The tidymodels ecosystem

MODELING WITH TIDYMODELS IN R

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Collection of machine learning packages

Collection of machine learning packages

Data resampling

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Data resampling

Feature engineering

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Model fitting

Data resampling

Feature engineering

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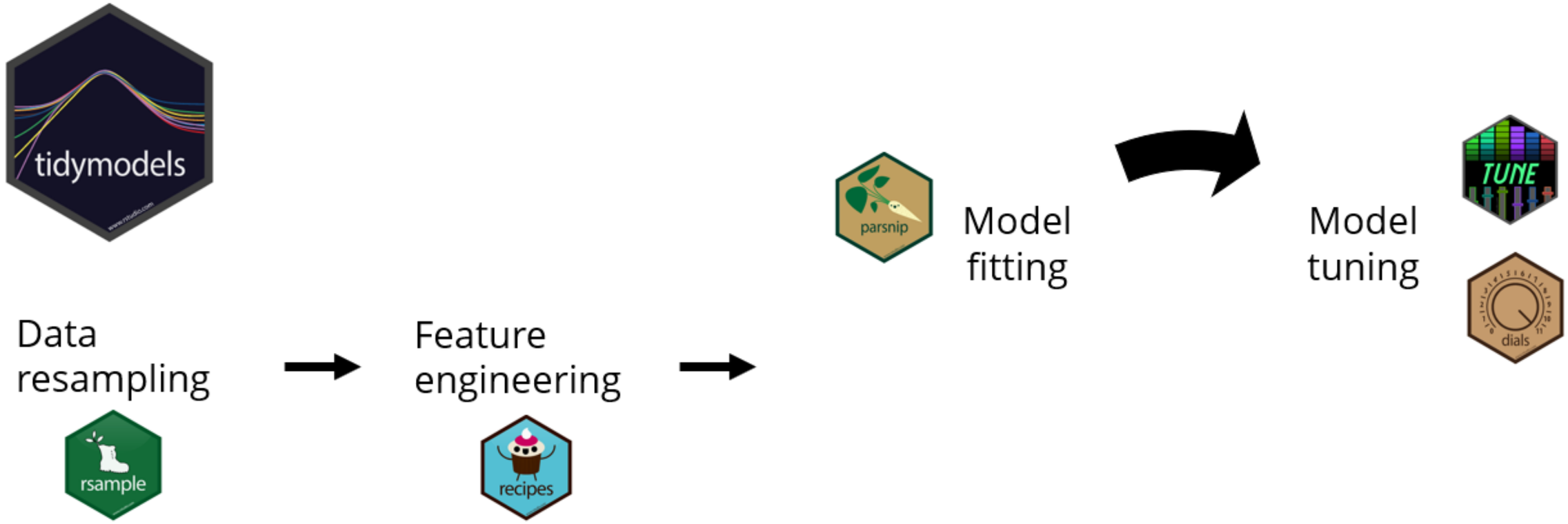
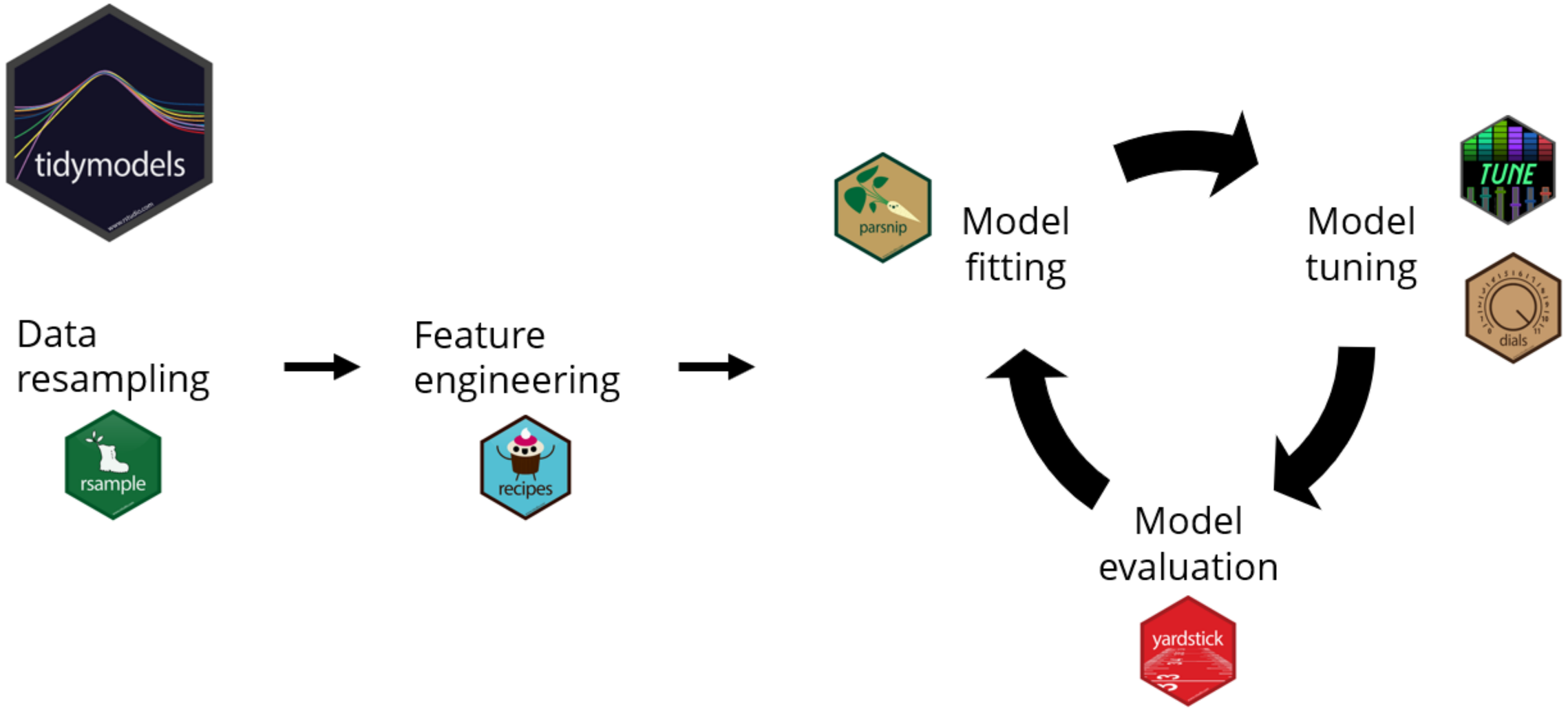


Collection of machine learning packages



Supervised machine learning

Branch of machine learning that uses labeled data for model fitting

Regression

- Predicting **quantitative** outcomes
  - Selling price of a home

Classification

- Predicting **categorical** outcomes
  - Whether an employee will leave a company

left_company	miles_from_home	salary
no	1	84500
yes	10	64820
no	5	76490
yes	19	68540

`tidymodels` **variable roles**

- *left_company* is an outcome variable
- *miles_from_home* and *salary* are predictor variables

Data resampling

Create training and test sets

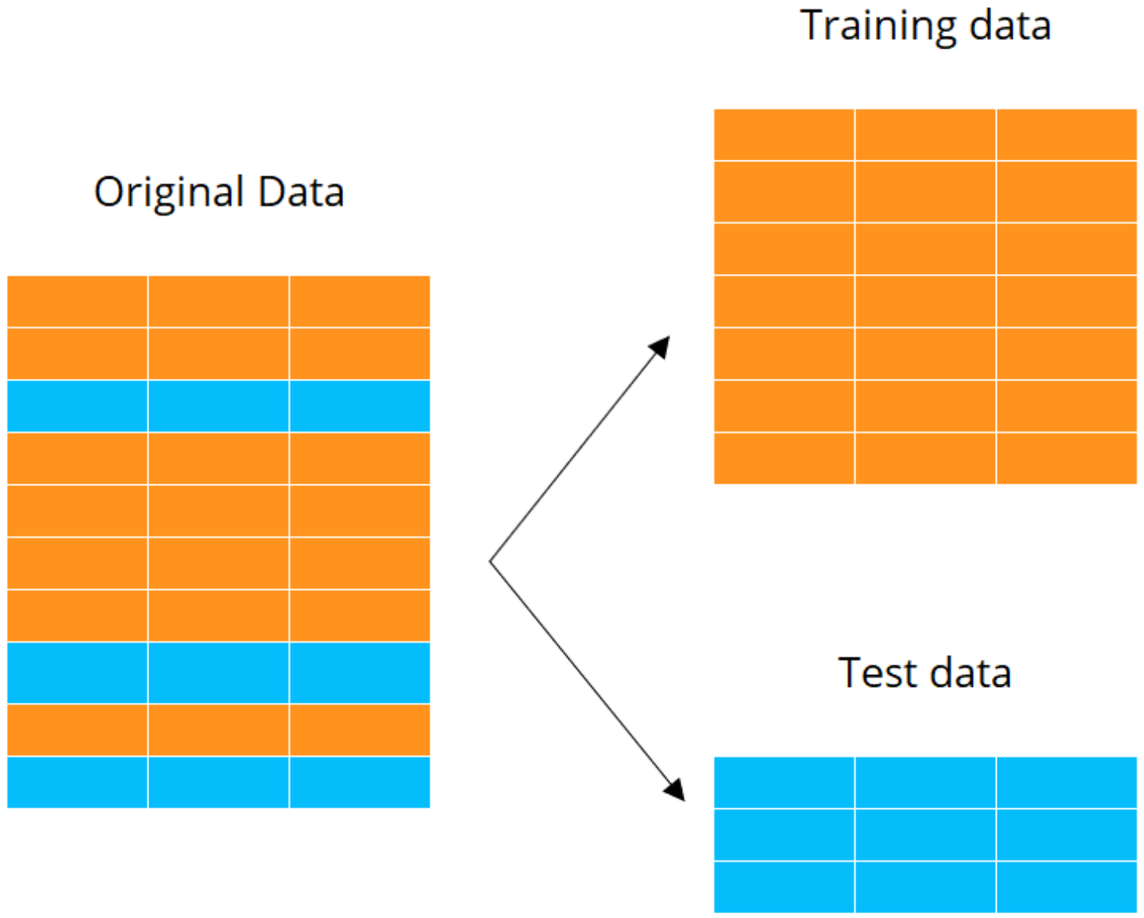
- Guards against **overfitting**
- Common ratio is 75% training, 25% test

Training data

- Feature engineering
- Model fitting and tuning

Test data

- Estimate model performance on new data



Fuel efficiency data

Vehicle fuel efficiency data from the U.S. Environmental Protection Agency

- Outcome variable is `hwy` - highway fuel efficiency in miles per gallon (mpg)

```
mpg
```

```
# A tibble: 234 x 11
     hwy   cty displ   cyl manufacturer model       year trans      drv   fl    class
   <int> <int> <dbl> <int> <chr>        <chr>      <int> <chr>      <chr> <chr> <chr>
 1    29    18   1.8     4 audi         a4          1999 auto(l5)   f     p     compact
 2    29    21   1.8     4 audi         a4          1999 manual(m5) f     p     compact
 3    31    20   2       4 audi         a4          2008 manual(m6) f     p     compact
 4    30    21   2       4 audi         a4          2008 auto(av)   f     p     compact
 5    26    16   2.8     6 audi         a4          1999 auto(l5)   f     p     compact
# ... with 224 more rows
```

Data resampling with tidymodels

- `initial_split()`
  - Specifies instructions for creating training and test datasets
  - `prop` specifies the proportion to place into training
  - `strata` provides stratification by the outcome variable
- Pass split object to `training()` function
- Pass split object to `testing()` function

```
library(tidymodels)
```

```
mpg_split <- initial_split(mpg,
                           prop = 0.75,
                           strata = hwy)
```

```
mpg_training <- mpg_split %>%
  training()
```

```
mpg_test <- mpg_split %>%
  testing()
```

Home sales data

Home sales from the Seattle, Washington area between 2015 and 2016

```
home_sales
```

```
# A tibble: 1,492 x 8
   selling_price home_age bedrooms bathrooms sqft_living sqft_lot sqft_basement floors
           <dbl>    <dbl>    <dbl>     <dbl>       <dbl>    <dbl>          <dbl>  <dbl>
 1        487000       10        4       2.5        2540     5001              0      2
 2        465000       10        3      2.25        1530     1245            480      2
 3        411000       18        2         2        1130     1148            330      2
 4        635000        4        3       2.5        3350     4007            800      2
 5        380000       24        5       2.5        2130     8428              0      2
# ... with 1,482 more rows
```

Let's practice!

MODELING WITH TIDYMODELS IN R

Linear regression with tidymodels

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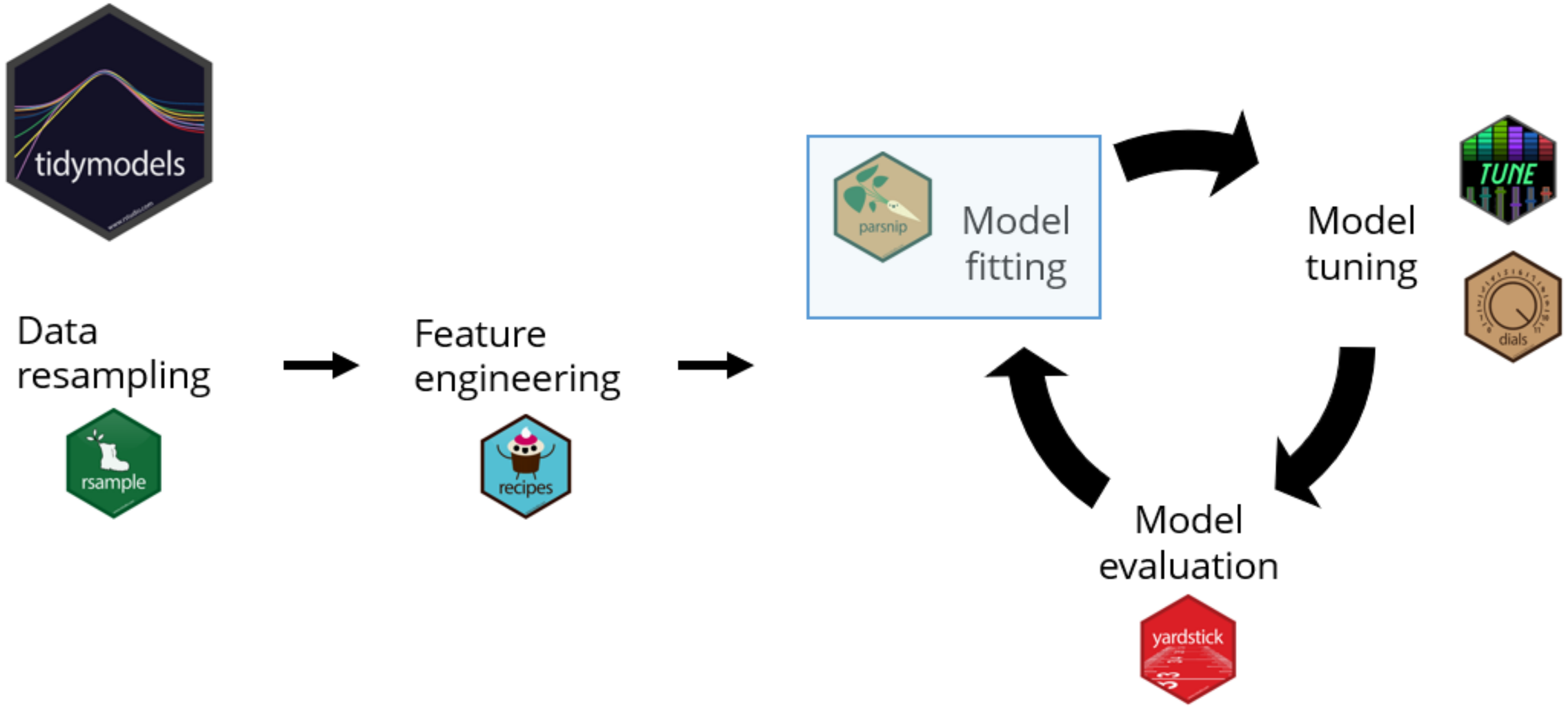
Model fitting with parsnip



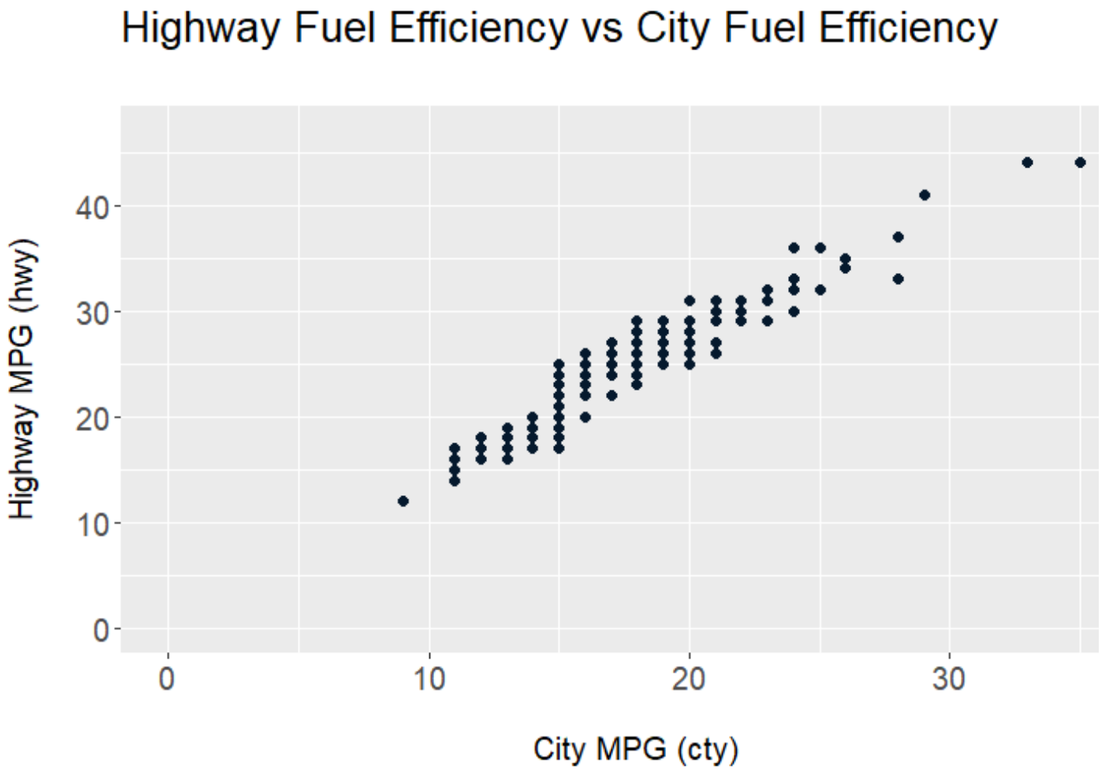
Linear regression model

Predicting `hwy` using `cty` as a predictor

$$hwy = \beta_0 + \beta_1 cty$$

Model parameters

- β_0 is the intercept
- β_1 is the slope



Linear regression model

Predicting `hwy` using `cty` as a predictor

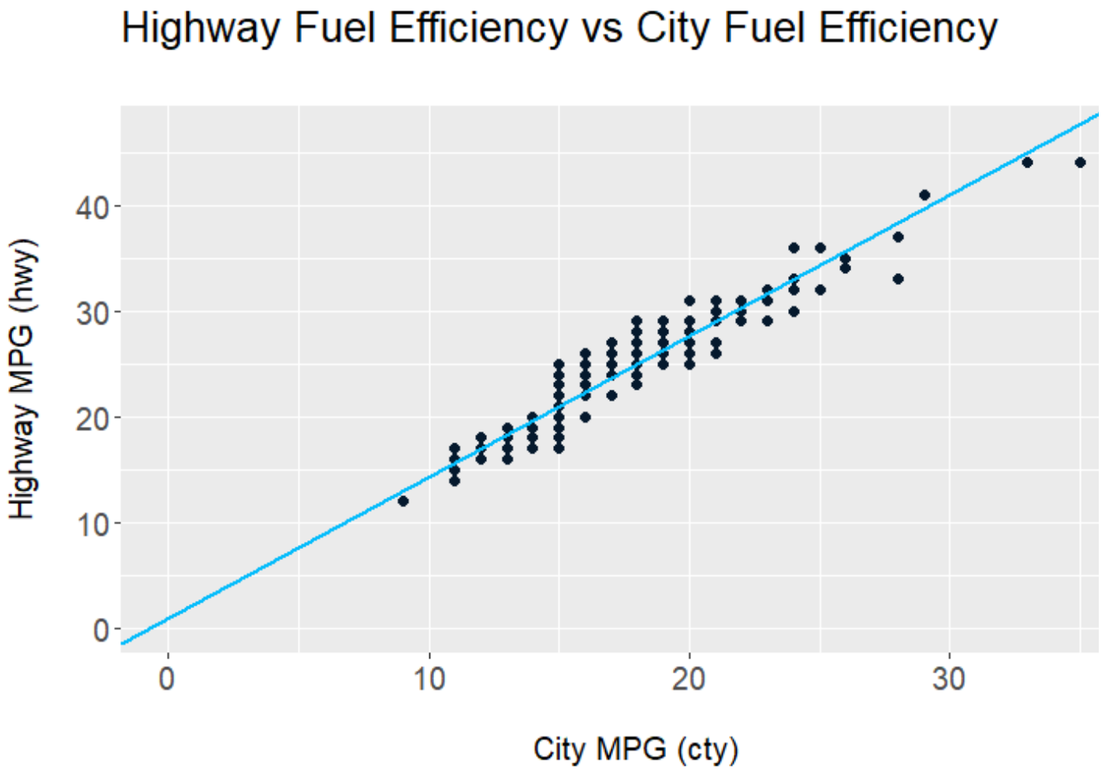
$$hwy = \beta_0 + \beta_1 cty$$

Model parameters

- β_0 is the intercept
- β_1 is the slope

Estimated paramters from training data

$$hwy = 0.77 + 1.35(cty)$$



Model formulas

Model formulas in `parsnip`

- Used to assign column roles
  - Outcome variable
  - Predictor variables

General form

```
outcome ~ predictor_1 + predictor_2 + ...
```

Shorthand notation

```
outcome ~ .
```

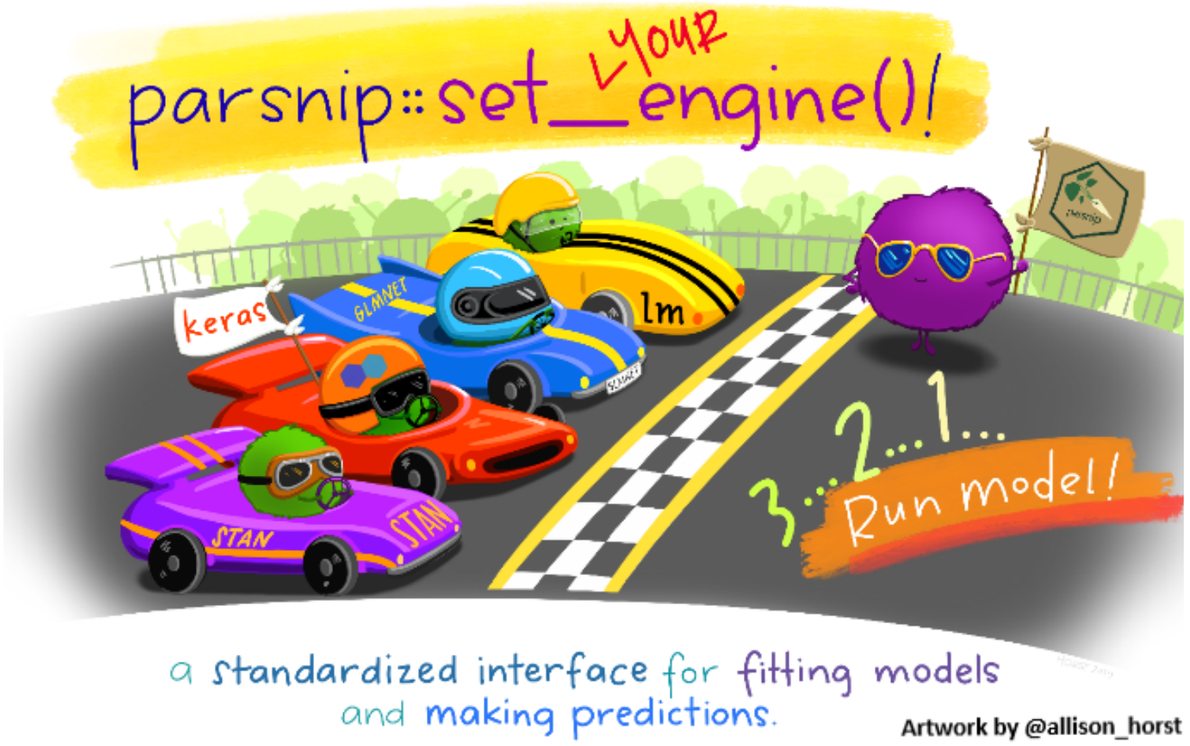
Predicting `hwy` using `cty` as a predictor variable

```
hwy ~ cty
```

The parsnip package

Unified syntax for model specification in R

1. Specify the **model type**
   - Linear regression or other model type
2. Specify the **engine**
   - Different engines correspond to different underlying R packages
3. Specify the **mode**
   - Either regression or classification



Fitting a linear regression model

Define model specification with `parsnip`

- `linear_reg()`

```
lm_model <- linear_reg() %>%
  set_engine('lm') %>%
  set_mode('regression')
```

Pass `lm_model` to the `fit()` function

- Specify model formula
- `data` to use for model fitting

```
lm_fit <- lm_model %>%
  fit(hwy ~ cty, data = mpg_training)
```

Obtaining the estimated parameters

The `tidy()` function

- Takes a trained `parsnip` model object
- Creates a model summary tibble
- `term` and `estimate` column provide estimated parameters

```
tidy(lm_fit)
```

```
# A tibble: 2 x 5
  term        estimate std.error statistic  p.value
  <chr>          <dbl>     <dbl>     <dbl>    <dbl>
1 (Intercept)    0.769    0.528       1.46 1.47e- 1
2 cty            1.35     0.0305     44.2  6.32e-97
```

Making predictions

Pass trained `parsnip` model to the `predict()` function

- `new_data` specifies dataset on which to predict new values

```
hwy_predictions <- lm_fit %>%
  predict(new_data = mpg_test)

hwy_predictions
```

```
# A tibble: 57 x 1
   .pred
   <dbl>
 1  25.0
 2  27.7
 3  25.0
 4  25.0
 5  22.3
# ... with 47 more rows
```

Standardized output from `predict()`

1. Returns a tibble
2. Keep rows in the same order as `new_data` input
3. Names prediction column `.pred`

Adding predictions to the test data

The `bind_cols()` function

- Combines two or more tibbles along the column axis
- Useful for creating a model results tibble

Steps

- Select `hwy` and `cty` from `mpg_test`
- Pass to `bind_cols()` and add predictions column

```
mpg_test_results <- mpg_test %>%
  select(hwy, cty) %>%
  bind_cols(hwy_predictions)

mpg_test_results
```

```
# A tibble: 57 x 3
     hwy   cty .pred
   <int> <int> <dbl>
 1    29    18  25.0
 2    31    20  27.7
 3    27    18  25.0
 4    26    18  25.0
 5    25    16  22.3
# ... with 47 more rows
```

Let's model!

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Evaluating model performance

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Input to yardstick functions

All `yardstick` functions require a tibble with model results

- Column with the true outcome variable values
  - `hwy` for mpg data
- Column with model predictions
  - `.pred`

```
mpg_test_results
```

```
# A tibble: 57 x 3
     hwy   cty .pred
   <int> <int> <dbl>
 1    29    18  25.0
 2    31    20  27.7
 3    27    18  25.0
 4    26    18  25.0
 5    25    16  22.3
# ... with 47 more rows
```

Root mean squared error (RMSE)

RMSE estimates the average prediction error

- Calculated with the `rmse()` function from `yardstick`
  - Takes a tibble with model results
  - `truth` is the column with true outcome values
  - `estimate` is the column with predicted outcome values

```
mpg_test_results %>%
  rmse(truth = hwy, estimate = .pred)
```

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 rmse    standard        1.93
```

R squared metric

Measures the squared correlation between actual and predicted values

- Also called the **coefficient of determination**
- Ranges from 0 to 1
  - When all predictions equal the true outcome values, R squared is 1
- Calculated with the `rsq()` function from `yardstick`

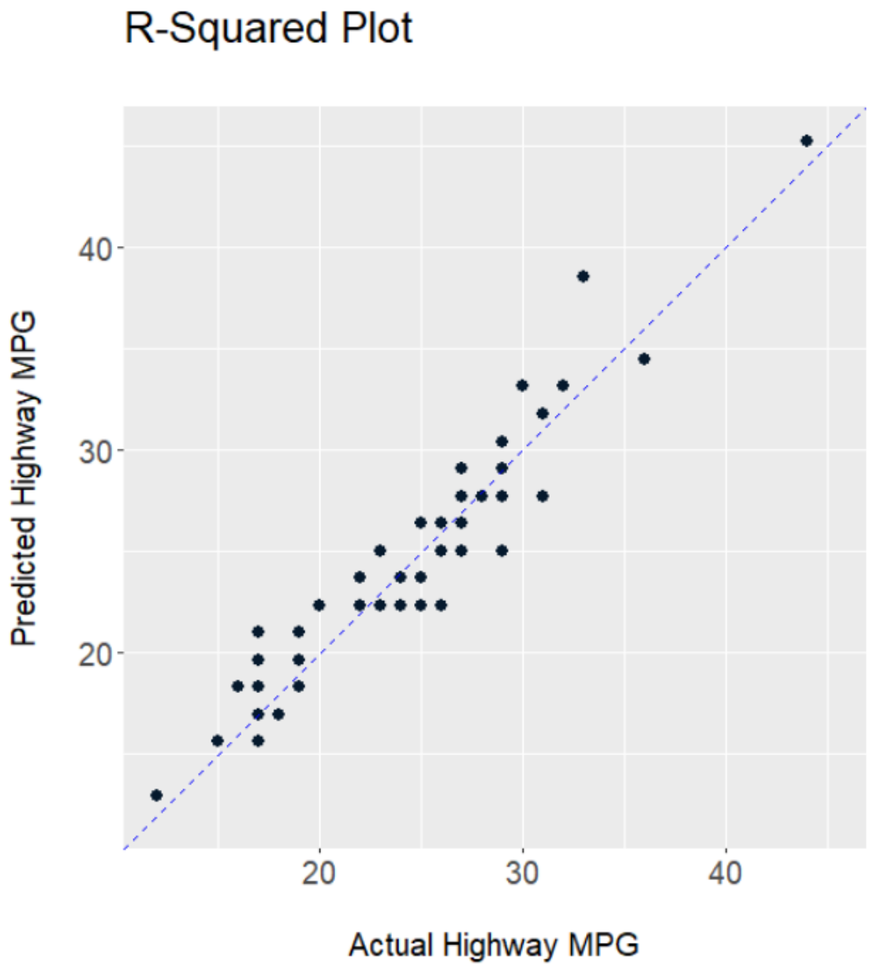
```
mpg_test_results %>%
  rsq(truth = hwy, estimate = .pred)
```

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 rsq     standard       0.904
```

R squared plots

Visualization of the R squared metric

- Model predictions versus the true outcome
- The line y = x
  - Represents R squared of 1
- Used to find potential problems with model performance
  - Non-linear patterns
  - Regions where model is predicting poorly

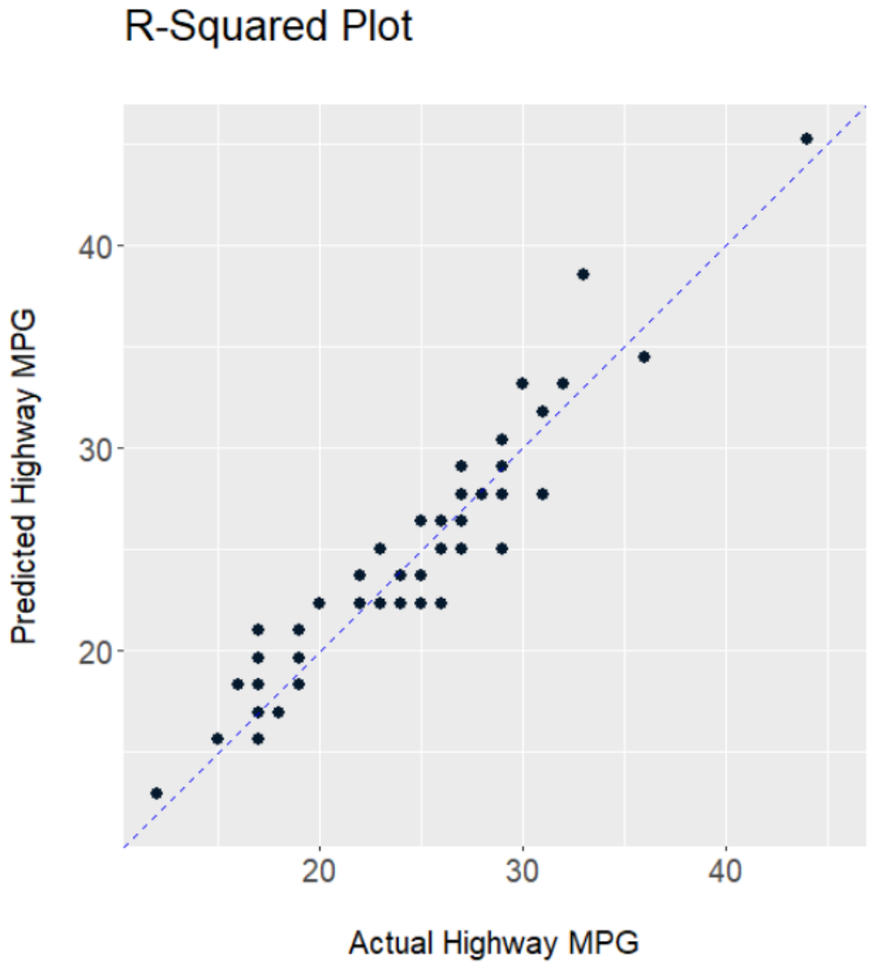


Plotting R squared plots

Making R squared plots with `ggplot2`

- Tibble of model results
- `geom_point()`
- `geom_abline()`
- `coord_obs_pred()`

```
ggplot(mpg_test_results, aes(x = hwy, y = .pred)) +
  geom_point() +
  geom_abline(color = 'blue', linetype = 2) +
  coord_obs_pred() +
  labs(title = 'R-Squared Plot',
       y = 'Predicted Highway MPG',
       x = 'Actual Highway MPG')
```



Streamlining model fitting

The `last_fit()` function

- Takes a model specification, model formula, and data split object
- Performs the following:
  1. Creates training and test datasets
  2. Fits the model to the training data
  3. Calculates metrics and predictions on the test data
  4. Returns an object with all results

```
lm_last_fit <- lm_model %>%
  last_fit(hwy ~ cty,
           split = mpg_split)
```

Collecting metrics

The `collect_metrics()` function

- Takes the results of `last_fit()`
  - Returns a tibble with performance metrics obtained on the test dataset
- Default regression model metrics
  - RMSE
  - R squared

```
lm_last_fit %>%
  collect_metrics()
```

```
# A tibble: 2 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 rmse    standard        1.93
2 rsq     standard        0.904
```

Collecting predictions

The `collect_predictions()` function

- Takes the results of `last_fit()`
  - Returns a tibble with test dataset predictions
  - Predictions column is named `.pred`
  - Outcome variable and other row identifier columns included

```
lm_last_fit %>%
  collect_predictions()
```

```
# A tibble: 57 x 4
   id                .pred  .row   hwy
   <chr>             <dbl> <int> <int>
 1 train/test split  25.0      1    29
 2 train/test split  27.7      3    31
 3 train/test split  25.0      7    27
 4 train/test split  25.0      8    26
 5 train/test split  22.3      9    25
# ... with 47 more rows
```

Let's evaluate some models!

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