

Data Cleaning

Fundamental Techniques in Data Science



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Outline

Data Analytic Lifecycle

Missing Data

Outliers

- Univariate Outliers

- Multivariate Outliers

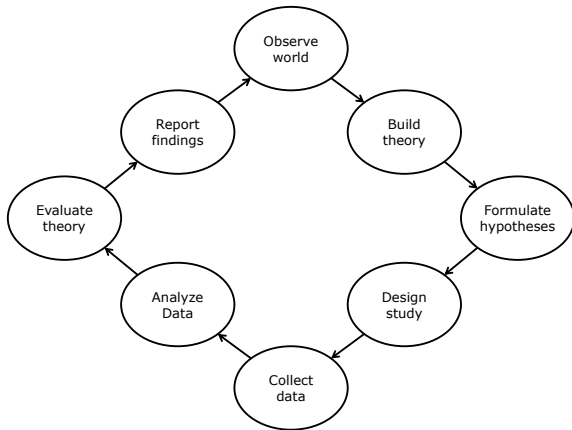


DATA ANALYTIC LIFECYCLE



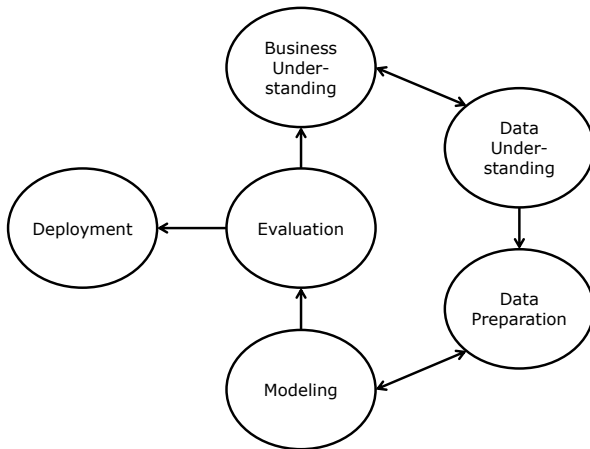
Research Cycle

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



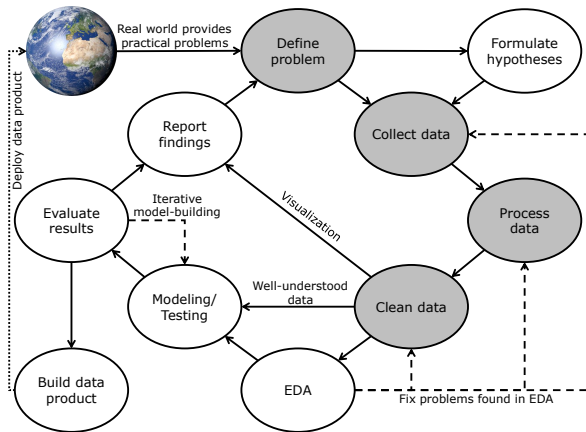
CRISP-DM

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



Data Science Cycle

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.



MISSING DATA



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 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
- 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

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

Example

We can calculate basic response rates with simple base R commands.

```
## Load some example data:
data(boys, package = "mice")

## Compute variable-wise proportions missing:
mMat <- is.na(boys)
mMat %>% colMeans() %>% round(3)

  age   hgt   wgt   bmi   hc   gen   phb   tv   reg
0.000 0.027 0.005 0.028 0.061 0.672 0.672 0.698 0.004
```

Example

```
## Compute observation-wise proportions missing:
```

```
pmRow <- rowMeans(mMat)
```

```
## Summarize the above:
```

```
range(pmRow)
```

```
[1] 0.0000000 0.7777778
```

```
range(pmRow[pmRow > 0])
```

```
[1] 0.1111111 0.7777778
```

```
median(pmRow)
```

```
[1] 0.3333333
```

```
## Compute the proportion of complete cases:
```

```
mean(pmRow == 0)
```

```
[1] 0.2981283
```

Example

We can use routines from the **mice** package to calculate covariance coverage and response patterns.

```
## Compute the covariance coverage:
cc <- mice::md.pairs(boys)$rr / nrow(boys)

## Check the result:
round(cc, 2)
```

	age	hgt	wgt	bmi	hc	gen	phb	tv	reg
age	1.00	0.97	0.99	0.97	0.94	0.33	0.33	0.3	1.00
hgt	0.97	0.97	0.97	0.97	0.92	0.32	0.32	0.3	0.97
wgt	0.99	0.97	0.99	0.97	0.94	0.32	0.32	0.3	0.99
bmi	0.97	0.97	0.97	0.97	0.91	0.32	0.32	0.3	0.97
hc	0.94	0.92	0.94	0.91	0.94	0.33	0.33	0.3	0.93
gen	0.33	0.32	0.32	0.32	0.33	0.33	0.33	0.3	0.33
phb	0.33	0.32	0.32	0.32	0.33	0.33	0.33	0.3	0.33
tv	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.3	0.30
reg	1.00	0.97	0.99	0.97	0.93	0.33	0.33	0.3	1.00

Example

```
## Range of coverages:
```

```
range(cc)
```

```
[1] 0.2994652 1.0000000
```

```
range(cc[cc < 1])
```

```
[1] 0.2994652 0.9959893
```

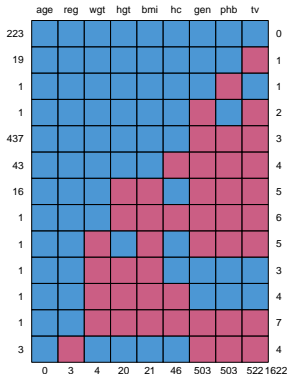
```
## How many coverages fall below some threshold?
```

```
(cc[lower.tri(cc)] < 0.7) %>% sum()
```

```
[1] 21
```


Example

```
## Compute missing data patterns:  
pats <- mice::md.pattern(boys)
```



Example

pats

	age	reg	wgt	hgt	bmi	hc	gen	phb	tv	
223	1	1	1	1	1	1	1	1	1	0
19	1	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	1	1	0	1	1
1	1	1	1	1	1	1	0	1	0	2
437	1	1	1	1	1	1	0	0	0	3
43	1	1	1	1	1	0	0	0	0	4
16	1	1	1	0	0	1	0	0	0	5
1	1	1	1	0	0	0	0	0	0	6
1	1	1	0	1	0	1	0	0	0	5
1	1	1	0	0	0	1	1	1	1	3
1	1	1	0	0	0	0	1	1	1	4
1	1	1	0	0	0	0	0	0	0	7
3	1	0	1	1	1	1	0	0	0	4
	0	3	4	20	21	46	503	503	522	1622

Example

```
## How many unique response patterns?
```

```
nrow(pats) - 1
```

```
[1] 13
```

```
## What is the most common response patterns?
```

```
maxPat <- rownames(pats) %>% as.numeric() %>% which.max()
```

```
pats[maxPat, ]
```

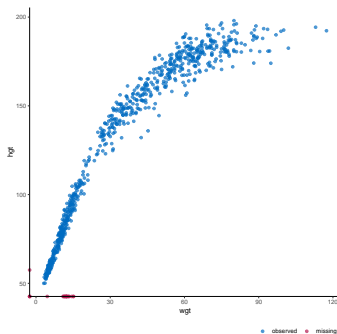
```
age reg wgt hgt bmi hc gen phb tv  
1 1 1 1 1 1 0 0 0 3
```

Visualizing Incomplete Data

The **ggmice** package provides some nice ways to visualize incomplete data and objects created during missing data treatment.

```
library(ggmice); library(ggplot2)

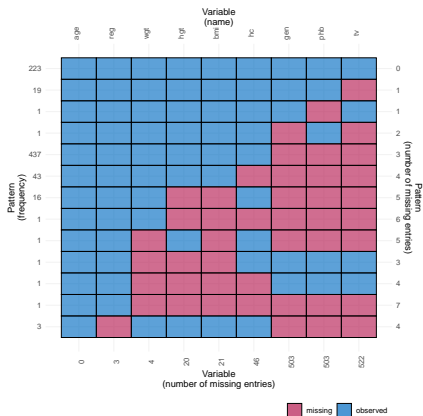
ggmice(boys, aes(wgt, hgt)) + geom_point()
```



Visualizing Incomplete Data

We can also create a nicer version of the response pattern plot.

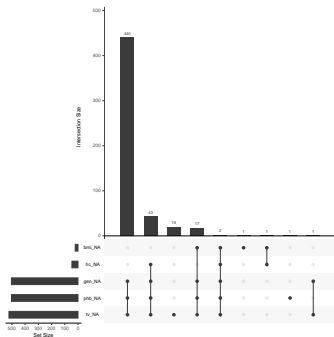
```
plot_pattern(boys, rotate = TRUE)
```



Visualizing Incomplete Data

The **naniar** package also provides some nice visualization and numerical summary routines for incomplete data.

```
naniar::gg_miss_upset(boys)
```



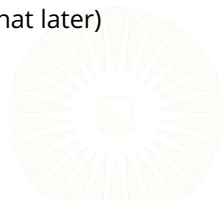
OUTLIERS



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)

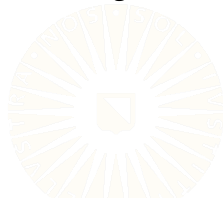


What is an outlier?

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.

- Today, we'll only discuss three of the simplest:
 1. Z-score method
 2. Tukey's boxplot method
 3. Adjusted boxplot method



Z-Score Method

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

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

- Z_n represents the distance between X_n and the sample mean in standard deviation units.
- Assuming a large sample, if $T_n > C$ (where C is usually 3), we label X_n as an outlier.



Z-Score Method

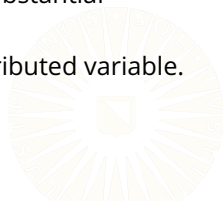
For each observation, X_n , we compute the following quantity:

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

- Z_n represents the distance between X_n and the sample mean in standard deviation units.
- Assuming a large sample, if $T_n > C$ (where C is usually 3), we label X_n as an outlier.

Although simple (and popular), this method has some substantial limitations.

- The logic of the filtering rule assumes a normally distributed variable.
- Both \bar{X} and SD_X are highly sensitive to outliers.



Example

We can implement the z-score method via the `scale()` function.

```
## Compute the absolute standardized residuals:
```

```
z <- boys %$% scale(bmi) %>% abs()
```

```
## Which observations are potential outliers?
```

```
which(z > 3)
```

```
[1] 544 574 608 610 668 708 716 733
```

```
## View the potentially outlying cases:
```

```
boys %>% filter(z > 3)
```

	age	hgt	wgt	bmi	hc	gen	phb	tv	reg
1	14.967	174.1	88.0	29.03	54.4	G3	P4	10	east
2	15.493	182.5	102.0	30.62	57.7	<NA>	<NA>	NA	west
3	16.090	180.6	90.4	27.71	58.8	<NA>	<NA>	NA	south
4	16.156	194.3	113.0	29.93	58.4	G3	P5	6	north
5	17.749	174.0	94.9	31.34	56.3	G5	P5	25	west
6	19.060	180.8	93.8	28.69	55.8	G4	P5	15	south
7	19.290	180.9	94.4	28.84	58.6	<NA>	<NA>	NA	south
8	19.926	192.3	117.4	31.74	57.6	G5	P6	18	north

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 $1/N$.

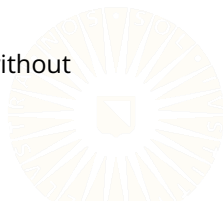
- Replacing a single value with ∞ will produce an infinite mean.

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 a box-and-whiskers plot.

- Does not require normally distributed X
- Not sensitive to outliers



Boxplot Method

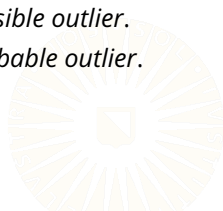
A *fence* is an interval defined as the following function of the *first quartile*, the *third quartile*, and the *inner quartile range* ($IQR = Q_3 - Q_1$):

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

- 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*.



Example

We can implement the boxplot method via `boxplot.stats()` .

```
## Find potentially outlying cases:  
(out <- boys %$% boxplot.stats(bmi, coef = 3)$out)
```

```
[1] 30.62 31.34 31.74
```

```
## Which observations are potential outliers?  
boys %$% which(bmi %in% out)
```

```
[1] 574 668 733
```

```
## View the potentially outlying cases:  
boys %>% filter(bmi %in% out)
```

	age	hgt	wgt	bmi	hc	gen	phb	tv	reg
1	15.493	182.5	102.0	30.62	57.7	<NA>	<NA>	NA	west
2	17.749	174.0	94.9	31.34	56.3	G5	P5	25	west
3	19.926	192.3	117.4	31.74	57.6	G5	P6	18	north

Adjusted Boxplot Method

The original boxplot method uses symmetric fences, so it will tend to flag too many outliers when the true distribution is skewed.

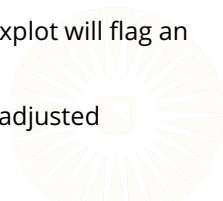
- Hubert and Vandervieren (2008) developed an adjusted boxplot method that accounts for skewness when estimating the fences.

The adjusted boxplot incorporates a robust estimate of skewness (the *medcouple*, MC) when defining the fences:

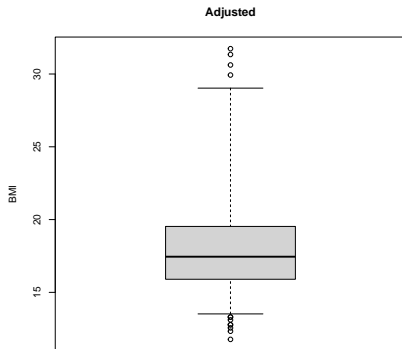
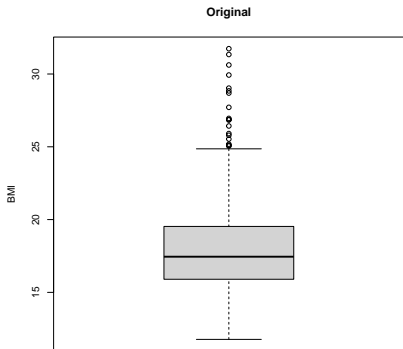
$$F = \{Q_1 - C \times e^{(a \times MC)} IQR, Q_3 + C \times e^{(b \times MC)} IQR\}$$

The adjusted boxplot usually performs quite well.

- When the true distribution is skewed, the adjusted boxplot will flag an “appropriate” proportion of outliers.
- If the true distribution is symmetric, $\hat{MC} \approx 0$, and the adjusted boxplot reduces to the normal boxplot.



Boxplot: Original vs. Adjusted



Example

We can implement the adjusted boxplot method via the `adjboxStats()` function from the **robustbase** package.

```
library(robustbase)

## Find potentially outlying cases:
(out <- boys %$% adjboxStats(bmi, coef = 2)$out)

[1] 11.77 12.56 12.33

## Which observations are potential outliers?
boys %$% which(bmi %in% out)

[1] 2 3 44

## View the potentially outlying cases:
boys %>% filter(bmi %in% out)

  age  hgt  wgt  bmi   hc  gen  phb tv   reg
1 0.038 53.5 3.37 11.77 35.0 <NA> <NA> NA south
2 0.057 50.0 3.14 12.56 35.2 <NA> <NA> NA south
3 0.164 55.0 3.73 12.33 37.8 <NA> <NA> NA  west
```

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

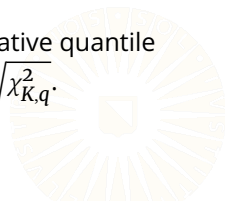
One of the most common distance metrics is the *Mahalanobis Distance*.

- The Mahalanobis distance, Δ , is a multivariate generalization of the z-score method:

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

As with z-scores, if $\Delta_n > C$, we label \mathbf{x}_n as a potential 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: $C = \sqrt{\chi_{K,q}^2}$.



Example

We can compute Mahalanobis distances with `mahalanobis()` .

```
## Compute the squared Mahalanobis distances for height and weight:
md <- boys %>%
  select(hgt, wgt) %>%
  mahalanobis(center = colMeans(., na.rm = TRUE),
              cov = cov(., use = "pairwise")
              )

## Check the first few values:
head(md)
```

	3	4	18	23	28	36
	4.373667	3.642861	4.266050	3.648161	3.270584	3.546730

Example

We compare to some critical χ^2 value to flag potential outliers.

```
out <- md > qchisq(0.999, df = 2)
```

```
which(out)
```

```
5800 6064 6641 7135 7161 7293  
574 610 668 716 720 733
```

```
boys %>% filter(out)
```

	age	hgt	wgt	bmi	hc	gen	phb	tv	reg
1	15.493	182.5	102.0	30.62	57.7	<NA>	<NA>	NA	west
2	16.156	194.3	113.0	29.93	58.4	G3	P5	6	north
3	17.749	174.0	94.9	31.34	56.3	G5	P5	25	west
4	19.290	180.9	94.4	28.84	58.6	<NA>	<NA>	NA	south
5	19.408	192.7	100.1	26.95	58.2	G5	P5	25	east
6	19.926	192.3	117.4	31.74	57.6	G5	P6	18	north

Problems with Mahalanobis Distance

Like the z-score method it generalizes, 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.



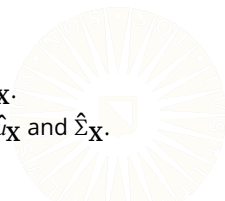
Problems with Mahalanobis Distance

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- 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 $\hat{\Sigma}_{\mathbf{X}}$.



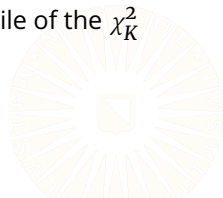
Robust Mahalanobis Distance

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: $C = \sqrt{\chi_{K,q}^2}$.



Example

We can get robust estimates of the sufficient statistics from the

`cov.mcd()` function provided by the **MASS** package.

```
## The MCD method is stochastic, so we should set a seed:
set.seed(235711)

## Compute robust, MCD estimates of the sufficient stats:
stats <- boys %>%
  select(hgt, wgt) %>%
  na.omit() %>% # cov.mcd() won't accept missing values
  MASS::cov.mcd(quantile.used = floor(0.9 * nrow(.)))
```

Example

Now, we can use the robust estimates of location and scale to estimate the Mahalanobis distances.

```
## Compute the robust squared Mahalanobis distances:
```

```
md <- boys %>%  
  select(hgt, wgt) %>%  
  mahalanobis(center = stats$center, cov = stats$cov)
```

```
## Check the first few values:
```

```
head(md)
```

	3	4	18	23	28	36
	4.439179	3.543098	4.277634	3.591591	3.178271	3.488979

Example

We flag potential outliers using the usual method.

```
out <- md > qchisq(0.999, df = 2)
```

```
which(out)
```

```
4646 5585 5602 5710 5800 6040 6064 6566 6641 6686 6693 6724
  441  544  547  560  574  608  610  658  668  671  672  674
6878 6964 7066 7135 7161 7293 7300 7308 7362 7444
  686  695  708  716  720  733  735  736  740  745
```

```
boys %>% filter(out) %>% slice_head(n = 6)
```

	age	hgt	wgt	bmi	hc	gen	phb	tv	reg
1	12.741	172.0	79.5	26.87	55.0	G2	P3	8	south
2	14.967	174.1	88.0	29.03	54.4	G3	P4	10	east
3	15.003	188.0	91.6	25.91	59.8	G4	P4	12	south
4	15.249	188.0	89.0	25.18	56.0	G5	P5	20	west
5	15.493	182.5	102.0	30.62	57.7	<NA>	<NA>	NA	west
6	16.090	180.6	90.4	27.71	58.8	<NA>	<NA>	NA	south

Example

```
boys %>% filter(out) %>% slice_head(n = -6)
```

	age	hgt	wgt	bmi	hc	gen	phb	tv	reg
1	12.741	172.0	79.5	26.87	55.0	G2	P3	8	south
2	14.967	174.1	88.0	29.03	54.4	G3	P4	10	east
3	15.003	188.0	91.6	25.91	59.8	G4	P4	12	south
4	15.249	188.0	89.0	25.18	56.0	G5	P5	20	west
5	15.493	182.5	102.0	30.62	57.7	<NA>	<NA>	NA	west
6	16.090	180.6	90.4	27.71	58.8	<NA>	<NA>	NA	south
7	16.156	194.3	113.0	29.93	58.4	G3	P5	6	north
8	17.555	190.0	97.0	26.86	59.0	<NA>	<NA>	NA	south
9	17.749	174.0	94.9	31.34	56.3	G5	P5	25	west
10	17.911	181.2	86.8	26.43	58.3	G5	P5	15	north
11	17.938	180.3	83.0	25.53	55.4	<NA>	<NA>	NA	west
12	18.039	187.1	87.7	25.05	58.8	<NA>	<NA>	NA	south
13	18.507	193.5	92.0	24.57	59.0	<NA>	<NA>	NA	north
14	18.743	192.0	99.0	26.85	59.5	G5	P6	25	east
15	19.060	180.8	93.8	28.69	55.8	G4	P5	15	south
16	19.290	180.9	94.4	28.84	58.6	<NA>	<NA>	NA	south

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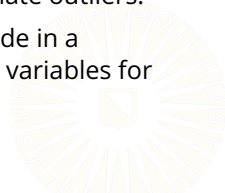
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Maybe check the variables in a single model for multivariate outliers.

- 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.

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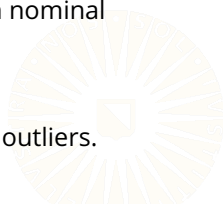
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Binary

- 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.



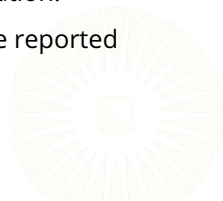
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The most direct solution is to delete any outlying observation.

- 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.

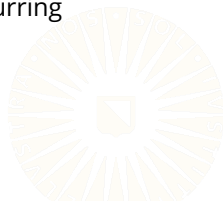
- Delete outlying values (but not the entire observation).
- These empty cells then become missing data.

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



References

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