

Data Cleaning, Data Visualization, & Functions

Fundamental Techniques in Data Science



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Outline

Functions

Data Visualization

- Base R Graphics
- GGPlot

Data Cleaning

- Data Analytic Lifecycle
- Missing Data
- Outliers



FUNCTIONS



R Functions

Functions are the foundation of R programming.

- Other than data objects, almost everything else that you interact with when using R is a function.
- Any R command written as a word followed by parentheses `()` is a function.
 - `mean()`
 - `library()`
 - `mutate()`
- Infix operators are aliased functions.
 - `<-`
 - `+`, `-`, `*`
 - `%>%`, `$$`, `%<>%`



User-Defined Functions

We can define our own functions using the `function()` function.

```
square <- function(x) {  
  out <- x^2  
  out  
}
```

After defining a function, we use it in the same way as any other R function.

```
square(5)  
[1] 25
```



User-Defined Functions

One-line functions don't need braces

```
square <- function(x) x^2
```

```
square(5)
```

```
[1] 25
```

Function arguments are not strictly typed. R will try to work with whatever you provide as input.

```
square(1:5)
```

```
[1] 1 4 9 16 25
```

```
square(pi)
```

```
[1] 9.869604
```

```
square(TRUE)
```

```
[1] 1
```

```
square("bob") # But one can only try so hard
```

```
Error in x^2
```

User-Defined Functions

Functions can take multiple arguments.

```
mod <- function(x, y) x %% y
mod(10, 3)

[1] 1
```

Sometimes it's useful to specify a list of arguments that we unpack inside the function.

```
getLsBeta <- function(datList) {
  X <- datList$X
  y <- datList$y

  solve(crossprod(X)) %*% t(X) %*% y
}

X <- matrix(runif(500), ncol = 5)
datList <- list(y = X %*% rep(0.5, 5), X = X)

getLsBeta(datList = datList)

[,1]
[1,] 104 0.5
```

User-Defined Functions

Functions are first-class objects in R.

- We can treat them like any other R object.

R views an initialized, but unevaluated, function as a special object with type "closure"

```
class(getLsBeta)
[1] "function"

typeof(getLsBeta)
[1] "closure"
```

After evaluation, functions are simply equivalent to the objects they return.

```
class(getLsBeta(datList))
[1] "matrix" "array"

typeof(getLsBeta(datList))
[1] "double"
```


User-Defined Functions

We can use functions as arguments to other operations and functions.

```
fun1 <- function(x, y) x + y

## What will this command return?
fun1(1, fun1(1, 1))

[1] 3
```

Why would we care?

```
s2 <- var(runif(100))
x <- rnorm(100, 0, sqrt(s2))

x[1:10, ]

      [,1]      [,2]      [,3]      [,4]      [,5]
[1,] 0.52431382 0.67136447 0.28228726 0.7148383 0.54204681
[2,] 0.01926742 0.11693762 0.09148502 0.6929171 0.88371944
[3,] 0.05100735 0.18432074 0.43547799 0.6097462 0.09026598
[4,] 0.60566972 0.12944127 0.21000143 0.2441917 0.68141473
[5,] 0.48737303 0.94030405 0.23988619 0.4915910 0.36353771
[6,] 0.19941958 0.96670678 0.11455820 0.1243947 0.24253273
[7,] 0.95507004 0.88705000 0.48788585 0.8888170 0.81881888
```

DATA VISUALIZATION



Setup

```
dataDir <- "../../../data/"

diabetes <- readRDS(paste0(dataDir, "diabetes.rds"))
titanic <- readRDS(paste0(dataDir, "titanic.rds"))
bfi      <- readRDS(paste0(dataDir, "bfi.rds"))

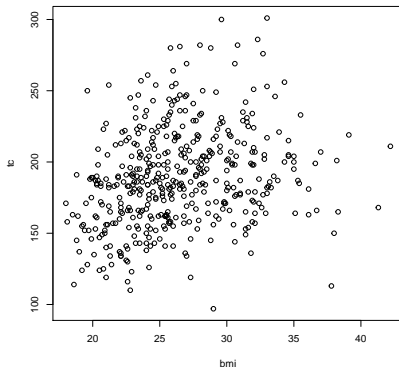
## Convert survival indicator to a numeric dummy code:
titanic <- titanic %>% mutate(survived = as.numeric(survived) - 1)
```



Base R Graphics: Scatterplots

We can create a basic scatterplot using the `plot()` function.

```
diabetes %>% plot(y = tc, x = bmi)
```

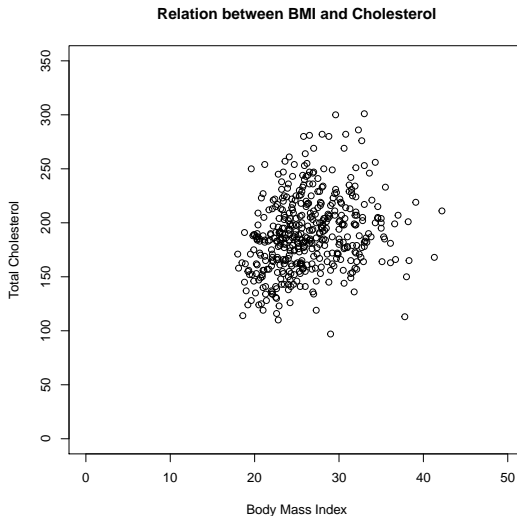


Base R Graphics: Scatterplots

```
diabetes %$% plot(y = tc,  
                 x = bmi,  
                 ylab = "Total Cholesterol",  
                 xlab = "Body Mass Index",  
                 main = "Relation between BMI and Cholesterol",  
                 ylim = c(0, 350),  
                 xlim = c(0, 50)  
                 )
```



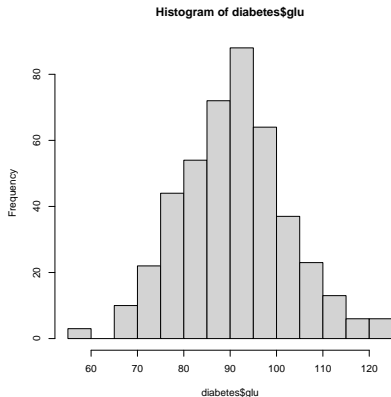
Base R Graphics: Scatterplots



Base R Graphics: Histograms

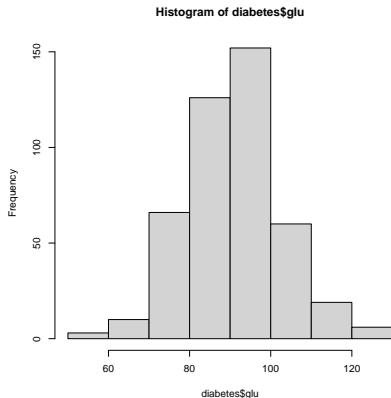
We can create a simple histogram with the `hist()` function.

```
hist(diabetes$glu)
```



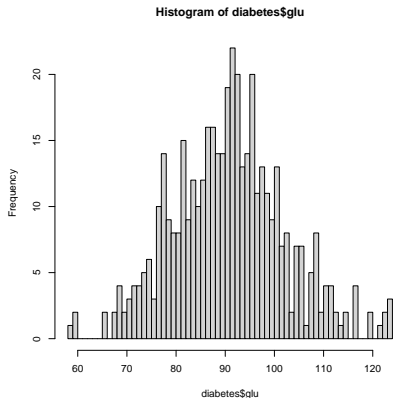
Base R Graphics: Histograms

```
hist(diabetes$glu, breaks = 5)
```



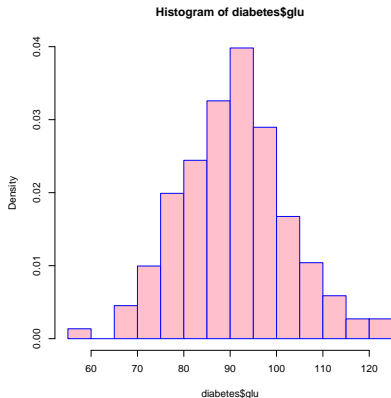
Base R Graphics: Histograms

```
hist(diabetes$glu, breaks = 50)
```



Base R Graphics: Histograms

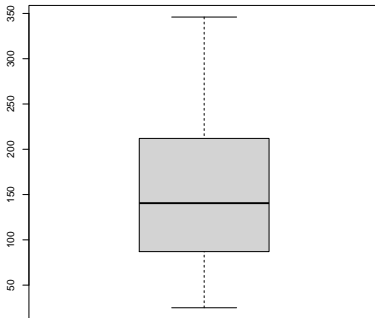
```
hist(diabetes$glu, col = "pink", border = "blue", probability = TRUE)
```



Base R Graphics: Boxplots

We can create simple boxplots via the `boxplot()` function.

```
boxplot(diabetes$progress)
```

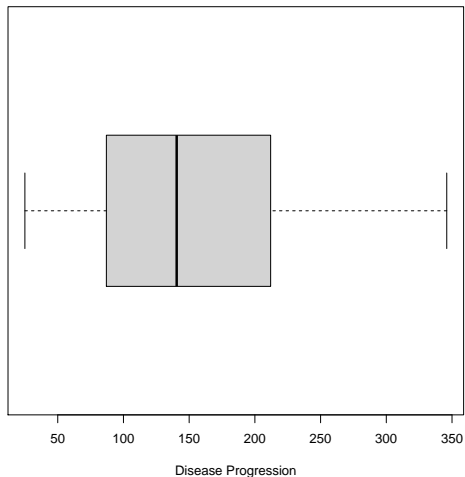


Base R Graphics: Boxplots

```
boxplot(diabetes$progress,  
        horizontal = TRUE,  
        range = 3,  
        xlab = "Disease Progression")
```



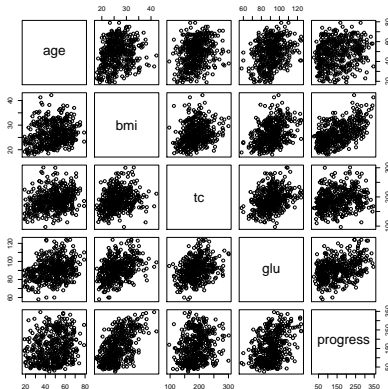
Base R Graphics: Boxplots



Base R Graphics: Fancy Things

Plotting an entire data frame produces a scatterplot matrix.

```
diabetes %>% select(age, bmi, tc, glu, progress) %>% plot()
```

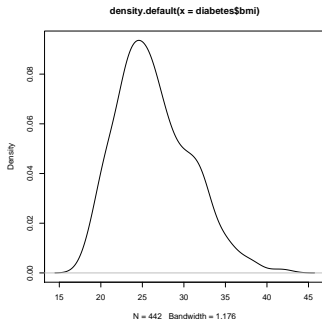


Base R Graphics: Fancy Things

The `density()` function estimates the density of a variable.

- If we plot a density object, we get a kernel density plot.

```
density(diabetes$bmi) %>% plot()
```



Base R Graphics: Fancy Things

```
d <- density(diabetes$bmi)
```

```
ls(d)
```

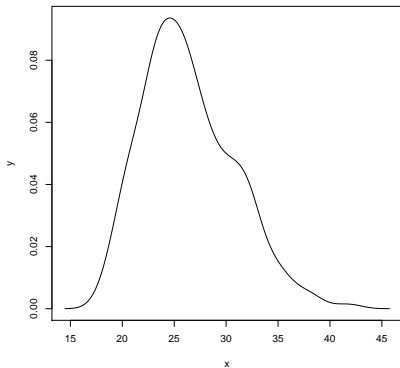
```
[1] "bw"          "call"        "data.name"  "has.na"
```

```
[5] "n"           "x"           "y"
```



Base R Graphics: Fancy Things

```
d %>% plot(y = y, x = x, type = "l")
```



Base R Graphics: Workflow

Base R graphics work by building up graphics from layers.

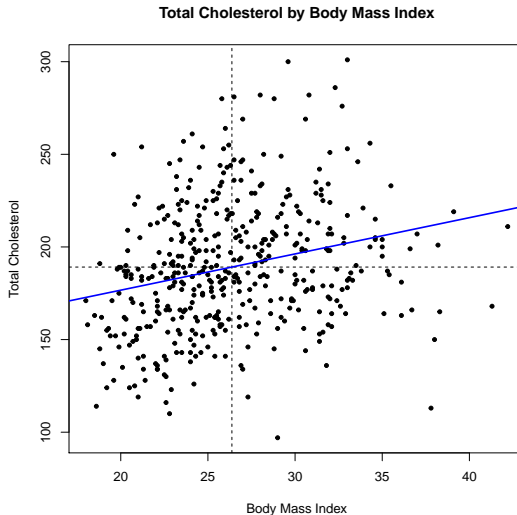
```
## Start with a simple scatterplot:
diabetes %$% plot(y = tc, x = bmi, pch = 20, xlab = "", ylab = "")

## Use the abline() function to add lines representing the means of x and y:
abline(h = mean(diabetes$tc), v = mean(diabetes$bmi), lty = 2)

## Add the best fit line from a linear regression of 'tc' onto 'bmi':
diabetes %$%
  lm(tc ~ bmi) %>%
  coef() %>%
  abline(coef = ., col = "blue", lwd = 2)

## Add titles:
title(main = "Total Cholesterol by Body Mass Index",
      ylab = "Total Cholesterol",
      xlab = "Body Mass Index")
```

Base R Graphics: Workflow



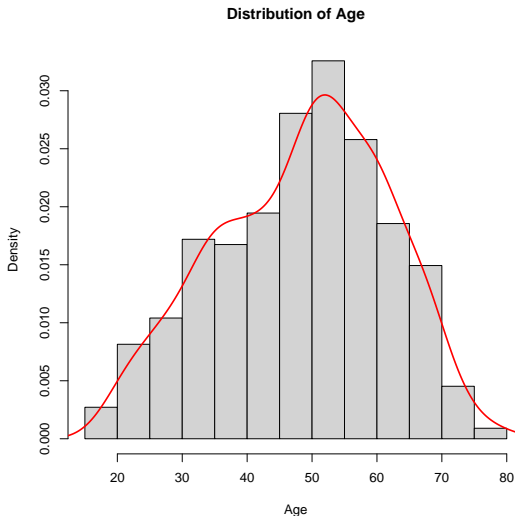
Base R Graphics: Workflow

Add a kernel density plot on top of a histogram.

```
diabetes %$%  
  hist(age,  
        probability = TRUE,  
        xlab = "Age",  
        main = "Distribution of Age")  
  
diabetes %$%  
  density(age) %>%  
  lines(col = "red", lwd = 2)
```



Base R Graphics: Workflow



GGPlot

Base R graphics are fine for quick-and-dirty visualizations (e.g., EDA, checking assumptions), but for publication quality graphics, we probably want to use GGPlot.

GGPlot uses the "grammar of graphics" and "tidy data" to build up a figure from modular components

Describes all the non-data ink
Plotting space for the data
Statistical models & summaries
Rows and columns of sub-plots
Shapes used to represent the data
Scales onto which data is mapped
The actual variables to be plotted

Theme
Coordinates
Statistics
Facets
Geometries
Aesthetics
Data



GGPlot: Basic Setup

We start by calling the `ggplot()` function.

- We must define a data source.
- We must also give some aesthetic via the `aes()` function.

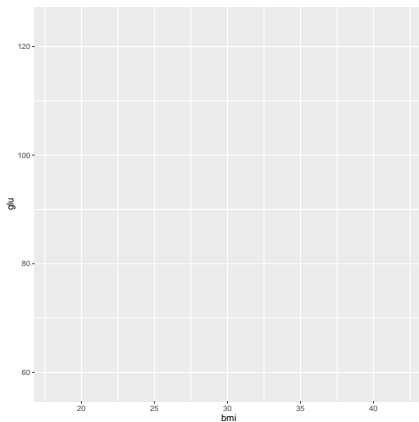
```
library(ggplot2)
p1 <- ggplot(data = diabetes, mapping = aes(x = bmi, y = glu))
```



GGPlot: Basic Setup

At this point, our plot is pretty boring.

p1



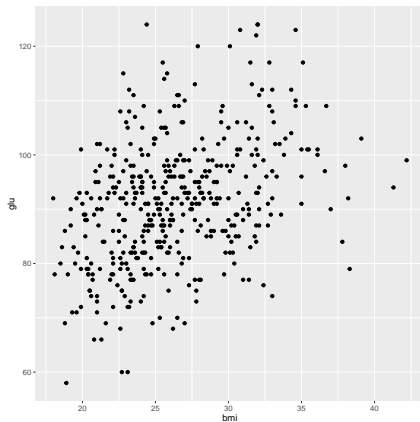
GGPlot: Geometries

We need to define some geometry via an appropriate `geom_X()` function.

```
p1 + geom_point()
```

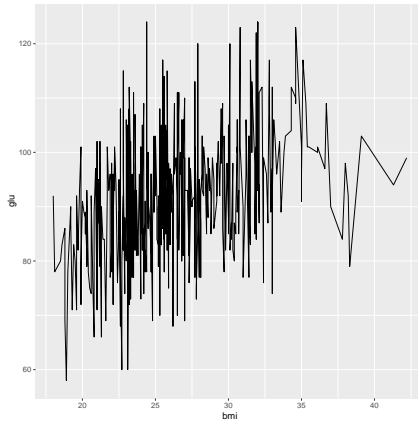


GGPlot: Geometries



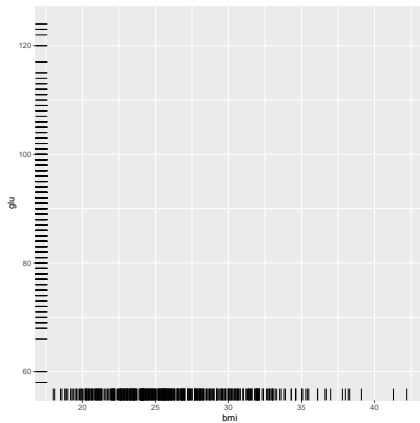
GGPlot: Geometries

```
p1 + geom_line()
```



GGPlot: Geometries

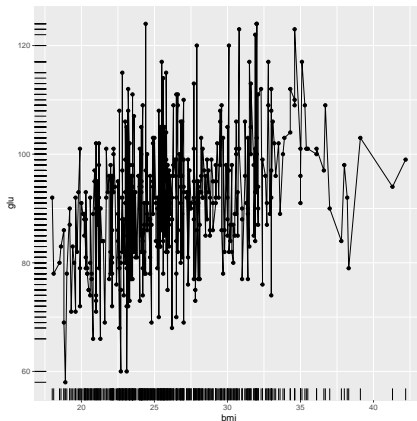
```
p1 + geom_rug()
```



GGPlot: Geometries

We can also combine different geoms into a single figure

```
p1 + geom_point() + geom_line() + geom_rug()
```



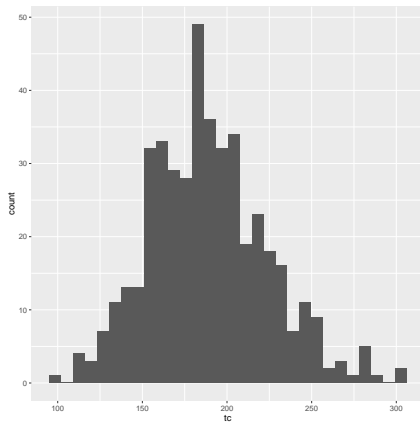
GGPlot: Geometries

We can use different flavors of geom for different types of data

```
p2 <- ggplot(diabetes, aes(tc))  
p2 + geom_histogram()
```

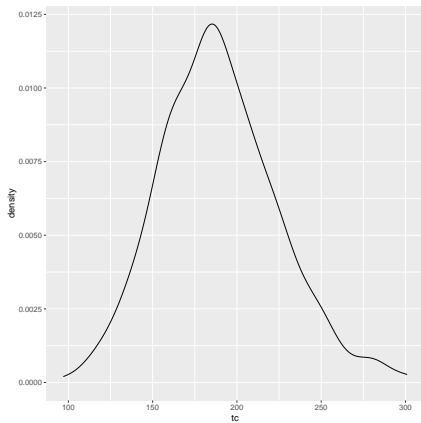


GGPlot: Geometries



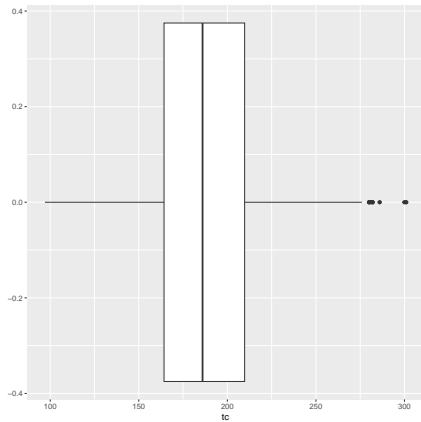
GGPlot: Geometries

```
p2 + geom_density()
```



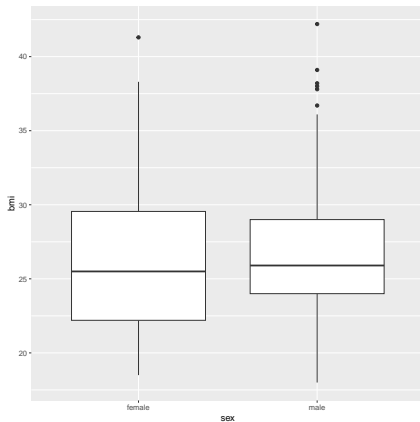
GGPlot: Geometries

```
p2 + geom_boxplot()
```



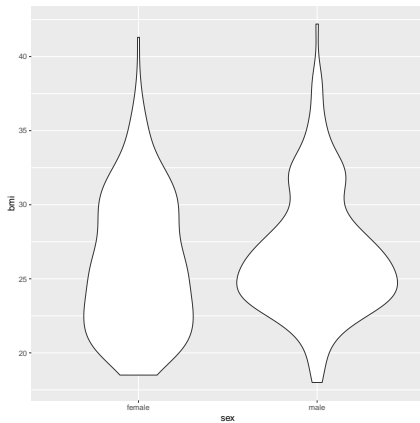
GGPlot: Geometries

```
p3 <- ggplot(diabetes, aes(sex, bmi))  
p3 + geom_boxplot()
```



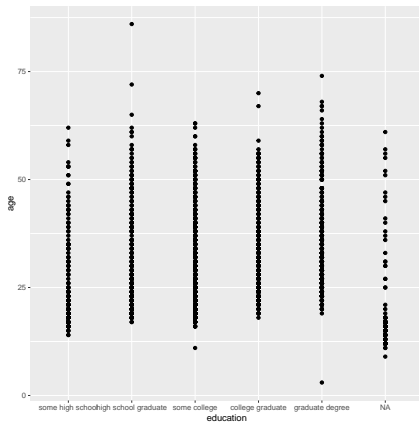
GGPlot: Geometries

```
p3 + geom_violin()
```



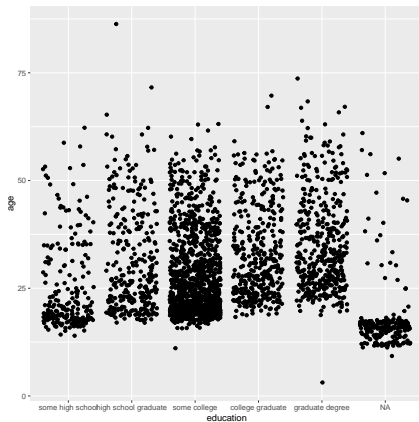
GGPlot: Geometries

```
p4 <- ggplot(bfi, aes(education, age))  
p4 + geom_point()
```



GGPlot: Geometries

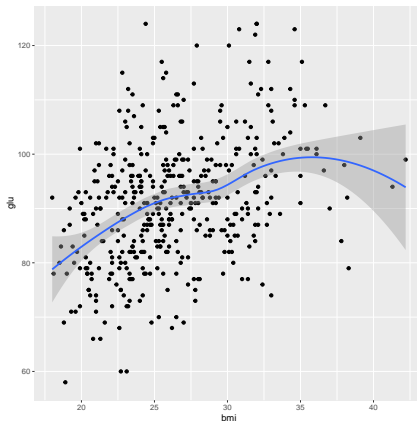
```
p4 + geom_jitter()
```



GGPlot: Statistics

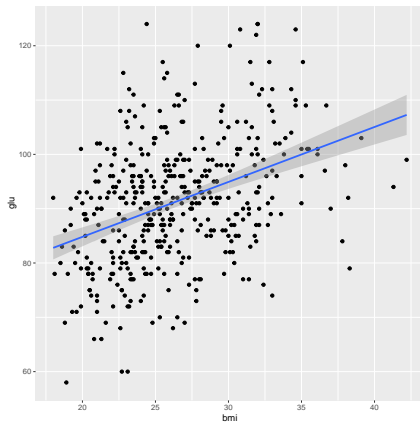
We can also add statistical summaries of the data

```
p1 + geom_point() + geom_smooth()
```



GGPlot: Statistics

```
p1 + geom_point() + geom_smooth(method = "lm")
```



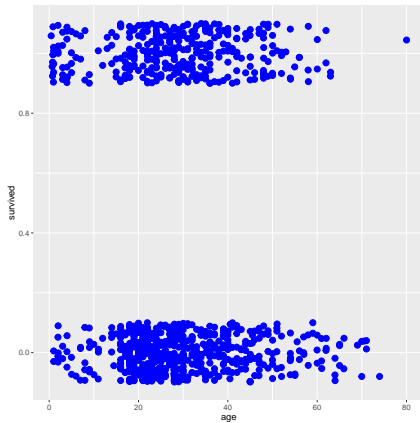
GGPlot: Styling

Changing style options outside of the `aes()` function applies the styling to the entire plot.

```
p5 <- ggplot(titanic, aes(age, survived))  
p5 + geom_jitter(color = "blue", size = 3, height = 0.1)
```



GGPlot: Styling



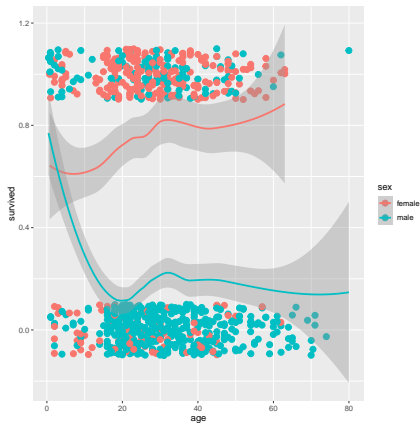
GGPlot: Styling

We can also apply styles as a function of variables by defining the style within the `aes()` function.

```
p6.1 <- ggplot(titanic, aes(age, survived, color = sex))  
p6.1 + geom_jitter(size = 3, height = 0.1) + geom_smooth()
```



GGPlot: Styling

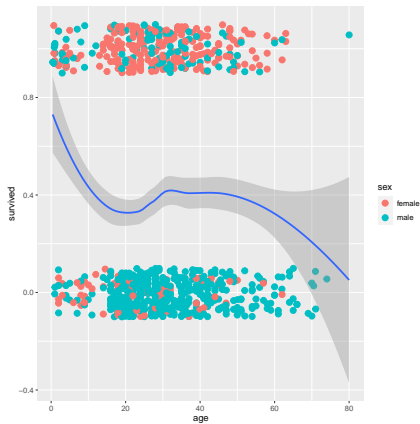


GGPlot: Styling

```
p6.2 <- ggplot(titanic, aes(age, survived))  
p6.2 + geom_jitter(aes(color = sex), size = 3, height = 0.1) +  
  geom_smooth()
```

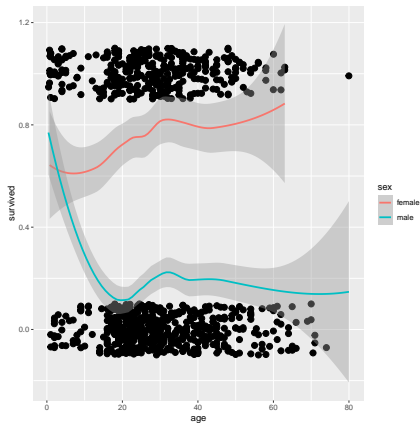


GGPlot: Styling



GGPlot: Styling

```
p6.2 + geom_jitter(size = 3, height = 0.1) +  
  geom_smooth(aes(color = sex))
```



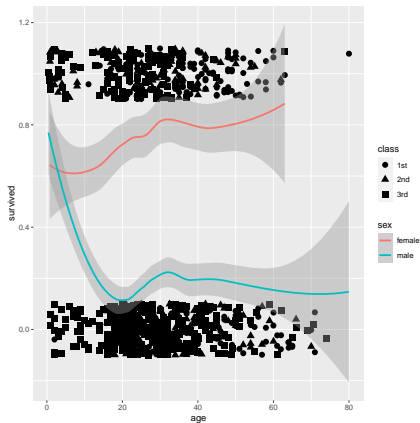
GGPlot: Styling

```
p6.2 + geom_jitter(aes(color = class), size = 3, height = 0.1) +  
  geom_smooth(aes(color = sex))
```



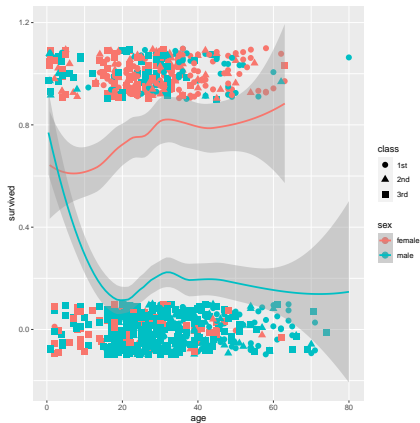
GGPlot: Styling

```
p6.2 + geom_jitter(aes(shape = class), size = 3, height = 0.1) +  
  geom_smooth(aes(color = sex))
```



GGPlot: Styling

```
p6.1 + geom_jitter(aes(shape = class), size = 3, height = 0.1) +  
  geom_smooth()
```



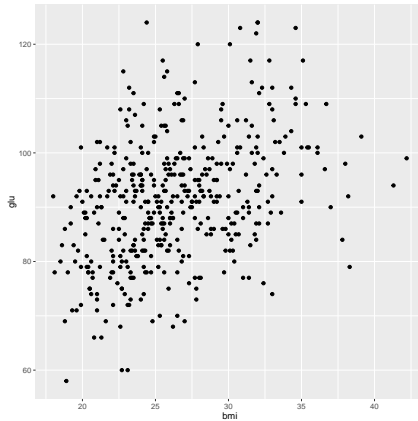
GGPlot: Themes

We can apply several pre-baked themes to adjust a plot's overall appearance

```
(p1.1 <- p1 + geom_point())
```

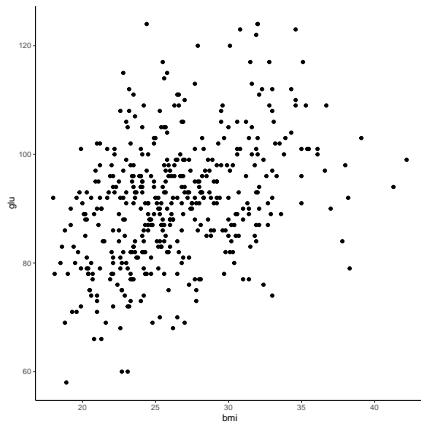


GGPlot: Themes



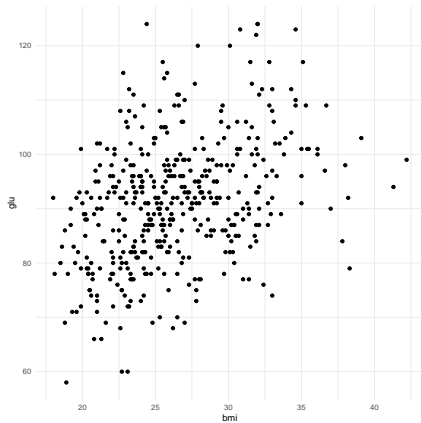
GGPlot: Themes

```
p1.1 + theme_classic()
```



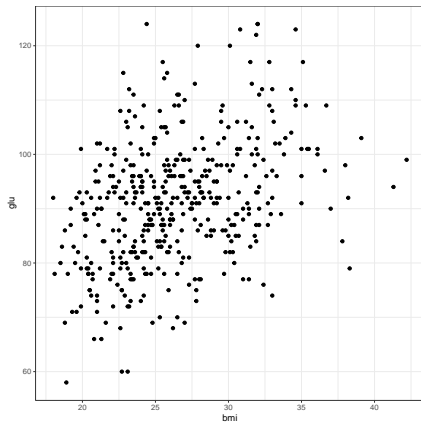
GGPlot: Themes

```
p1.1 + theme_minimal()
```



GGPlot: Themes

```
p1.1 + theme_bw()
```



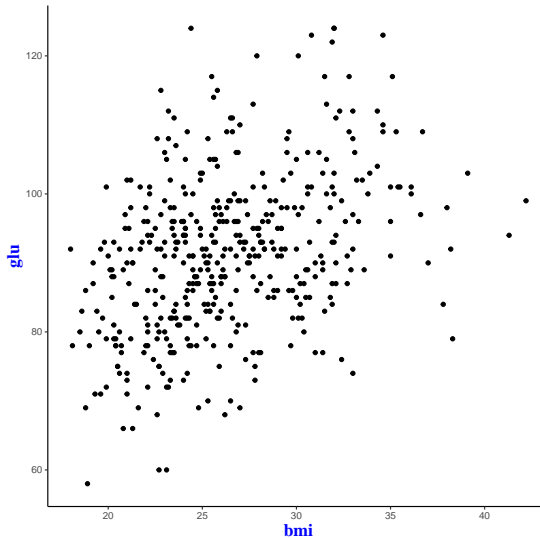
GGPlot: Themes

We can also moodifying individual theme elements.

```
p1.1 + theme_classic() +  
  theme(axis.title = element_text(size = 16,  
                                   family = "serif",  
                                   face = "bold",  
                                   color = "blue"),  
        aspect.ratio = 1)
```



GGPlot: Themes



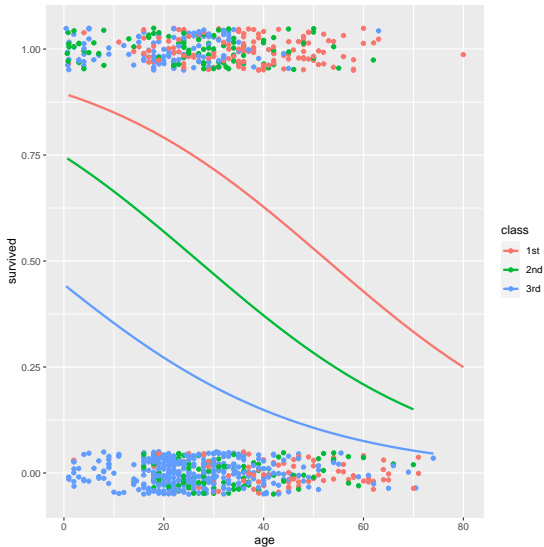
GGPlot: Facets

Facetting allow us to make arrays of conditional plots.

```
(p7 <- ggplot(titanic, aes(age, survived, color = class)) +  
  geom_jitter(height = 0.05) +  
  geom_smooth(method = "glm",  
              method.args = list(family = "binomial"),  
              se = FALSE)  
)
```



GGPlot: Facets



GGPlot: Joining Multiple Figures

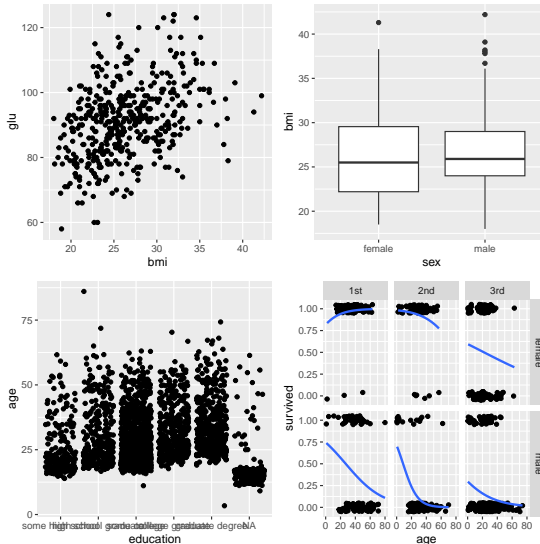
If we want to paste several different plots into a single figure (without facetting), we can use the utilities in the **gridExtra** package.

```
library(gridExtra)

grid.arrange(p1 + geom_point(),
             p3 + geom_boxplot(),
             p4 + geom_jitter(),
             p8 + facet_grid(vars(sex), vars(class)),
             ncol = 2)
```



GGPlot: Joining Multiple Figures



Saving Graphics

To save a graphic that we've created in R, we simply redirect the graphical output to a file using an appropriate function.

```
figDir <- "../figures/"

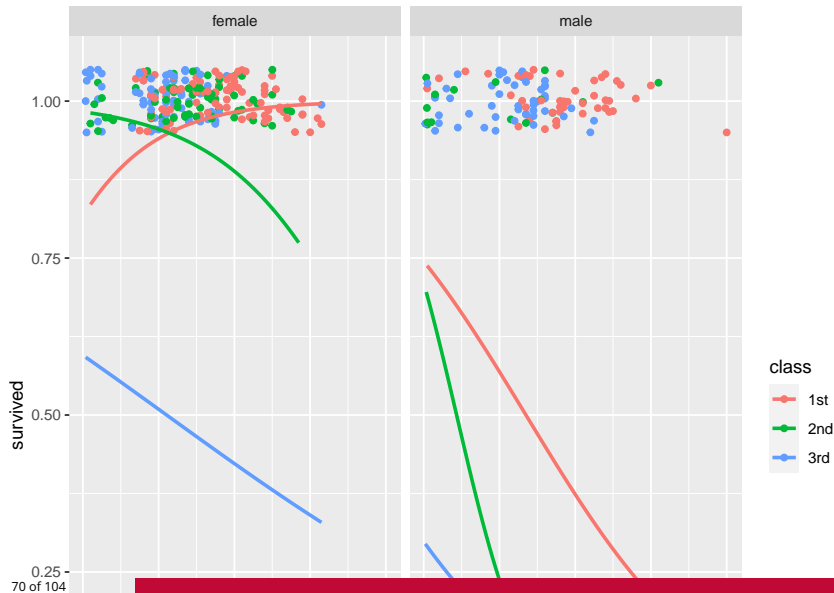
## Save as PDF
pdf(paste0(figDir, "example_plot.pdf"))

Error in pdf(paste0(figDir, "example_plot.pdf")): cannot open file
'../figures/example_plot.pdf'

p7 + facet_wrap(vars(sex))
```



Saving Graphics

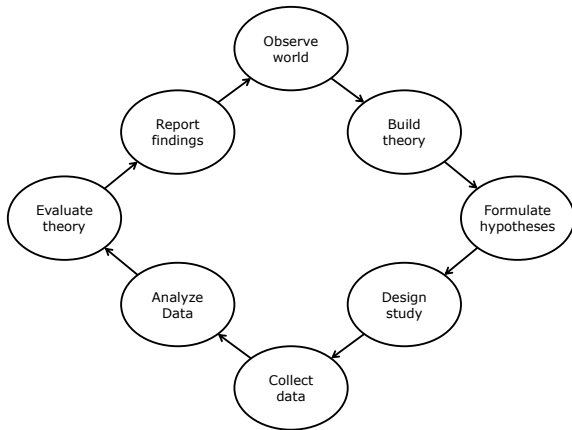


DATA CLEANING



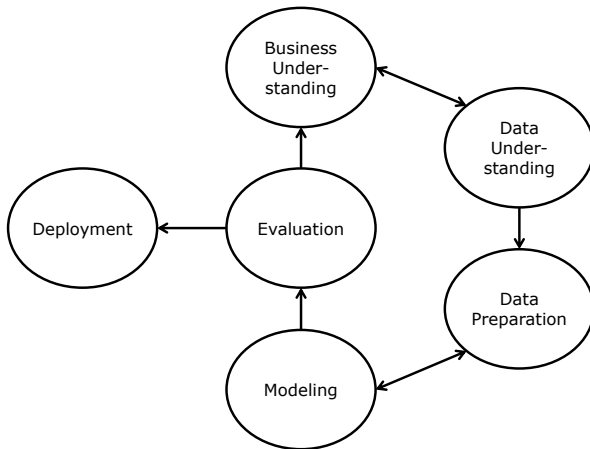
Research Cycle

The following is a representation of the *Research Cycle* used for empirical research in most of the sciences.



CRISP-DM

The *Cross-industry Standard Process for Data Mining* was developed to standardized the process of data mining in industry applications.



The *Data Science Cycle* represented here was adapted from O’Neil and Schutt (2014).

Data Cleaning

When we receive new data, they are generally messy and contaminated by various anomalies and errors.

- One of the first steps in processing a new set of data is *cleaning*.
- By cleaning the data, we ensure a few properties:
 - The data are in an analyzable format.
 - All data take legal values.
 - Any outliers are located and treated.
 - Any missing data are located and treated.



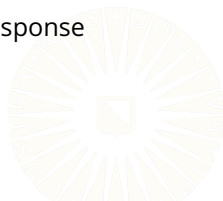
A Little Notation

$Y :=$ An $N \times P$ data matrix

$Y_{mis} :=$ The *missing* part of Y

$Y_{obs} :=$ The *observed* part of Y

$R :=$ An $N \times P$ pattern matrix encoding nonresponse



What are Missing Data?

Missing data are empty cells in a dataset where there should be observed values.

- The missing cells correspond to true population values, but we haven't observed those values.



What are Missing Data?

Missing data are empty cells in a dataset where there should be observed values.

- The missing cells correspond to true population values, but we haven't observed those values.

Not every empty cell is a missing datum.

- Quality-of-life ratings for dead patients in a mortality study
- Firm profitability after the company goes out of business
- Self-reported severity of menstrual cramping for men
- Empty blocks of data following "gateway" items



Missing Data Descriptives



Missing Data Pattern

Missing data (or response) patterns represent unique combinations of observed and missing items.

- P items $\Rightarrow 2^P$ possible patterns.

	X	Y
1	x	y
2	x	.
3	.	y
4	.	.

Patterns for $P = 2$

	X	Y	Z
1	x	y	z
2	x	y	.
3	x	.	z
4	.	y	z
5	x	.	.
6	.	.	z
7	.	y	.
8	.	.	.

Patterns for $P = 3$

Nonresponse Rates

Percent/Proportion Missing

- The proportion of cells containing missing data
- Good early screening measure
- Should be computed for each variable, not for the entire dataset

Attrition Rate

- The proportion of participants that drop-out of a study at each measurement occasion

Percent/Proportion of Complete Cases

- The proportion of observations with no missing data
- Often reported but nearly useless quantity



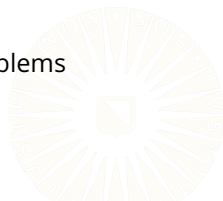
Nonresponse Rates

Covariance Coverage

- The proportion of cases available to estimate a given pairwise relationship (e.g., a covariance between two variables)
- Very important to have adequate coverage for the parameters you want to estimate

Fraction of Missing Information

- Associated with an estimated parameter, not with an incomplete variable
- Like an R^2 for the missing data
- Most important diagnostic value for missing data problems
- Can only be computed after treating the missing data



Covariance Coverage Examples

- What is the coverage for $\text{cov}(X, Y)$?
- What is the coverage for $\text{cov}(W, Y)$?
- What about $\text{cov}(X, Z)$?

	W	X	Y	Z
1	w	x	y	.
2	w	x	y	.
3	w	x	y	.
4	w	x	y	.
5	w	x	y	.
6	w	.	y	z
7	w	.	y	z
8	w	.	y	z
9	w	.	y	z
10	w	.	y	z

Nonresponse Rate Examples

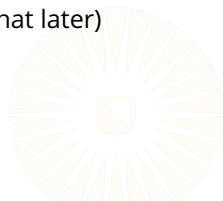
- What is the percent missing at Time 2?
- What is the attrition rate at Time 3?

	T1	T2	T3	T4
1	x1	x2	x3	x4
2	x1	x2	x3	x4
3	x1	x2	x3	x4
4	x1	x2	x3	.
5	x1	x2	x3	.
6	x1	x2	.	.
7	x1	x2	.	.
8	x1	.	.	.
9	x1	.	.	.
10	x1	.	.	.

What is an outlier?

For the time being, we're considering *univariate outliers*.

- Extreme values with respect to the distribution of a variable's other observations
 - A human height measurement of 3 meters
 - A high temperature in Utrecht of 50°
 - Annual income of €250,000 for a student
- Not accounting for any particular model (we'll get to that later)



What is an outlier?

A univariate outlier may, or may not, be an illegal value.

- Data entry errors are probably the most common cause.
- Outliers can also be legal, but extreme, values.

Key Point: We choose to view an outlier as arising from a different population than the one to which we want to generalize our findings.



Finding Univariate Outliers

We have many methods available to diagnose potential outliers.

- Four of the simplest and most popular are:
 1. Internally studentized residuals (AKA Z-score method)
 2. Externally studentized residuals
 3. Median absolute deviation method
 4. Tukey's boxplot method



Internally Studentized Residuals

For each observation, X_n , we compute the following quantity:

$$T_n = \frac{X_n - \bar{X}}{SD_X}$$

- T_n follows a Student's t distribution with $df = N - 1$.
 - We can do a formal test for “outlier” status.
- Assuming a large sample, if $T_n > C$ (where C is usually 2 or 3), we label X_n as an outlier.



Internally Studentized Residuals

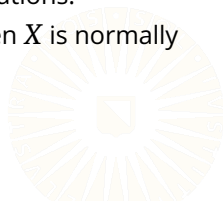
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Although simple, this method has some substantial limitations.

- The cutpoint, C , can only be meaningfully chosen when X is normally distributed.
- Both \bar{X} and SD_X are highly sensitive to outliers.



Externally Studentized Residual

The externally studentized residual method is essentially the same as the internally studentized residual method, but we adjust \bar{X} and SD_X to remove the influence of the observation we're evaluating.

- Let $\mathbb{N}_{(n)} = \{1, \dots, (n-1), (n+1), \dots, N\}$.
- Define the deletion mean, $\bar{X}_{(n)}$, and deletion SD, $SD_{X(n)}$, as:

$$\bar{X}_{(n)} = \frac{1}{N-1} \sum_{i \in \mathbb{N}_{(n)}} X_i$$
$$SD_{X(n)} = \sqrt{\frac{1}{N-2} \sum_{i \in \mathbb{N}_{(n)}} (X_i - \bar{X}_{(n)})^2}$$



Externally Studentized Residual

The externally studentized residual is defined in the same way as the internally studentized version:

$$T_{(n)} = \frac{X_n - \bar{X}_{(n)}}{SD_{X(n)}}$$

- $T_{(n)}$ follows a Student's t distribution with $df = N - 2$.
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Externally Studentized Residual

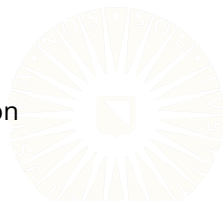
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$$T_{(n)} = \frac{X_n - \bar{X}_{(n)}}{SD_{X(n)}}$$

- $T_{(n)}$ follows a Student's t distribution with $df = N - 2$.
 - We can do a formal test for “outlier” status.
- Assuming a large sample, if $T_{(n)} > C$ (where C is usually 2 or 3), we label X_n as an outlier.

$T_{(n)}$ is immune to the influence of the n th observation.

- Still requires X to be normally distributed
- Still sensitive to outliers other than the n th observation



Median Absolute Deviation Method

The biggest limitation of studentized residuals is that their measures of central tendency and dispersion are sensitive to outliers.

- If we can replace the (deleted) mean and the (deleted) SD with more robust statistics, we can avoid this issue.
 - Replace the mean, \bar{X} , with the *median*, $\text{Med}(X)$
 - Replace the SD with the *median absolute deviation*:

$$MAD_X = b \times \text{Med} (|X_n - \text{Med}(X)|)$$

- We choose the coefficient as $b = 1/Q_{0.75}$
- For the normal distribution, $b \approx 1/0.6745 \approx 1.4826$



Median Absolute Deviation Method

We compute our test statistic by replacing the mean with the median and the SD with the MAD in the standard Wald test formula:

$$T_{MAD} = \frac{X_n - \text{Med}(X)}{MAD_X}$$

- T_{MAD} doesn't allow for formal statistical tests.
- We can use the same general cutoffs we would use for the studentized residual methods.
 - Assuming a large sample, if $T_{(n)} > C$ (where C is usually 2 or 3), we label X_n as an outlier.



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 - Assuming a large sample, if $T_{(n)} > C$ (where C is usually 2 or 3), we label X_n as an outlier.

T_{MAD} is immune to the influence of, up to, 50% outlying observations.

- Requires us to assume a parametric distribution for X
 - This assumption is necessary to compute b .

Breakdown Point

To compare robust statistics, we consider their *breakdown points*.

- The breakdown point is the minimum proportion of cases that must be replaced by ∞ to cause the value of the statistic to go to ∞ .

The mean has a breakdown point of $1/N$.

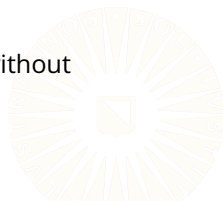
- Replacing a single value with ∞ will produce an infinite mean.

The deletion mean has a breakdown point of $2/N$.

- We can replace, at most, 1 value with ∞ without producing an infinite mean.

The median has breakdown point of 50%.

- We can replace $n < N/2$ of the observations with ∞ without producing an infinite median.



Boxplot Method

Tukey (1977) described a procedure for flagging potential outliers based on the familiar box-and-whiskers plot.

- Does not require normally distributed X
- Not sensitive to outliers
- Doesn't allow for formal statistical tests



Boxplot Method

A *fence* is an interval defined as the following function of the *first quartile*, the *third quartile*, and the *inner quartile range* ($IQR = Q_3 - Q_1$):

$$F = \{Q_1 - C \times IQR, Q_3 + C \times IQR\}$$

- Taking $C = 1.5$ produces the *inner fence*.
- Taking $C = 3.0$ produces the *outer fence*.

We can use these fences to identify potential outliers:

- Any value that falls outside of the inner fence is a *possible outlier*.
- Any value that falls outside of the outer fence is a *probable outlier*.

Multivariate Outliers

Sometimes, the combinations of values in an observation are very unlikely, even when no individual value is an outlier.

- These observations are *multivariate outliers*.
 - A person in the 95th percentile for height and the 5th percentile for weight
 - A person who simultaneously scores highly on scales of depression and positive affect

To detect multivariate outliers, we use *distance metrics*.

- Distance metrics quantify the similarity of two vectors.
 - Similarity between two observations
 - Similarity between an observation and the mean vector



Mahalanobis Distance

One of the most common distance metrics is the *Mahalanobis Distance*.

- The Mahalanobis distance, Δ , is a multivariate generalization of the internally studentized residual:

$$\Delta_n = \sqrt{(\mathbf{x}_n - \hat{\mu}_{\mathbf{X}})^T \hat{\Sigma}_{\mathbf{X}}^{-1} (\mathbf{x}_n - \hat{\mu}_{\mathbf{X}})}$$

As with studentized residuals, if $\Delta_n > C$, we label \mathbf{x}_n as an outlier.

- When \mathbf{X} is K -variate normally distributed, Δ_n^2 follows a χ^2 distribution with $df = K$.
- We take C to be the square-root of a suitably conservative quantile (e.g., $q \in \{99\%, 99.9\%\}$) of the χ_K^2 distribution: $C = \sqrt{\chi_{K,q}^2}$.

Problems with Mahalanobis Distance

Like the internally studentized residual, Mahalanobis distance is highly sensitive to outliers.

- The underlying estimates of central tendency, $\hat{\mu}_{\mathbf{X}}$, and dispersion, $\hat{\Sigma}_{\mathbf{X}}$, are computed using all observations.



Problems with Mahalanobis Distance

Like the internally studentized residual, Mahalanobis distance is highly sensitive to outliers.

- The underlying estimates of central tendency, $\hat{\mu}_{\mathbf{X}}$, and dispersion, $\hat{\Sigma}_{\mathbf{X}}$, are computed using all observations.

We want robust analogues of $\hat{\mu}_{\mathbf{X}}$ and $\hat{\Sigma}_{\mathbf{X}}$.

- We have several options for robust estimation of $\hat{\mu}_{\mathbf{X}}$ and $\hat{\Sigma}_{\mathbf{X}}$. E.g.:
 - Minimum covariance determinant method (MCD; Rousseeuw, 1985)
 - Minimum volume ellipsoid method (MVE; Rousseeuw, 1985)
 - M-estimation (Maronna, 1976)
- Conceptually, robust methods operate by either:
 - Using only a “good” subset of data to estimate $\hat{\mu}_{\mathbf{X}}$ and $\hat{\Sigma}_{\mathbf{X}}$.
 - Downweighting outlying observations when estimating $\hat{\mu}_{\mathbf{X}}$ and $\hat{\Sigma}_{\mathbf{X}}$.

Robust Mahalanobis Distance

Equipped with robust estimates of central tendency, $\hat{\mu}_{R,X}$, and dispersion, $\hat{\Sigma}_{R,X}$, we define the robust Mahalanobis distance in the natural way:

$$\Delta_{R,n} = \sqrt{(\mathbf{x}_n - \hat{\mu}_{R,X})^T \hat{\Sigma}_{R,X}^{-1} (\mathbf{x}_n - \hat{\mu}_{R,X})}$$

We use $\Delta_{R,n}$ in the same way as Δ_n .

- If $\Delta_{R,n} > C$, we label \mathbf{x}_n as an outlier.
- Again, we take C to be the square-root of some quantile of the χ_K^2 distribution: $C = \sqrt{\chi_{K,q}^2}$.

Practicalities: Univariate vs. Multivariate

Univariate outlier checks are safe for most variables.



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Don't include too many variables in multivariate outlier checks.

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Do use multivariate outlier checks for scales.

- E.g., if you have a psychometric scale measuring depression, you should check the items of that scale for multivariate outliers.



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Do use multivariate outlier checks for scales.

- E.g., if you have a psychometric scale measuring depression, you should check the items of that scale for multivariate outliers.

Maybe check the variables in a single model for multivariate outliers.

- E.g., if you have a small set of items that you will include in a regression model, it could make sense to check these variables for multivariate outliers.

Practicalities: Outliers for Categorical Data

Nominal, ordinal, and binary items *can* have outliers.

- Outliers on categorical variables are often more indicative of bad variables than outlying cases.



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Ordinal

- Most participant endorse one of the lowest categories on an ordinal item, but a few participants endorse the highest category.
- The participants who endorse the highest category may be outliers.



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Nominal

- Groups with very low membership may be outliers on nominal grouping variables.



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- Most participant endorse one of the lowest categories on an ordinal item, but a few participants endorse the highest category.
- The participants who endorse the highest category may be outliers.

Nominal

- Groups with very low membership may be outliers on nominal grouping variables.

Binary

- If most endorse the item, the few who do not may be outliers.

Treating Outliers

If we locate any outliers, they must be treated.

- Outliers caused by errors, mistakes, or malfunctions (i.e., *error outliers*) should be directly corrected.
- Labeling non-error outliers is a subjective task.
 - A (non-error) outlier must originate from a population separate from the one we care about.
 - Don't blindly automate the decision process.



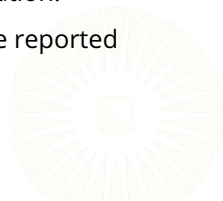
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 - Don't blindly automate the decision process.

The most direct solution is to delete any outlying observation.

- If you delete non-error outliers, the analysis should be reported twice: with outliers and without.



Treating Outliers

For univariate outliers, we can use less extreme types of deletion.

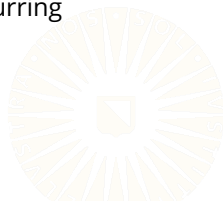
- Delete outlying values (but not the entire observation).
- These empty cells then become missing data.

Winsorization:

- Replace the missing values with the nearest non-outlying value.

Missing data analysis:

- Treat the missing values along with any naturally-occurring nonresponse.



Treating Outliers

We can also use robust regression procedures to estimate the model directly in the presence of outliers.

- Weight the objective function to reduce the impact of outliers
 - M-estimation
- Trim outlying observations during estimation
 - Least trimmed squares, MCD, MVE
- Take the median, instead of the mean, of the squared residuals
 - Least median of squares
- Model some quantile of the DV's distribution instead of the mean
 - Quantile regression
- Model the outcome with a heavy-tailed distribution
 - Laplacian, Student's T



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