

# Cross validation

Data Science in a Box  
[datasciencebox.org](https://datasciencebox.org)



# Data and exploration



# the office



# Data

```
office_ratings <- read_csv("data/office_ratings.csv")
office_ratings
```

```
## # A tibble: 188 × 6
##   season episode title          imdb_rating total_votes air_date
##   <dbl>   <dbl> <chr>          <dbl>         <dbl> <date>
## 1     1       1     Pilot             7.6           3706 2005-03-24
## 2     1       2 Diversity Day        8.3           3566 2005-03-29
## 3     1       3 Health Care         7.9           2983 2005-04-05
## 4     1       4 The Alliance        8.1           2886 2005-04-12
## 5     1       5 Basketball          8.4           3179 2005-04-19
## 6     1       6 Hot Girl            7.8           2852 2005-04-26
## # ... with 182 more rows
```

Source: The data come from [data.world](https://data.world), by way of TidyTuesday.



# IMDB ratings

Code

Plot

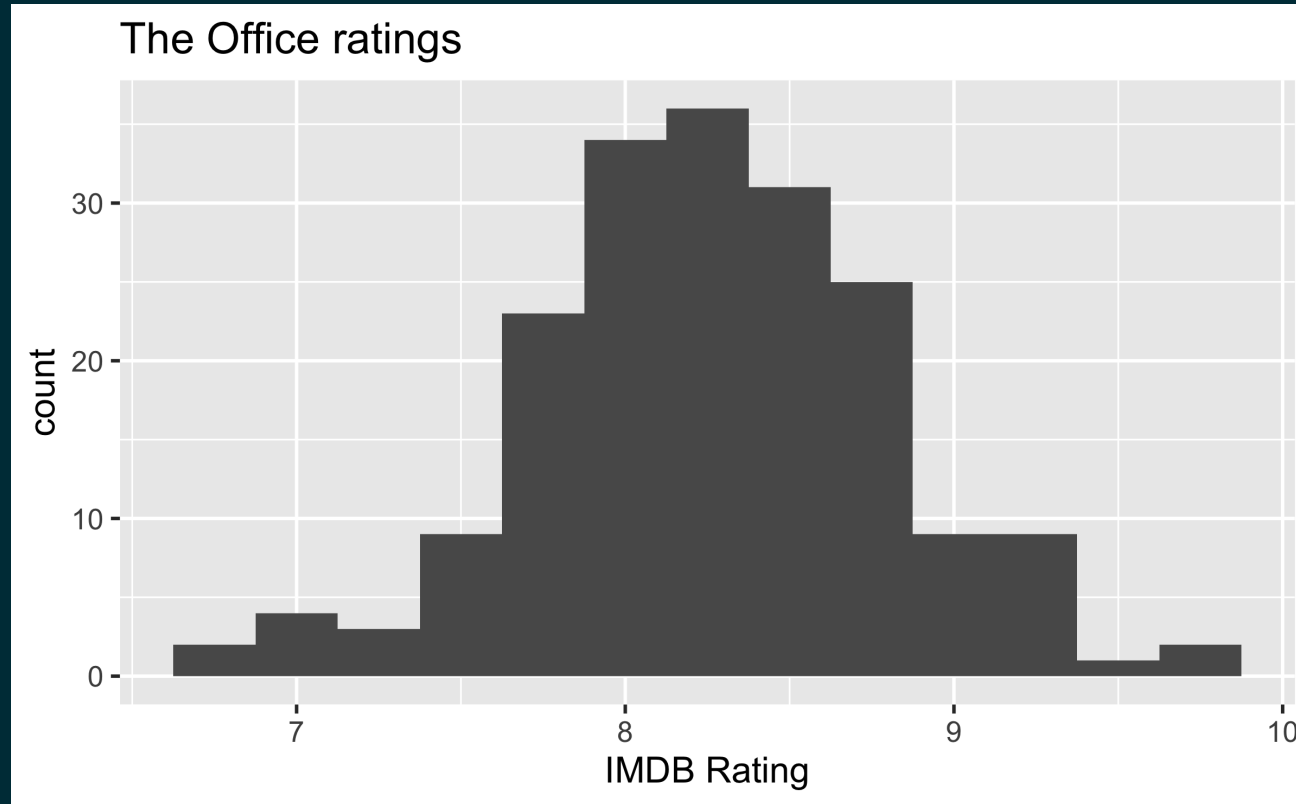
```
ggplot(office_ratings, aes(x = imdb_rating)) +  
  geom_histogram(binwidth = 0.25) +  
  labs(  
    title = "The Office ratings",  
    x = "IMDB Rating"  
  )
```



# IMDB ratings

Code

Plot



# IMDB ratings vs. number of votes

Code

Plot

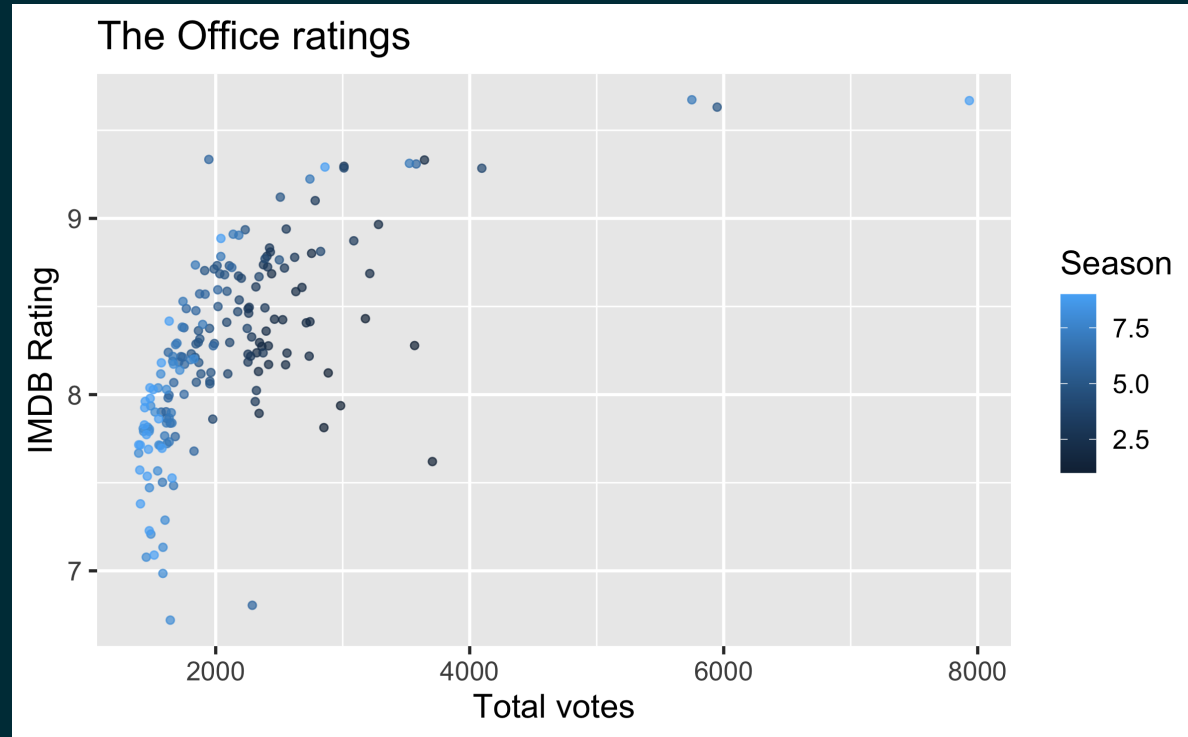
```
ggplot(office_ratings, aes(x = total_votes, y = imdb_rating, color = season)) +  
  geom_jitter(alpha = 0.7) +  
  labs(  
    title = "The Office ratings",  
    x = "Total votes",  
    y = "IMDB Rating",  
    color = "Season"  
  )
```



# IMDB ratings vs. number of votes

Code

Plot





# Outliers

Code

Plot

```
ggplot(office_ratings, aes(x = total_votes, y = imdb_rating)) +  
  geom_jitter() +  
  gghighlight(total_votes > 4000, label_key = title) +  
  labs(  
    title = "The Office ratings",  
    x = "Total votes",  
    y = "IMDB Rating"  
  )
```

If you like the Dinner Party episode, I highly recommend this "oral history" of the episode published on Rolling Stone magazine.



# Outliers

Code

Plot

```
## Warning: Using across() in filter() is deprecated, use
```

```
if_any() or if_all().
```

If you like the Dinner Party episode, I highly recommend this "oral history" of the episode published on Rolling Stone magazine.



# IMDB ratings vs. seasons

Code

Plot

```
ggplot(office_ratings, aes(x = factor(season), y = imdb_rating, color = season)) +  
  geom_boxplot() +  
  geom_jitter() +  
  guides(color = FALSE) +  
  labs(  
    title = "The Office ratings",  
    x = "Season",  
    y = "IMDB Rating"  
  )
```



# IMDB ratings vs. seasons

Code

Plot

```
## Warning: guides(<scale> = FALSE) is deprecated. Please use
```

```
guides(<scale> = "none");
```



# Modeling



# Train / test

- Create an initial split

```
set.seed(1122)  
office_split <- initial_split(office_ratings) # prop = 3/4 by default
```

- Save training data

```
office_train <- training(office_split)  
dim(office_train)
```

```
## [1] 141  6
```

- Save testing data

```
office_test <- testing(office_split)  
dim(office_test)
```

```
## [1] 47  6
```



# Specify model

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

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



# Build recipe

Code

Output

```
office_rec <- recipe(imdb_rating ~ ., data = office_train) %>%  
  # title isn't a predictor, but keep around to ID  
  update_role(title, new_role = "ID") %>%  
  # extract month of air_date  
  step_date(air_date, features = "month") %>%  
  step_rm(air_date) %>%  
  # make dummy variables of month  
  step_dummy(contains("month")) %>%  
  # remove zero variance predictors  
  step_zv(all_predictors())
```





# Build recipe

Code

Output

office\_rec

```
## Recipe
##
## Inputs:
##
##      role #variables
##      ID      1
## outcome      1
## predictor      4
##
## Operations:
##
## Date features from air_date
## Variables removed air_date
## Dummy variables from contains("month")
## Zero variance filter on all_predictors()
```



# Build workflow

Code

Output

```
office_wflow <- workflow() %>%  
  add_model(office_mod) %>%  
  add_recipe(office_rec)
```



# Build workflow

Code

Output

office\_wflow

```
## — Workflow —————
## Preprocessor: Recipe
## Model: linear_reg()
##
## — Preprocessor —————
## 4 Recipe Steps
##
## • step_date()
## • step_rm()
## • step_dummy()
## • step_zv()
##
## — Model —————
## Linear Regression Model Specification (regression)
##
## Computational engine: lm
```



# Fit model

Code

Output

```
office_fit <- office_wflow %>%  
  fit(data = office_train)
```



# Fit model

Code

Output

```
tidy(officer_fit) %>%  
  print(n = 12)
```

```
## # A tibble: 12 × 5  
##   term                estimate std.error statistic  p.value  
##   <chr>              <dbl>    <dbl>    <dbl>    <dbl>  
## 1 (Intercept)        7.23      0.205     35.4 3.14e-68  
## 2 season             -0.0499   0.0157     -3.18 1.86e- 3  
## 3 episode             0.0353   0.0101      3.50 6.44e- 4  
## 4 total_votes        0.000352 0.0000448    7.85 1.39e-12  
## 5 air_date_month_Feb  0.0242   0.147      0.165 8.69e- 1  
## 6 air_date_month_Mar -0.145    0.144     -1.01 3.16e- 1  
## 7 air_date_month_Apr -0.106    0.140     -0.759 4.49e- 1  
## 8 air_date_month_May  0.0575   0.175      0.329 7.43e- 1  
## 9 air_date_month_Sep  0.440    0.191      2.30 2.30e- 2  
## 10 air_date_month_Oct 0.321    0.150      2.13 3.50e- 2  
## 11 air_date_month_Nov 0.237    0.138      1.72 8.81e- 2  
## 12 air_date_month_Dec 0.443    0.190      2.34 2.09e- 2
```



# Evaluate model



# Make predictions for training data

```
office_train_pred <- predict(office_fit, office_train) %>%  
  bind_cols(office_train %>% select(imdb_rating, title))
```

```
office_train_pred
```

```
## # A tibble: 141 × 3  
##   .pred imdb_rating title  
##   <dbl>      <dbl> <chr>  
## 1  7.90         8.1 Garden Party  
## 2  8.43         7.9 The Chump  
## 3  7.81         7.1 Here Comes Treble  
## 4  7.94         6.7 Get the Girl  
## 5  7.92         7.9 Tallahassee  
## 6  8.29         7.7 The Inner Circle  
## # ... with 135 more rows
```



# R-squared

Percentage of variability in the IMDB ratings explained by the model

```
rsq(office_train_pred, truth = imdb_rating, estimate = .pred)
```

```
## # A tibble: 1 × 3
##   .metric .estimator .estimate
##   <chr>   <chr>      <dbl>
## 1 rsq     standard      0.500
```

Are models with high or low  $R^2$  more preferable?





# RMSE

An alternative model performance statistic: **root mean square error**

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}}$$

```
rmse(office_train_pred, truth = imdb_rating, estimate = .pred)
```

```
## # A tibble: 1 × 3  
##   .metric .estimator .estimate  
##   <chr>    <chr>        <dbl>  
## 1 rmse      standard      0.373
```

Are models with high or low RMSE are more preferable?



# Interpreting RMSE

Is this RMSE considered low or high?

```
rmse(office_train_pred, truth = imdb_rating, estimate = .pred)
```

```
## # A tibble: 1 × 3  
##   .metric .estimator .estimate  
##   <chr>   <chr>       <dbl>  
## 1 rmse    standard     0.373
```

```
office_train %>%  
  summarise(min = min(imdb_rating), max = max(imdb_rating))
```

```
## # A tibble: 1 × 2  
##   min    max  
##   <dbl> <dbl>  
## 1  6.7   9.7
```



but, really, who cares about predictions on **training** data?



# Make predictions for testing data

```
office_test_pred <- predict(office_fit, office_test) %>%  
  bind_cols(office_test %>% select(imdb_rating, title))
```

```
office_test_pred
```

```
## # A tibble: 47 × 3  
##   .pred imdb_rating title  
##   <dbl>      <dbl> <chr>  
## 1  8.52        8.4 Office Olympics  
## 2  8.54        8.6 The Client  
## 3  8.90        8.8 Christmas Party  
## 4  8.71         9 The Injury  
## 5  8.50        8.2 Boys and Girls  
## 6  8.46        8.4 Dwight's Speech  
## # ... with 41 more rows
```



# Evaluate performance on testing data

- RMSE of model fit to testing data

```
rmse(office_test_pred, truth = imdb_rating, estimate = .pred)
```

```
## # A tibble: 1 × 3
##   .metric .estimator .estimate
##   <chr>    <chr>         <dbl>
## 1 rmse     standard         0.386
```

- $R^2$  of model fit to testing data

```
rsq(office_test_pred, truth = imdb_rating, estimate = .pred)
```

```
## # A tibble: 1 × 3
##   .metric .estimator .estimate
##   <chr>    <chr>         <dbl>
## 1 rsq     standard         0.556
```



# Training vs. testing

metric	train	test	comparison
RMSE	0.373	0.386	RMSE lower for training
R-squared	0.500	0.556	R-squared higher for training



# Evaluating performance on training data

- The training set does not have the capacity to be a good arbiter of performance.
- It is not an independent piece of information; predicting the training set can only reflect what the model already knows.
- Suppose you give a class a test, then give them the answers, then provide the same test. The student scores on the second test do not accurately reflect what they know about the subject; these scores would probably be higher than their results on the first test.

Source: [tidymodels.org](https://tidymodels.org)



[datasciencebox.org](https://datasciencebox.org)

# Cross validation





# Cross validation

More specifically, **v-fold cross validation**:

- Shuffle your data  $v$  partitions
- Use 1 partition for validation, and the remaining  $v-1$  partitions for training
- Repeat  $v$  times

You might also heard of this referred to as k-fold cross validation.



# Cross validation



# Split data into folds

```
set.seed(345)
```

```
folds <- vfold_cv(office_train, v = 5)  
folds
```

```
## # 5-fold cross-validation  
## # A tibble: 5 × 2  
##   splits      id  
##   <list>    <chr>  
## 1 <split [112/29]> Fold1  
## 2 <split [113/28]> Fold2  
## 3 <split [113/28]> Fold3  
## 4 <split [113/28]> Fold4  
## 5 <split [113/28]> Fold5
```

	training					testing
fold 1	validate	train	train	train	train	
fold 2	train	validate	train	train	train	
fold 3	train	train	validate	train	train	
fold 4	train	train	train	validate	train	
fold 5	train	train	train	train	validate	



# Fit resamples

```
set.seed(456)

office_fit_rs <- office_wflow %>%
  fit_resamples(folds)

office_fit_rs
```



```
## # Resampling results
## # 5-fold cross-validation
## # A tibble: 5 × 4
##   splits          id    .metrics          .nc
##   <list>         <chr> <list>         <list>
## 1 <split [112/29]> Fold1 <tibble [2 × 4]> <tibble [0 × 3]>
## 2 <split [113/28]> Fold2 <tibble [2 × 4]> <tibble [0 × 3]>
## 3 <split [113/28]> Fold3 <tibble [2 × 4]> <tibble [0 × 3]>
## 4 <split [113/28]> Fold4 <tibble [2 × 4]> <tibble [0 × 3]>
## 5 <split [113/28]> Fold5 <tibble [2 × 4]> <tibble [0 × 3]>
```



# Collect CV metrics

```
collect_metrics(office_fit_rs)
```

```
## # A tibble: 2 × 6
##   .metric .estimator mean      n std_err .config
##   <chr>   <chr>      <dbl> <int>   <dbl> <chr>
## 1 rmse    standard    0.403     5  0.0336 Preprocessor1_Model1
## 2 rsq     standard    0.413     5  0.0727 Preprocessor1_Model1
```



# Deeper look into CV metrics

Raw

Tidy

```
collect_metrics(office_fit_rs, summarize = FALSE) %>%  
  print(n = 10)
```

```
## # A tibble: 10 × 5  
##   id      .metric .estimator .estimate .config  
##   <chr> <chr>      <chr>          <dbl> <chr>  
## 1 Fold1 rmse      standard      0.430 Preprocessor1_Model1  
## 2 Fold1 rsq      standard      0.134 Preprocessor1_Model1  
## 3 Fold2 rmse      standard      0.368 Preprocessor1_Model1  
## 4 Fold2 rsq      standard      0.496 Preprocessor1_Model1  
## 5 Fold3 rmse      standard      0.452 Preprocessor1_Model1  
## 6 Fold3 rsq      standard      0.501 Preprocessor1_Model1  
## 7 Fold4 rmse      standard      0.289 Preprocessor1_Model1  
## 8 Fold4 rsq      standard      0.529 Preprocessor1_Model1  
## 9 Fold5 rmse      standard      0.475 Preprocessor1_Model1  
## 10 Fold5 rsq      standard      0.403 Preprocessor1_Model1
```



# Deeper look into CV metrics

Raw

Tidy

Fold	RMSE	R-squared
Fold1	0.430	0.134
Fold2	0.368	0.496
Fold3	0.452	0.501
Fold4	0.289	0.529
Fold5	0.475	0.403



# How does RMSE compare to y?

- Cross validation RMSE stats

```
## # A tibble: 1 × 6
##   min    max  mean  med    sd   IQR
##   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 0.289 0.475 0.403 0.430 0.0751 0.0841
```

- Training data IMDB score stats

```
## # A tibble: 1 × 6
##   min    max  mean  med    sd   IQR
##   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1  6.7   9.7  8.24  8.2 0.530 0.600
```





# What's next?

