

## Multiple Linear Regression Review

Rebecca C. Steorts (slide adaption from Maria Tacket) and material from Chapter 1 of Roback and Legler text.

# Reading

BMLR: Chapter 1:

<https://bookdown.org/roback/bookdown-BeyondMLR/>

## Computing set up

```
library(tidyverse)
library(tidymodels)
library(GGally)
library(xaringanExtra)
library(knitr)
library(patchwork)
library(viridis)
library(ggfortify)
library(dplyr)

ggplot2::theme_set(ggplot2::theme_bw(base_size = 16))

colors <- tibble::tibble(green = "#B5BA72")
```

# Topics

- ▶ Define statistical models
- ▶ Motivate generalized linear models and multilevel models
- ▶ Review multiple linear regression

Notes based on Chapter 1 of Roback and Legler (2021) unless noted otherwise.

# Statistical models

We first review/define some concepts on statistical models.

# Models and statistical models

Suppose we have observations  $y_1, \dots, y_n$

- ▶ **Model:** Mathematical description of the process we think generates the observations
- ▶ **Statistical model:** Model that includes an equation describing the impact of explanatory variables (**deterministic part**) and probability distributions for parts of the process that are assumed to be random variation (**random part**)

Definitions adapted from Stroup (2012)

# Statistical models

A statistical model must include

1. The observations
2. The deterministic (systematic) part of the process
3. The random part of the process with a statement of the presumed probability distribution

Definitions adapted from Stroup (2012)

## Example

Suppose we have the model for comparing two means:

$$y_{ij} = \mu_i + \epsilon_{ij}$$

where

- ▶  $i = 1, 2$ : group
- ▶  $j = 1, \dots, n$ : observation number
- ▶  $n_i$ : number of observations in group  $i$
- ▶  $\mu_i$ : mean of group  $i$
- ▶  $y_{ij}$ :  $j^{th}$  observation in the  $i^{th}$  group
- ▶  $\epsilon_{ij}$ : random error (variation) associated with  $ij^{th}$  observation

Adapted from Stroup (2012)



## Example

$$y_{ij} = \mu_i + \epsilon_{ij}$$

- ▶  $y_{ij}$ : the observations
- ▶  $\mu_i$ : deterministic part of the model, no random variability
- ▶  $\epsilon_{ij}$  : random part of the model, indicating observations vary about their mean
- ▶ Typically assume  $\epsilon_{ij}$  are independent and identically distributed (i.i.d.)  $N(0, \sigma^2)$

Adapted from Stroup (2012)

## Practice

Suppose  $y_{ij}$ 's are observed outcome data and  $x_i$ 's are values of the explanatory variable. Assume a linear regression model can be used to describe the process of generating  $y_{ij}$  based on the  $x_i$ .

1. Write the specification of the statistical model.
2. Label the 3 components of the model equation (observation, deterministic part, random part)
3. What is  $E(y_{ij})$ , the expected value of the observations?

## Solution to Practice

1. Write the specification of the statistical model.

Solution:

$$y_{ij} = \mu_i + \epsilon_{ij}$$

2. Label the 3 components of the model equation (observation, deterministic part, random part)

Solution:

- ▶ observations:  $y_{ij}$ ,
  - ▶ deterministic component:  $\mu_i$
  - ▶ random component:  $\epsilon_{ij}$
3. What is  $E(y_{ij})$ , the expected value of the observations?  
Solution:  $\mu_i$ .

# Motivating generalized linear models (GLMs) and multilevel models

Now, we review the basic assumptions for linear regression that often do not hold in practice.

This motivates introducing generalized linear models.

# Assumptions for linear regression

- ▶ **Linearity:** Linear relationship between mean response and predictor variable(s)
- ▶ **Independence:** Residuals are independent. There is no connection between how far any two points lie above or below regression line.
- ▶ **Normality:** Response follows a normal distribution at each level of the predictor (or combination of predictors)
- ▶ **Equal variance:** Variability (variance or standard deviation) of the response is equal for all levels of the predictor (or combination of predictors)

# Assumptions for linear regression

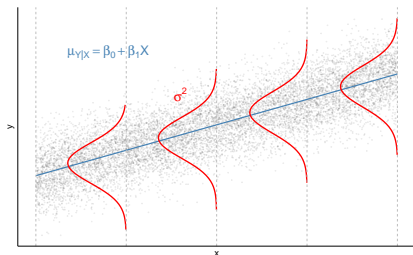


Figure 1: Modified from Figure 1.1. in BMLR

- ▶ **Linearity:** Linear relationship between mean of the response  $Y$  and the predictor  $X$
- ▶ **Independence:** No connection between how far any two points lie from regression line
- ▶ **Normality:** Response  $Y$  follows a normal distribution at each level of the predictor  $X$  (red curves)
- ▶ **Equal variance:** Variance of the response  $Y$  is equal for all levels of the predictor  $X$

## Violations in assumptions

*Is the time studying predictive of success on an exam?* The time spent studying for an exam (in hours) and success (pass/fail) are recorded for randomly selected students.

- ▶ The response variable is the exam outcome (pass/fail).
- ▶ The explanatory variable is the time spent studying in hours.

Which assumption(s) are obviously violated, if any?

## Solution

The response variable is a binary outcome, which violates the assumption that the response is normally distributed. (Chapter 6 introduces logistic regression, which is more suitable for binary data).



## Violations in assumptions

*Do wealthy households tend to have fewer children compared to households with lower income?* Annual income and family size are recorded for a random sample of households.

- ▶ The response variable is number of children in the household.
- ▶ The predictor variable is annual income in US dollars.

Which assumption(s) are obviously violated, if any?

## Solution

Family size is a count taking on any integer value (with no upper bound).

The normality assumption may be problematic as the distribution of family size may be skewed. For example, think of how family sizes may occur in practice (one or two children versus five/six children).

This concern along with the discrete nature of the response variable raise issues with the normality assumption. (Chapter 4 will introduce Poisson models, which may be more appropriate).

## Violations in assumptions

Medical researchers investigated the outcome of a particular surgery for patients with comparable stages of disease but different ages. The 10 hospitals in the study had at least two surgeons performing the surgery of interest. Patients were randomly selected for each surgeon at each hospital. The surgery outcome was recorded on a scale of 1 - 10.

- ▶ The response variable is surgery outcome, 1 - 10.
- ▶ The predictor variable is patient age in years.

Which assumption(s) are obviously violated, if any?

## Solution

- ▶ Outcomes for patients operated on by the same surgeon are more likely to be similar and have similar results.
- ▶ Outcomes at one hospital may be more similar due to factors associated with different patient populations.

The structure of the data suggests that the independence assumption may be violated.

## Beyond linear regression

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  - ▶ Response variable can be non-normal



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  - ▶ Relationship between response and predictor(s) can be nonlinear
  - ▶ Response variable can be non-normal
  - ▶ Variance in response can differ at each level of predictor(s)
  - ▶ **The independence assumption still must hold!**
- ▶ **Multilevel models** and other types of models are used to model data that violate the independence assumption, i.e. correlated observations.

# Multiple linear regression

For the rest of the lecture, we will focus on reviewing some important parts of multiple linear regression.

# Data: Kentucky Derby Winners

Today's data is from the Kentucky Derby, an annual 1.25-mile horse race held at the Churchill Downs race track in Louisville, KY. The data is in the file derbyplus.csv and contains information for races 1896 - 2017.

## Response variable

- ▶ speed: Average speed of the winner in feet per second (ft/s)

## Additional variable

- ▶ winner: Winning horse

## Predictor variables

- ▶ year: Year of the race
- ▶ condition: Condition of the track (good, fast, slow)
- ▶ starters: Number of horses who raced

**Goal: Understand variability in average winner speed based on characteristics of the race.**

# Data

```
derby <- read_csv("data/derbyplus.csv")
```

```
derby |>  
  head(5) |> kable()
```

year	winner	condition	speed	starters
1896	Ben Brush	good	51.66	8
1897	Typhoon II	slow	49.81	6
1898	Plaudit	good	51.16	4
1899	Manuel	fast	50.00	5
1900	Lieut. Gibson	fast	52.28	7

# Data science workflow

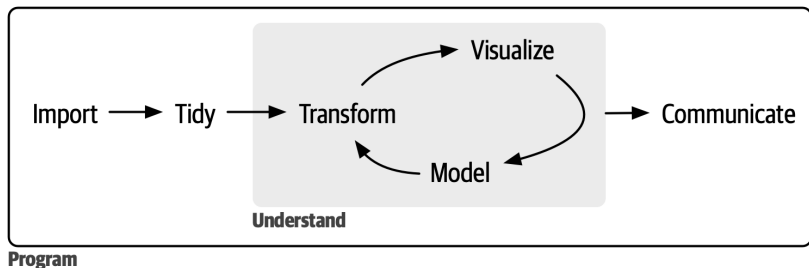


Figure 2: Image source: Wickham, Çetinkaya-Rundel, and Grolemund (2023)

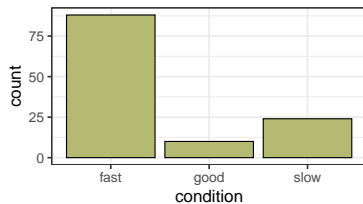
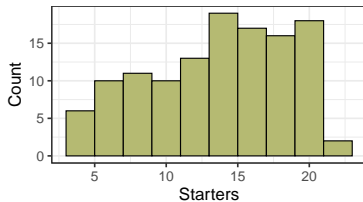
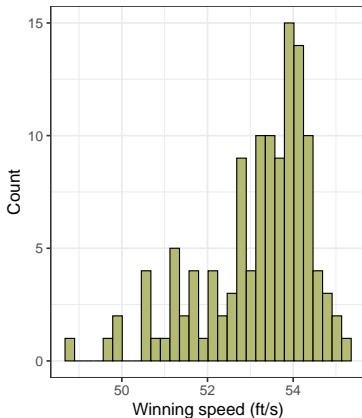
# Exploratory data analysis (EDA)

- ▶ Once you're ready for the statistical analysis, the first step should always be **exploratory data analysis**.
- ▶ The EDA will help you
  - ▶ begin to understand the variables and observations
  - ▶ identify outliers or potential data entry errors
  - ▶ begin to see relationships between variables
  - ▶ identify the appropriate model and identify a strategy
- ▶ The EDA is exploratory; formal modeling and statistical inference are used to draw conclusions.



# Univariate EDA

## Univariate data analysis

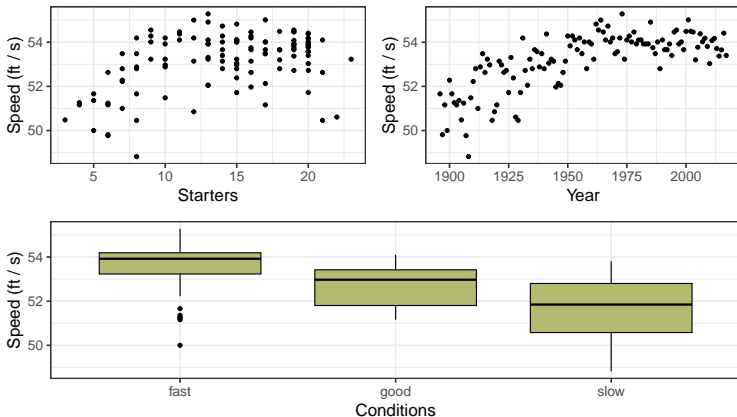


## Univariate EDA code

```
p1 <- ggplot(data = derby, aes(x = speed)) +  
  geom_histogram(fill = colors$green, color = "black") +  
  labs(x = "Winning speed (ft/s)", y = "Count")  
  
p2 <- ggplot(data = derby, aes(x = starters)) +  
  geom_histogram(fill = colors$green, color = "black",  
    binwidth = 2) +  
  labs(x = "Starters", y = "Count")  
  
p3 <- ggplot(data = derby, aes(x = condition)) +  
  geom_bar(fill = colors$green, color = "black", aes(x = ))  
  
p1 + (p2 / p3) +  
  plot_annotation(title = "Univariate data analysis")
```

# Bivariate EDA

## Bivariate data analysis

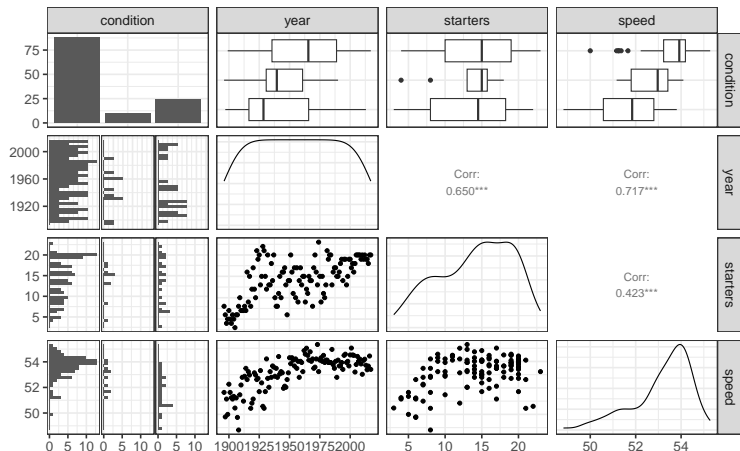


## Bivariate EDA code

```
p4 <- ggplot(data = derby, aes(x = starters, y = speed)) +  
  geom_point() +  
  labs(x = "Starters", y = "Speed (ft / s)")  
  
p5 <- ggplot(data = derby, aes(x = year, y = speed)) +  
  geom_point() +  
  labs(x = "Year", y = "Speed (ft / s)")  
  
p6 <- ggplot(data = derby, aes(x = condition, y = speed)) +  
  geom_boxplot(fill = colors$green, color = "black") +  
  labs(x = "Conditions", y = "Speed (ft / s)")  
  
(p4 + p5) + p6 +  
  plot_annotation(title = "Bivariate data analysis")
```

# Scatterplot matrix

A **scatterplot matrix** helps quickly visualize relationships between many variable pairs. They are particularly useful to identify potentially correlated predictors.



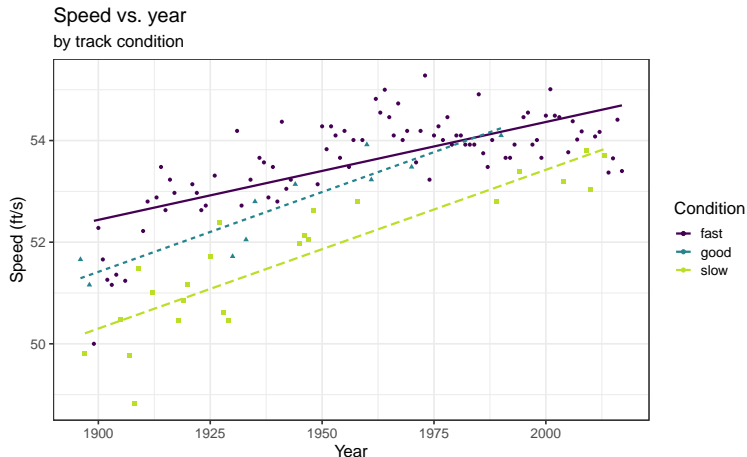
## Scatterplot matrix code

Create using the `ggpairs()` function in the `GGally` package.

```
library(GGally)
ggpairs(data = derby,
        columns = c("condition", "year",
                    "starters", "speed"))
```

# Multivariate EDA

Plot the relationship between the response and a predictor based on levels of another predictor to assess potential interactions.



## Multivariate EDA code

```
library(viridis)
ggplot(data = derby, aes(x = year, y = speed, color = condition,
                          shape = condition, linetype = condition)) +
  geom_point() +
  geom_smooth(method = "lm", se = FALSE, aes(linetype = condition)) +
  labs(x = "Year", y = "Speed (ft/s)", color = "Condition",
       title = "Speed vs. year",
       subtitle = "by track condition") +
  guides(lty = FALSE, shape = FALSE) +
  scale_color_viridis_d(end = 0.9)
```



## Candidate models

Model 1: Main effects model (year, condition, starters)

```
model1 <- lm(speed ~ starters + year +  
              condition, data = derby)
```

Model 2: Main effects +  $year^2$ , the quadratic effect of year

```
model2 <- lm(speed ~ starters +  
              year + I(year^2) +  
              condition, data = derby)
```

Model 3: Main effects + interaction between year and condition

```
model3 <- lm(speed ~ starters + year +  
              condition + year * condition,  
              data = derby)
```

# Inference for regression

Use statistical inference to

- ▶ Evaluate if predictors are statistically significant (not necessarily practically significant!)
- ▶ Quantify uncertainty in coefficient estimates
- ▶ Quantify uncertainty in model predictions

If LINE assumptions are met, we can use inferential methods based on mathematical models. If at least linearity and independence are met, we can use simulation-based inference methods.

# Inference for regression

When LINE assumptions are met... . . .

- ▶ Use least squares regression to obtain the estimates for the model coefficients  $\beta_0, \beta_1, \dots, \beta_j$  and for  $\sigma^2$
- ▶  $\hat{\sigma}$  is the **regression standard error**

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

where  $p$  is the number of non-intercept terms in the model (e.g.,  $p = 1$  in simple linear regression)

- ▶ Goal is to use estimated values to draw conclusions about  $\beta_j$
- ▶ Use  $\hat{\sigma}$  to calculate  $SE_{\hat{\beta}_j}$ . [Click here for more detail.](#)

## Hypothesis testing for $\beta_j$

1. **State the hypotheses.**  $H_0 : \beta_j = 0$  vs.  $H_a : \beta_j \neq 0$ , given the other variables in the model.
2. **Calculate the test statistic.**

$$t = \frac{\hat{\beta}_j - 0}{SE_{\hat{\beta}_j}}$$

3. **Calculate the p-value.** The p-value is calculated from a  $t$  distribution with  $n - p - 1$  degrees of freedom.

$$\text{p-value} = 2P(T > |t|) \quad T \sim t_{n-p-1}$$

4. **State the conclusion in context of the data.**
  - Reject  $H_0$  if p-value is sufficiently small.

## Confidence interval for $\beta_j$

The  $C\%$  confidence interval for  $\beta_j$  is

$$\hat{\beta}_j \pm t^* \times SE_{\hat{\beta}_j}$$

where the critical value  $t^* \sim t_{n-p-1}$

### **General interpretation for the confidence interval**

$LB, UB$

:

We are  $C\%$  confident that for every one unit increase in  $x_j$ , the response is expected to change by LB to UB units, holding all else constant.

# Measures of model performance

- ▶  $R^2$ : Proportion of variability in the response explained by the model
  - ▶ Will always increase as predictors are added, so it shouldn't be used to compare models
- ▶  $Adj.R^2$ : Similar to  $R^2$  with a penalty for extra terms
- ▶  $AIC$ : Likelihood-based approach balancing model performance and complexity
- ▶  $BIC$ : Similar to  $AIC$  with stronger penalty for extra terms

## Model summary statistics

Use the `glance()` function to get model summary statistics

model	r.squared	adj.r.squared	AIC	BIC
Model1	0.730	0.721	259.478	276.302
Model2	0.827	0.819	207.429	227.057
Model3	0.751	0.738	253.584	276.016

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Which model do you choose based on these statistics?



## Characteristics of a “good” final model

- ▶ Model can be used to answer primary research questions
- ▶ Predictor variables control for important covariates
- ▶ Potential interactions have been investigated
- ▶ Variables are centered, as needed, for more meaningful interpretations
- ▶ Unnecessary terms are removed
- ▶ Assumptions are met and influential points have been addressed
- ▶ Model tells a “persuasive story parsimoniously”

List from Section 1.6.7 of Roback and Legler (2021)

# References

- Roback, Paul, and Julie Legler. 2021. *Beyond multiple linear regression: applied generalized linear models and multilevel models in R*. CRC Press.
- Stroup, Walter W. 2012. *Generalized Linear Mixed Models: Modern Concepts, Methods and Applications*. CRC press.
- Wickham, Hadley, Mine Çetinkaya-Rundel, and Garrett Grolemund. 2023. *R for Data Science*. " O'Reilly Media, Inc."