04 - A Typical (Supervised) ML Workflow

ml4econ, HUJI 2021

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April 4, 2021 (updated: 2021-04-01)

Packages and setup

Use the pacman package that automatically loads and installs packages:

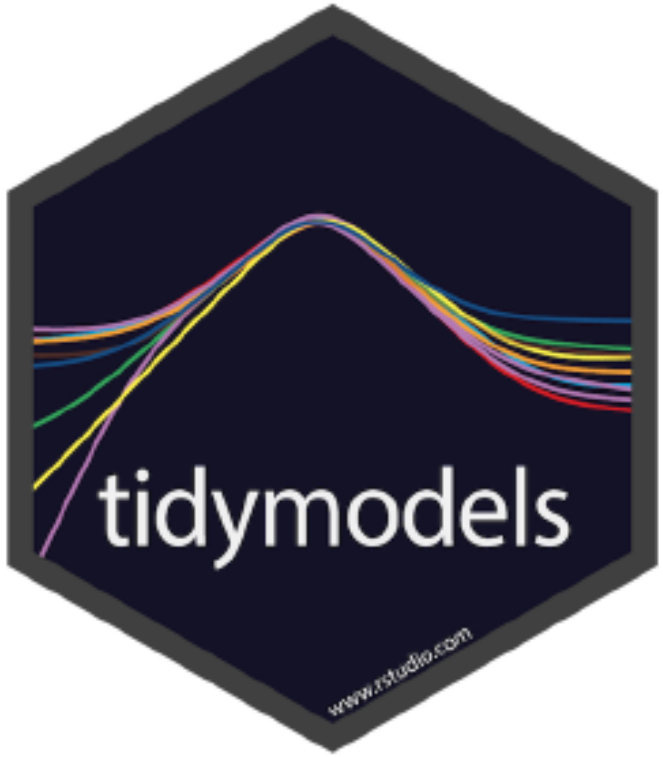
```
if (!require("pacman")) install.packages("pacman")

pacman::p_load(
  tidyverse,   # for data wrangling and visualization
  tidymodels,  # for data modeling
  GGally,      # for pairs plot
  skimr,       # for summary statistics
  here         # for referencing folders and files
  )
```

Set a theme for `ggplot` (Relevant only for the presentation)

```
theme_set(theme_grey(20))
```

The `tidymodels` package



> "`tidymodels` is a "meta-package" for modeling and statistical analysis that share the underlying design philosophy, grammar, and data structures of the tidyverse."

Supervised ML Workflow

Step 1: Define the Prediton Task

Step 2: Explore the Data

Step 3: Set Model and Tuning Parameters

Step 4: Cross-validation

Step 5: Evaluate the Model

Step 1: Define the Prediction Task

Predicting Boston Housing Prices

We will use the `BostonHousing`: housing data for 506 census tracts of Boston from the 1970 census (Harrison and Rubinfeld, 1978).

- `medv` (target): median value of owner-occupied homes in USD 1000's.
- `lstat`(predictor): percentage of lower status of the population.
- `chas` (predictor): Charles River dummy variable (= 1 if tract bounds river; 0 otherwise).

OBJECTIVE: Predict `medv`.

Source: https://www.bostonusa.com/

Load the Data

Load the data

```
boston_raw <- read_csv(here("04-ml-workflow/data","BostonHousing.csv"))
```

```
## Parsed with column specification:
## cols(
##   crim = col_double(),
##   zn = col_double(),
##   indus = col_double(),
##   chas = col_double(),
##   nox = col_double(),
##   rm = col_double(),
##   age = col_double(),
##   dis = col_double(),
##   rad = col_double(),
##   tax = col_double(),
##   ptratio = col_double(),
##   b = col_double(),
##   lstat = col_double(),
##   medv = col_double()
## )
```

What Type of Data?

We can use the `glimpse()` function in order to better understand the data structure:

```
glimpse(boston_raw)
```

```
## Rows: 506
## Columns: 14
## $ crim    <dbl> 0.00632, 0.02731, 0.02729, 0.03237, 0.06905, 0.02985, 0.08829, ...
## $ zn      <dbl> 18.0, 0.0, 0.0, 0.0, 0.0, 0.0, 12.5, 12.5, 12.5, 12.5, 12.5, 12...
## $ indus   <dbl> 2.31, 7.07, 7.07, 2.18, 2.18, 2.18, 7.87, 7.87, 7.87, 7.87, 7.8...
## $ chas    <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, ...
## $ nox     <dbl> 0.538, 0.469, 0.469, 0.458, 0.458, 0.458, 0.524, 0.524, 0.524, ...
## $ rm      <dbl> 6.575, 6.421, 7.185, 6.998, 7.147, 6.430, 6.012, 6.172, 5.631, ...
## $ age     <dbl> 65.2, 78.9, 61.1, 45.8, 54.2, 58.7, 66.6, 96.1, 100.0, 85.9, 94...
## $ dis     <dbl> 4.0900, 4.9671, 4.9671, 6.0622, 6.0622, 6.0622, 5.5605, 5.9505,...
## $ rad     <dbl> 1, 2, 2, 3, 3, 3, 5, 5, 5, 5, 5, 5, 5, 4, 4, 4, 4, 4, 4, 4, 4, ...
## $ tax     <dbl> 296, 242, 242, 222, 222, 222, 311, 311, 311, 311, 311, 311, 311...
## $ ptratio <dbl> 15.3, 17.8, 17.8, 18.7, 18.7, 18.7, 15.2, 15.2, 15.2, 15.2, 15....
## $ b       <dbl> 396.90, 396.90, 392.83, 394.63, 396.90, 394.12, 395.60, 396.90,...
## $ lstat   <dbl> 4.98, 9.14, 4.03, 2.94, 5.33, 5.21, 12.43, 19.15, 29.93, 17.10,...
## $ medv    <dbl> 24.0, 21.6, 34.7, 33.4, 36.2, 28.7, 22.9, 27.1, 16.5, 18.9, 15....
```

The chas variable is mostly zero $\Rightarrow$ should be a factor.

Initial Data Filtering

Select `medv` and `lstat`

```
boston <- boston_raw %>%
  as_tibble() %>%
  select(medv, lstat, chas) %>%
  mutate(chas = as_factor(chas))

head(boston)
```

```
## # A tibble: 6 x 3
##    medv lstat chas
##   <dbl> <dbl> <fct>
## 1  24    4.98 0
## 2  21.6  9.14 0
## 3  34.7  4.03 0
## 4  33.4  2.94 0
## 5  36.2  5.33 0
## 6  28.7  5.21 0
```

Step 2: Split the Data

Initial Split

We will use the `initial_split()`, `training()` and `testing()` functions from the rsample package to perform an initial train-test split

Set seed for reproducibility

```
set.seed(1203)
```

Initial split:

```
boston_split <- boston %>%
  initial_split(prop = 2/3, strata = medv)

boston_split
```

```
## <Training/Validation/Total>
## <338/168/506>
```

Prepare Training and Test Sets

```
boston_train_raw <- training(boston_split)
boston_test_raw  <- testing(boston_split)

head(boston_train_raw, 5)
```

```
## # A tibble: 5 x 3
##    medv lstat chas
##   <dbl> <dbl> <fct>
## 1  24    4.98 0
## 2  34.7  4.03 0
## 3  33.4  2.94 0
## 4  36.2  5.33 0
## 5  28.7  5.21 0
```

```
head(boston_test_raw, 5)
```

```
## # A tibble: 5 x 3
##    medv lstat chas
##   <dbl> <dbl> <fct>
## 1  21.6  9.14 0
## 2  16.5 29.9  0
## 3  18.9 17.1  0
## 4  18.9 13.3  0
## 5  20.4  8.26 0
```

Step 3: Explore the Data

Summary Statistics Using `skimr`

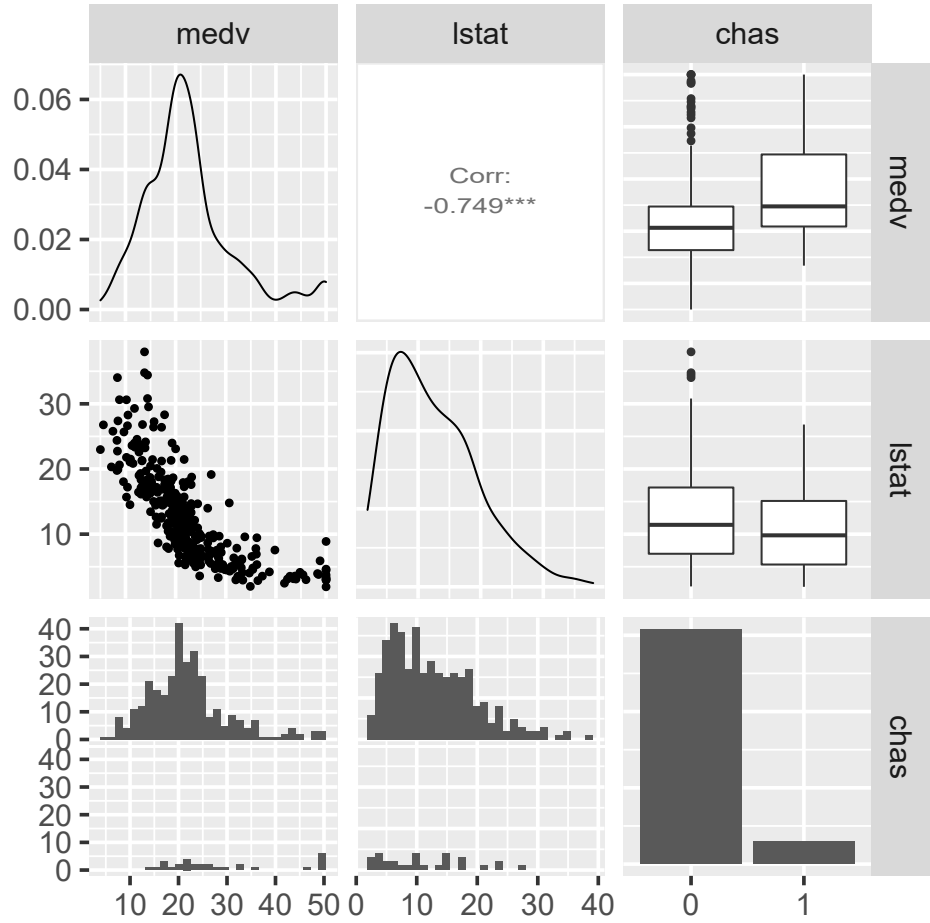
```
boston_train_raw %>%
  skim()
```

(Does not come out well on these slides)

Pairs Plot Using GGally

We now use a **pairs plot** which compactly plots every variable in a dataset against every other one.

```
boston_train_raw %>% ggpairs()
```



Select a Model

We choose the class of polynomial models:

$$medv_i = \beta_0 + \sum_{j=1}^{\lambda} \beta_j lstat_i^j + \varepsilon_i$$

```
boston_train_raw %>% ggplot(aes(lstat, medv)) +
  geom_point() +
  geom_smooth(
    method = lm,
    formula = y ~ poly(x,1),
    se = FALSE,
    color = "blue"
  ) +
  geom_smooth(
    method = lm,
    formula = y ~ poly(x,10),
    se = FALSE,
    color = "red"
  )
```

Step 4: Set Model and Tuning Parameters

Data Preprocessing using `recipes`

The `recipes` package is a great tool for data preprocessing that fits in naturally with the tidy approach to ML.

```
boston_rec <-
  recipe(medv ~ lstat + chas, data = boston_train_raw) %>%
  step_poly(lstat, degree = tune("lambda")) %>%
  step_dummy(chas)

boston_rec
```

```
## Data Recipe
##
## Inputs:
##
##       role #variables
##    outcome           1
##  predictor           2
##
## Operations:
##
## Orthogonal polynomials on lstat
## Dummy variables from chas
```

Set a Grid for λ

What are our tuning parameters?

```
boston_rec %>% parameters()
```

```
## Collection of 1 parameters for tuning
##
##      id parameter type object class
##  lambda         degree    nparam[+]
```

We need to tune the polynomial degree parameter (λ) when building our models on the train data. In this example, we will set the range between 1 and 8:

```
lambda_grid <- expand_grid("lambda" = 1:8)
```

Define the Model

We will use the linear regression model

```
lm_mod <- linear_reg()%>%
  set_engine("lm")

lm_mod
```

```
## Linear Regression Model Specification (regression)
##
## Computational engine: lm
```

Note that there are no tuning parameters here.

Step 5: Cross-validation

Split the Training Set to 5-folds

We will use the `vfold-cv()` function from the rsample package to split the training set to 5-folds:

```
cv_splits <- boston_train_raw %>%
  vfold_cv(v = 5)

cv_splits
```

```
## #  5-fold cross-validation
## # A tibble: 5 x 2
##   splits           id
##   <named list>     <chr>
## 1 <split [270/68]> Fold1
## 2 <split [270/68]> Fold2
## 3 <split [270/68]> Fold3
## 4 <split [271/67]> Fold4
## 5 <split [271/67]> Fold5
```

Estimate CV-RMSE Over the λ Grid

We now estimate the CV-RMSE for each value of λ.

```
boston_results <- tune_grid(
  boston_rec,
  model     = lm_mod,
  resamples = cv_splits,
  grid      = lambda_grid
)

boston_results
```

```
## #  5-fold cross-validation
## # A tibble: 5 x 4
##   splits           id    .metrics          .notes
##   <named list>     <chr> <list>            <list>
## 1 <split [270/68]> Fold1 <tibble [16 x 4]> <tibble [0 x 1]>
## 2 <split [270/68]> Fold2 <tibble [16 x 4]> <tibble [0 x 1]>
## 3 <split [270/68]> Fold3 <tibble [16 x 4]> <tibble [0 x 1]>
## 4 <split [271/67]> Fold4 <tibble [16 x 4]> <tibble [0 x 1]>
## 5 <split [271/67]> Fold5 <tibble [16 x 4]> <tibble [0 x 1]>
```

Find the Optimal λ

Let's find the top-3 performing models

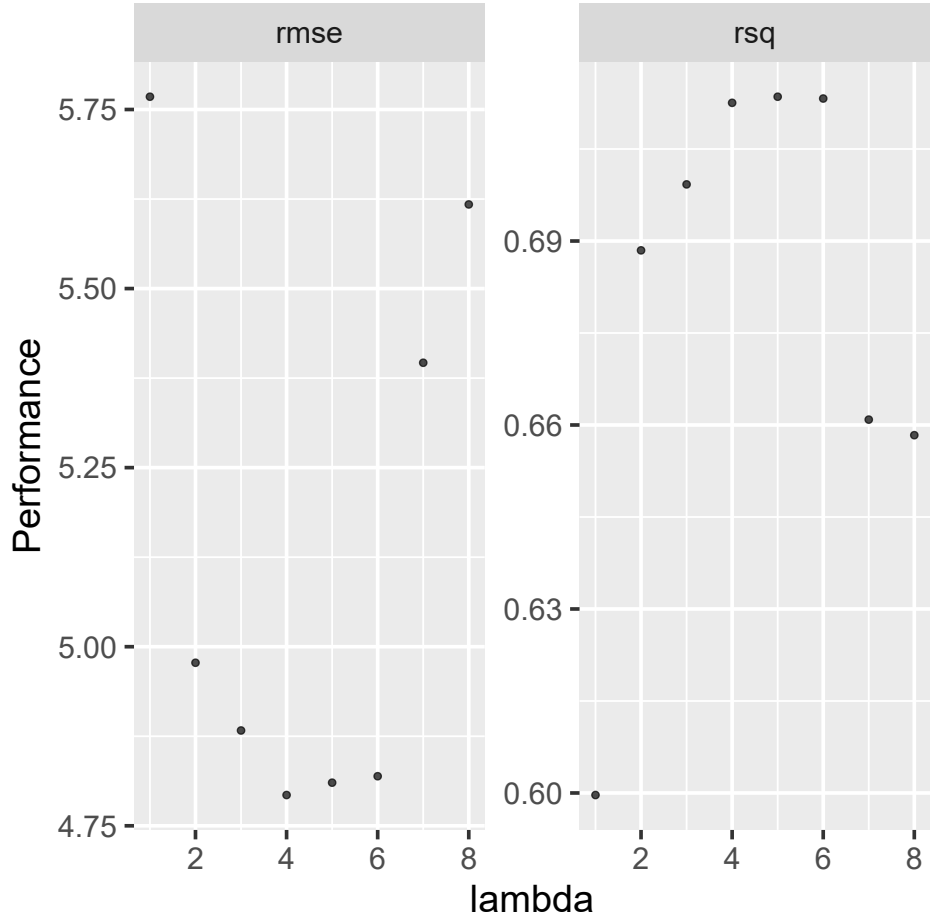
```
boston_results %>%
 show_best(metric = "rmse", n = 3, maximize = FALSE)
```

```
## # A tibble: 3 x 6
##   lambda .metric .estimator  mean     n std_err
##    <int> <chr>   <chr>      <dbl> <int>   <dbl>
## 1      4 rmse    standard    4.79     5   0.260
## 2      5 rmse    standard    4.81     5   0.273
## 3      6 rmse    standard    4.82     5   0.268
```

> *"[I]n reality there is rarely if ever a true underlying model, and even if there was a true underlying model, selecting that model will not necessarily give the best forecasts..."*
>
> — **Rob J. Hyndman**

And Now Using a Graph

```
boston_results %>%
  autoplot()
```



Step 6: Evaluate the Model

Use the Test Set to Evaluate the Best Model

Select the optimal λ

```
best_lambda <- boston_results %>%
  select_best(metric = "rmse", maximize = FALSE)

best_lambda
```

```
## # A tibble: 1 x 1
##   lambda
##    <int>
## 1      4
```

Prepare a recipe with the optimal $\lambda = 4$

```
boston_final <- boston_rec %>%
  finalize_recipe(best_lambda)
```

Apply the Recipe to the Training and Test Sets

`juice()` applies the recipe to the training set and `bake()` to the test set.

```
boston_train <- boston_final %>%
  prep() %>%
  juice()

boston_test <- boston_final %>%
  prep() %>%
  bake(new_data = boston_test_raw)
```

For example, let's take a look at the training set:

```
head(boston_train, 3)
```

```
## # A tibble: 3 x 6
##    medv lstat_poly_1 lstat_poly_2 lstat_poly_3 lstat_poly_4 chas_X1
##   <dbl>        <dbl>        <dbl>        <dbl>        <dbl>   <dbl>
## 1  24        -0.0586       0.0449      -0.0214     -0.00896       0
## 2  34.7      -0.0660       0.0627      -0.0515      0.0283        0
## 3  33.4      -0.0744       0.0851      -0.0940      0.0917        0
```

Fit the Model to the Training Set

Fit the optimal model ($\lambda = 4$)) to the training set:

```
boston_fit <- lm_mod %>%
  fit(medv ~ ., data = boston_train)
```

Here are the estimated coefficients:

```
boston_fit %>% tidy()
```

```
## # A tibble: 6 x 5
##   term         estimate std.error statistic   p.value
##   <chr>           <dbl>     <dbl>     <dbl>     <dbl>
## 1 (Intercept)     22.1      0.272     81.3  3.10e-221
## 2 lstat_poly_1  -123.       4.78     -25.8  3.59e- 81
## 3 lstat_poly_2    53.3      4.78      11.1  9.85e- 25
## 4 lstat_poly_3   -20.1      4.80      -4.19 3.59e-  5
## 5 lstat_poly_4    20.3      4.79       4.24 2.94e-  5
## 6 chas_X1          4.76     0.924      5.15 4.43e-  7
```

Make Predictions Using the Test Set

Create a tibble with the predictions and ground-truth

```
boston_pred <- boston_fit %>%
  predict(new_data = boston_test) %>%
  bind_cols(boston_test) %>%
  select(medv, .pred)

head(boston_pred)
```

```
## # A tibble: 6 x 2
##    medv .pred
##   <dbl> <dbl>
## 1  21.6 22.9
## 2  16.5  9.80
## 3  18.9 16.6
## 4  18.9 18.7
## 5  20.4 24.3
## 6  18.2 21.4
```

Note that this is the first time we make use of the test set!

Test-RMSE

Calculate the test root mean square error (test-RMSE):

```
boston_pred %>%
  rmse(medv, .pred)
```

```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard        5.94
```

The above is a measure of our model's performance on "general" data.

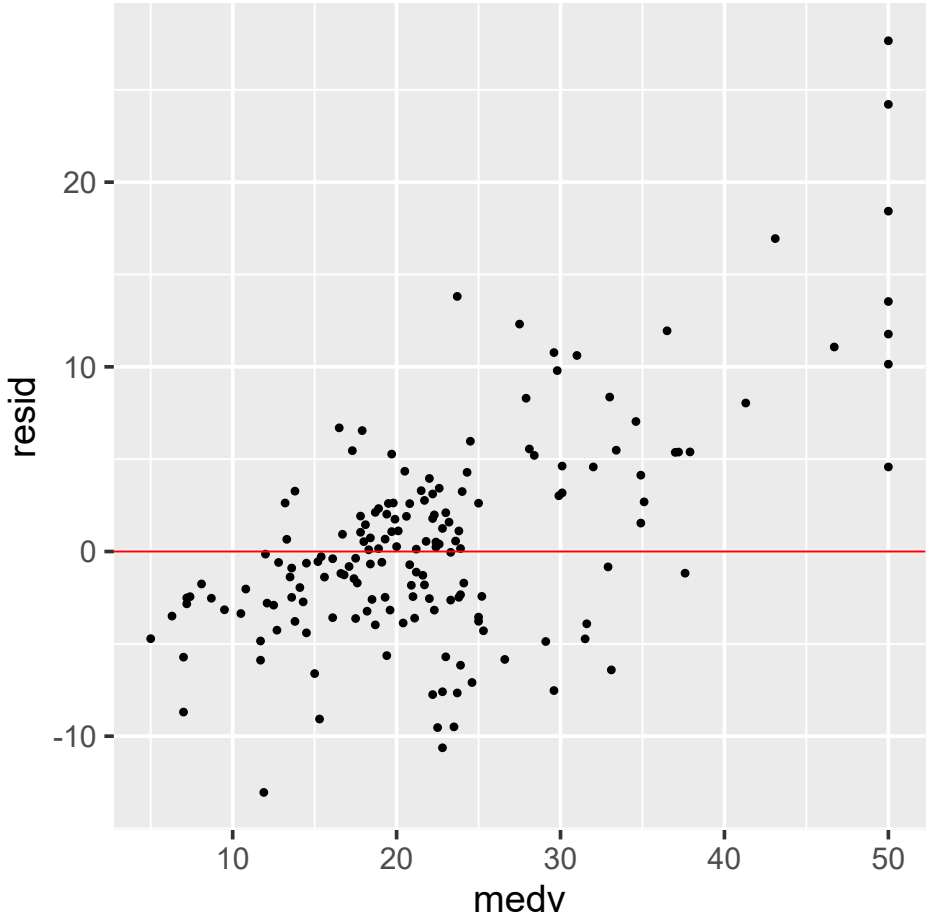
> **NOTE:** the test set RMSE estimates the expected squared prediction error on unseen data *given* the best model.

Always plot your prediction errors

Plotting the prediction errors $(y_i - \hat{y}_i)$ vs. the target provides valuable information about prediction quality.

```
boston_pred %>%
  mutate(resid = medv - .pred) %>%
  ggplot(aes(medv, resid)) +
  geom_point() +
  geom_hline(yintercept = 0, color = "red")
```

For example, our predictions for high-end levels of `medv` are extremely biased ⇒ there's room for improvement...



(A shortcut)

A much quicker way to get the test-set RMSE is using `tune`'s `final_fit()` function:

```
boston_final %>%
  last_fit(lm_mod, split = boston_split) %>%
  collect_metrics() %>%
  filter(.metric == "rmse")
```

```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard        5.94
```

`slides::end()`

Source code