

Data Cleaning, Data Visualization, & Functions

Fundamental Techniques in Data Science



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Outline

Data Analytic Lifecycle

Data Cleaning

Missing Data

Outliers

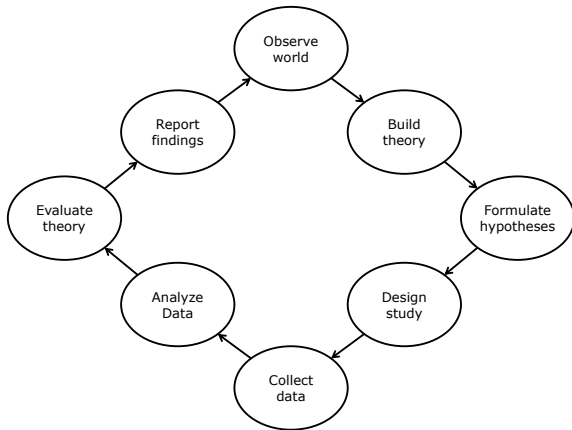


DATA ANALYTIC LIFECYCLE



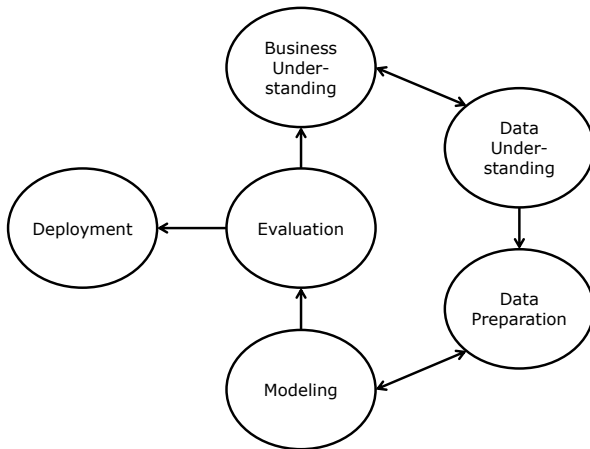
Research Cycle

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.



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

DATA CLEANING



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.



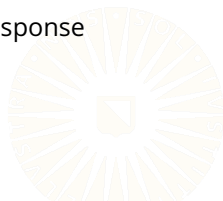
A Little Notation

$Y :=$ 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.



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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



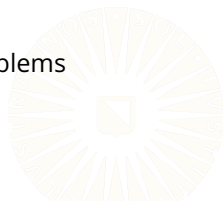
Nonresponse Rates

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

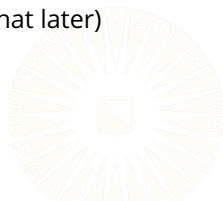
- What is the percent missing at Time 2?
- What is the attrition rate at Time 3?

	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 Tilburg of 50°
 - Annual income of €250,000 for a student
- Not accounting for any particular model (we'll get to that later)

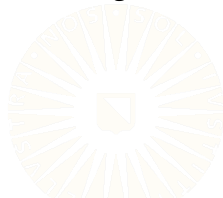


What is an outlier?

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

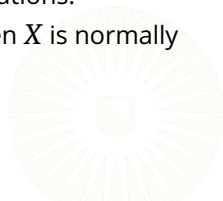
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Although simple, this method has some substantial limitations.

- 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

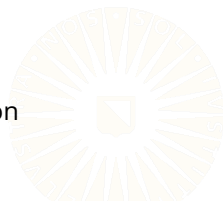
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 - We can do a formal test for “outlier” status.
- Assuming a large sample, if $T_{(n)} > C$ (where C is usually 2 or 3), we label X_n as an outlier.

$T_{(n)}$ 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 $1/N$.

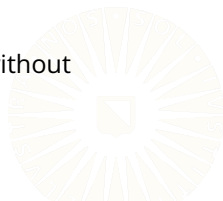
- Replacing a single value with ∞ will produce an infinite mean.

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

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Error in eval(m$data,  
parent.frame()): object 'Salaries'  
not found
```

Boxplot Method

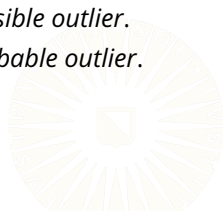
A *fence* is an interval defined as the following function of the *first quartile*, the *third quartile*, and the *inner quartile range* ($IQR = Q_3 - Q_1$):

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

- 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

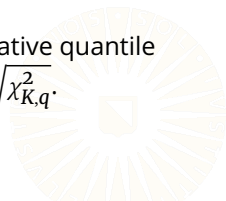
One of the most common distance metrics is the *Mahalanobis Distance*.

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

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

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.



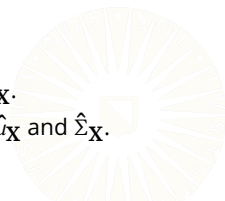
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We want robust analogues of $\hat{\mu}_{\mathbf{X}}$ and $\hat{\Sigma}_{\mathbf{X}}$.

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



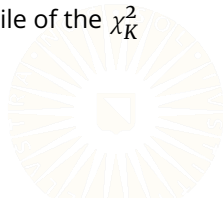
Robust Mahalanobis Distance

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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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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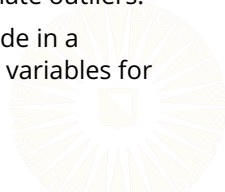
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Do use multivariate outlier checks for scales.

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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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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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Ordinal

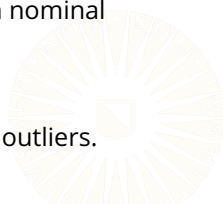
- Most participant endorse one of the lowest categories on an ordinal item, but a few participants endorse the highest category.
- The participants who endorse the highest category may be outliers.

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.



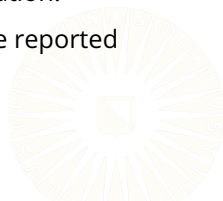
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The most direct solution is to delete any outlying observation.

- 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.

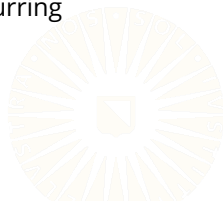
- Delete outlying values (but not the entire observation).
- These empty cells then become missing data.

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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