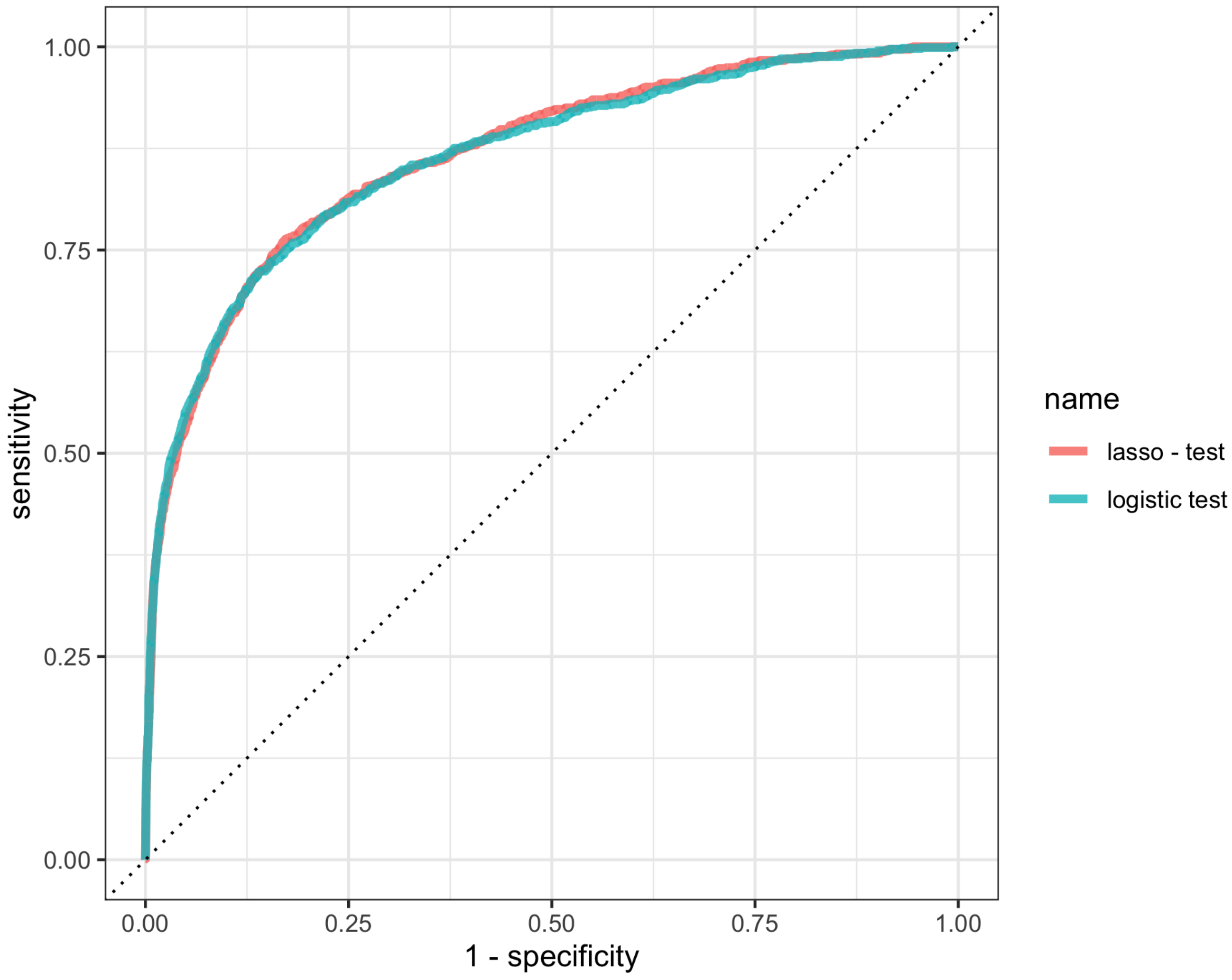
```r
lasso_test_perf %>%
  roc_auc(children, .pred_children)
```

```
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.866
```

```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

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

```
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.parameters` for more information.
```

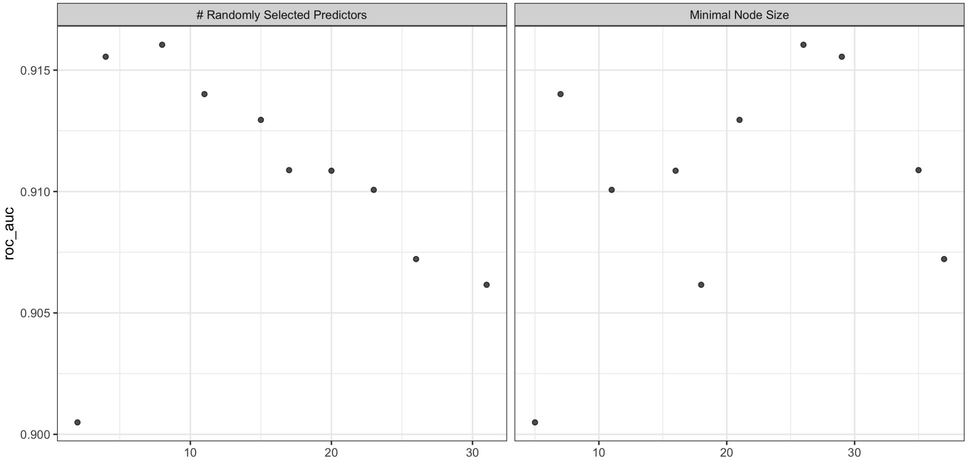
```
rf_grid = rf_work %>%
  tune_grid(
    hotel_vf,
    grid = 10,
    control = control_grid(save_pred = TRUE),
    metrics = metric_set(roc_auc)
  )
```

“Best” parameters

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

```
# A tibble: 5 × 8
   mtry min_n .metric .estimator  mean     n
std_err .config
  <int> <int> <chr>   <chr>      <dbl> <int>
<dbl> <chr>
1      8     26 roc_auc binary     0.916     5
0.00172 Prepro…
2      4     29 roc_auc binary     0.916     5
0.00190 Prepro…
3     11      7 roc_auc binary     0.914     5
0.00182 Prepro…
4     15     21 roc_auc binary     0.913     5
0.00118 Prepro…
5     17     35 roc_auc binary     0.911     5
0.00191 Prepro…
```

```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
```

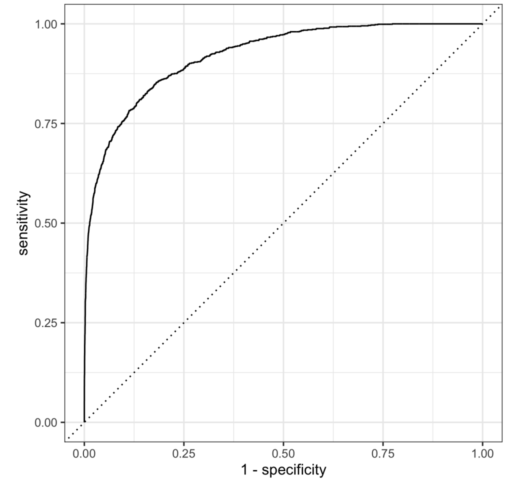
```r
rf_test_perf %>%
  precision(children, .pred_class)
```

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

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

```
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.920
```

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



Comparing models