Model assessment and selection

MODELING WITH DATA IN THE TIDYVERSE

Albert Y. Kim Assistant Professor of Statistical and Data Sciences



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Refresher: Multiple regression

Two models with different pairs of explanatory/predictor variables:

```
# Model 1 - Two numerical:
model_price_1 <- lm(log10_price ~ log10_size + yr_built,</pre>
                     data = house_prices)
# Model 3 - One numerical & one categorical:
model_price_3 <- lm(log10_price ~ log10_size + condition,</pre>
                     data = house_prices)
```



Refresher: Sum of squared residuals

3D scatterplot, regression plane, and residuals





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Refresher: Sum of squared residuals

#	A tibble: 1 x 1
	sum_sq_residuals
	<dbl></dbl>
1	595



Refresher: Sum of squared residuals

get_regression_points(model_price_3) %>%
mutate(sq_residuals = residual^2) %>%
summarize(sum_sq_residuals = sum(sq_residuals))

```
# A tibble: 1 x 1
    sum_sq_residuals
        <dbl>
1 608.
```



Let's practice! MODELING WITH DATA IN THE TIDYVERSE



Assessing model fit with R-squared

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R-squared

 $R^2 = 1 - rac{\operatorname{Var}(\operatorname{residuals})}{\operatorname{Var}(y)}$

- R^2 is between 0 & 1
- Smaller R^2 ~ "poorer fit"
- $R^2=1$ ~ "perfect fit" and $R^2=0$ ~ "no fit"



High R-squared value example

 $R^2 = 1 - rac{ ext{Var}(ext{residuals})}{ ext{Var}(y)}$

High R-squared example



Х



High R-squared value: "Perfect" fit

 $R^2 = 1 - rac{ ext{Var}(ext{residuals})}{ ext{Var}(y)}$

High R-squared example



Х



Low R-squared value example

 $R^2 = 1 - rac{ ext{Var(residuals)}}{ ext{Var}(y)}$

Low R-squared example



Х



Low R-squared value example

 $R^2 = 1 - rac{ ext{Var(residuals)}}{ ext{Var}(y)}$

Low R-squared example



Х



Numerical interpretation

Since $Var(y) \ge Var(residuals)$ and

 $R^2 = 1 - rac{\operatorname{Var}(\operatorname{residuals})}{\operatorname{Var}(y)} = rac{\operatorname{Var}(y) - \operatorname{Var}(\operatorname{residuals})}{\operatorname{Var}(y)}$

 R^2 's interpretation is: the proportion of the total variation in the outcome variable y that the model explains.



Computing R-squared

get_regression_points(model_price_1) %>%
 summarize(r_squared = 1 - var(residual)/var(log10_price))

```
# A tibble: 1 x 1
    r_squared
        <dbl>
1 0.483
```



Computing R-squared

get_regression_points(model_price_3) %>%
 summarize(r_squared = 1 - var(residual)/var(log10_price))

```
# A tibble: 1 x 1
    r_squared
        <dbl>
1 0.462
```



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Assessing predictions with RMSE

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Refresher: Residuals

3D scatterplot, regression plane, and residuals





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Mean squared error

```
# Sum of squared residuals:
get_regression_points(model_price_1) %>%
mutate(sq_residuals = residual^2) %>%
summarize(sum_sq_residuals = sum(sq_residuals))
```

#	A tibble:	1 x 1
	sum_sq_re	siduals
		<dbl></dbl>
1		585.

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Mean squared error

Mean squared error: use mean() instead of sum():
get_regression_points(model_price_1) %>%
mutate(sq_residuals = residual^2) %>%
summarize(mse = mean(sq_residuals))

# A tibble: 1 x 1	
mse	
<dbl></dbl>	
1 0.0271	



Root mean squared error

```
# Root mean squared error:
get_regression_points(model_price_1) %>%
mutate(sq_residuals = residual^2) %>%
summarize(mse = mean(sq_residuals)) %>%
mutate(rmse = sqrt(mse))
```

```
# A tibble: 1 x 2
    mse rmse
    <dbl> <dbl>
1 0.0271 0.164
```



RMSE of predictions on new houses

```
# Recreate data frame of "new" houses
new_houses <- data_frame(
   log10_size = c(2.9, 3.6),
   condition = factor(c(3, 4))
)
new_houses
```

#	A tibble: 2 x 2	
	log10_size conditior	ן
	<dbl> <fct></fct></dbl>	
1	2.9 3	
2	3.6 4	

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RMSE of predictions on new houses

Get predictions

get_regression_points(model_price_3,

newdata = new_houses)

#	A tibb	le: 2 x 4			
	ID	log10_size	condition	log10_price_hat	
	<int></int>	<dbl></dbl>	<fct></fct>	<dbl></dbl>	
1	1	2.9	3	5.34	
2	2	3.6	4	5.94	



RMSE of predictions on new houses

```
# Compute RMSE
get_regression_points(model_price_3,
                      newdata = new_houses) %>%
  mutate(sq_residuals = residual^2) %>%
  summarize(mse = mean(sq_residuals)) %>%
  mutate(rmse = sqrt(mse))
```

Error in mutate_impl(.data, dots) : Evaluation error: object 'residual' not found.



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Validation set prediction framework

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Validation set approach

Use two independent datasets to:

- 1. Train/fit your model
- 2. Evaluate your model's predictive power i.e. validate your model



Training/test set split

Randomly split all n observations (white) into

- 1. A *training set* (blue) to fit models
- 2. A *test set* (orange) to make predictions on





Training/test set split in R

```
library(dplyr)
```

```
# Randomly shuffle order of rows:
house_prices_shuffled <- house_prices %>%
sample_frac(size = 1, replace = FALSE)
```

```
# Split into train and test:
train <- house_prices_shuffled %>%
    slice(1:10000)
test <- house_prices_shuffled %>%
    slice(10001:21613)
```



Training models on training data

get_regression_table(train_model_price_1)

#	A tibble: 3	3 x 7					
	term	estimate	std_error	statistic	p_value	lower_ci	
	<chr></chr>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	
1	intercept	5.34	0.111	48.3	0	5.13	
2	log10_size	0.923	0.009	97.5	0	0.905	
3	yr_built	-0.001	0	-23.0	0	-0.001	



Making predictions on test data

Get predictions on test: get_regression_points(train_model_price_1, newdata = test)

# A tibble: 11,613 x 6								
	ID log10_price log10_size yr_built log10_price_hat							
	<int></int>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>			
1	1	5.83	3.29	1951	5.71			
2	2	5.88	3.40	1922	5.84			
3	3	6.15	3.67	2002	5.99			
4	4	5.62	3	1953	5.43			
•••								
# with 11,603 more rows								

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Assessing predictions with RMSE

summarize(rmse = sqrt(mean(sq_residuals)))





Comparing RMSE



A tibble: 1 x 1
 rmse
 <dbl>
1 0.168



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Conclusion - Where to go from here?

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R source code for all videos

Available at http://bit.ly/modeling_tidyverse

R source code for "Modeling with Data in the Tidyverse" DataCamp course

```
modeling_with_data_tidyverse.R
      # R source code for all slides/videos in Albert Y. Kim's "Modeling with Data in
   1
       # the Tidyverse" DataCamp course:
   2
   3
      # Load all necessary packages -----
   4
       library(ggplot2)
   5
       library(dplyr)
   6
       library(moderndive)
   7
   8
       # Chapter 1 - Video 1: Background on modeling for explanation -----
   9
       ## Modeling for explanation example
  10
       glimpse(evals)
  11
  12
       ## Exploratory data analysis
  13
       ggplot(evals, aes(x = score)) +
  14
         geom_histogram(binwidth = 0.25) +
  15
         labs(x = "teaching score", y = "count")
  16
  17
```

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Other Tidyverse courses

Available here and here

Tidyverse Fundamentals with R

Experience the whole data science pipeline from importing and tidying data to wrangling and visualizing data to modeling and communicating with data. Gain exposure to each component of this pipeline from a variety of different perspectives in this tidyverse R track.

skill TRACK Intermediate Tidyverse Toolbox

Take your tidyverse skills to the next level. This track covers getting your data in the right condition to start your analyses, writing better code with functional programming, and generating, exploring, and evaluating machine learning models. And you'll do all of this in the wonderful and clean world of the tidyverse.

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Refresher: General modeling framework

- In general: $y = f(ec{x}) + \epsilon$
- Linear regression models: $y=eta_0+eta_1\cdot x_1+\epsilon$



Parallel slopes model

House prices in Seattle





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Polynomial model

House prices in Seattle





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Tree models

Tree model for log10 price





DataCamp courses using other models

Courses with different f() in $y = f(\vec{x}) + \epsilon$:

- Machine Learning with Tree-Based Models in R
- Supervised Learning in R: Case Studies



Refresher: Regression table

Fit model: model_score_1 <- lm(score ~ age, data = evals)</pre>

Output regression table: get_regression_table(model_score_1)

#	A tibble:	2 x 7					
	term	estimate	std_error	statistic	p_value	lower_ci	upper_ci
	<chr></chr>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>
1	intercept	4.46	0.127	35.2	0	4.21	4.71
2	age	-0.006	0.003	-2.31	0.021	-0.011	-0.001



ModernDive: Online textbook **ST Modern Dive**

- Uses tidyverse tools: ggplot2 and dplyr \bullet
- Expands on the regression models from this course
- Uses evals and house_prices datasets (and more) ${}^{\bullet}$
- **Goal:** Statistical inference via data science
- Available at ModernDive.com



Good luck!

