Understanding Dataset elements of science misbehaviour

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LIG Grenoble – November 2020





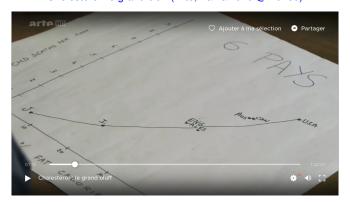
DATA STATISTICS INTRODUCTION

- CAUSALITY: The Question
- 2 DATA SET : A so Simple Object
 - THE PROBLEM: Building of data set
 - SET OF VARIABLES
 - Types of Variables
 - BOLF OF VARIABLES
- 3 THE PROBLEM: The Data Set
 - THE PROBLEM: How data were produced
 - SET OF VARIABLES
 - Missing Values
- A EXPLORATIONS
 - ANALYSIS OF DATASET
 - SAMPLE ANALYSIS
 - CENTRAL TENDENCY
 - VARIABILITY
- 5 SYNTHESIS



A VIVID DEBATE: CHOLESTEROL AND STATINS

Cholesterol: le grand bluff (Arte, 18/10/2016 @ 20h50)





CAUSALITY DATA SET DATA PRODUCTION EXPLORATIONS SYNTHESIS

A VIVID DEBATE: CHOLESTEROL AND STATINS

Cholesterol: le grand bluff (Arte, 18/10/2016 @ 20h50)



"Careful" selection of data and influence from the industry

What happens?



SCIENTIFIC FACTS

Scientific Hypothesis

- A Theory is a contemplative and rational type of abstract or generalizing thinking about a phenomenon, or the results of such thinking (wikipedia)
- Falsifiability is the logical possibility that an assertion can be shown false by an observation or a physical experiment. [Popper 1930]

Observations

Data set produced by an experiment (or a survey)

- Experimental Design (lectures of SMPE) the design is driven by the scientific question
- Existing Data the scientific question is driven by the Dataset



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DATA PRODUCTION

First question: Why this dataset has been produced? (purpose)

- ► Who organized the study?
- ▶ What was the guestion to be answered by the statistical analysis?
- ► Who will be the target of the analysis?



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- Designed survey on a population
- Designed Experiments



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Third question: How this dataset has been practically produced? (observations)

- Nature of the items in the Data set
- Characterization of data
- Semantic of Data

Take time to analyse the production process



ANALYSIS OF THE SET OF VARIABLES

Identification of the variables types

- ► Type of the variables (numbers, identifiers, ...)
- ► Set of values taken by the variables (bounds, sets,...)
- ► Properties of the variables (positive,...)



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- When these variables has been collected?
- Why these variables have been chosen?



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- Why these variables have been chosen?

Identification of the variables semantic

- ▶ What is the interpretation of the variables values? (size, weight, ...)
- ▶ What are the relations between variables (structure)?

Take time to build a serious metadata document



ANALYSIS OF THE TYPE OF VARIABLES

Nominal Variables: classification, membership (qualitative)

- Values in an unstructured set
- Examples : color, gender, ...
- ► Methods : grouping
- \triangleright Operators : =, \neq



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Quantitative Variables: Quantities

- Real values (ratio is significant)
- Examples : amount, duration, cost ...
- Methods : sum, difference
- \triangleright Operators : +, -, (×, /)



Take time to define precisely the variables properties

USAGE OF VARIABLES

Response Variables

- Quantity asked by the question
- Examples : response time, iteration duration, ...



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- Examples : size, load, ...

Univariate or Multivariate

Univariate : one variable is involved

Multivariate : several variables are involved

Take time to identify the response/explanatory variables



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DATA PRODUCTION PROCESS

Global Process

 $\textbf{Question} \Longrightarrow \textbf{Experiment, Survey} \Longrightarrow \textbf{Decision}$

Decision = Risk



DATA PRODUCTION PROCESS

Global Process

Question \Longrightarrow Experiment, Survey \Longrightarrow Decision

Decision = Risk

Quality of Data

Specification of the Data

- Error model for the values
- Experimental/Survey bias
- Analysis limitations

Evaluate the Quality of the Decision



Relevance

- degree to which statistics meet current and potential needs
- could extend to varying needs



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Accuracy

- ▶ Closeness of computations or estimates to the (unknown) exact or true values
- Variability (random error) and bias (systematic error)
- ► Sources of errors (experimental, coverage sampling...)



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Timeliness

- be delay between the reference point and the availability date
- trade-off against accuracy,



Comparability

measuring the impact of differences in applied statistical concepts and measurement tools/procedures when statistics are compared between geographical areas, non-geographical domains, or over time



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Accessibility

- Accessibility refers to the physical conditions under which users can obtain data
- Clarity refers to the data's information environment

Extracted from Handbook on Data Quality Assessment Methods and Tools EuroStat Report (2013)



OTHER CRITERIA FOR THE QUALITY OF DATA (FROM BERTI-EQUILLE (2007))

Interpretability

- availability of the supplementary information and metadata
- covers the underlying concepts

Unicity

- one physical observation is represented by a unique object in the Dataset
- no duplicates

Conformity to Norm

use the standardized encoding (reals, strings, statistical variables)

Consistency

duplicated informations have the same value



PRE-PROCESSING OF DATA

Before any analysis: check the Data

Question on the Quality

- ► Are there missing values? almost yes
- ► How many sampling are missing?
- ls there a bias for missing data or randomly spread?
- ls the bias in the dataset sufficiently important to modify the analysis (estimators, tests,...)?

Give potential explanations



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- ▶ Is the bias in the dataset sufficiently important to modify the analysis (estimators, tests....)?

Give potential explanations

Identification of Data Problems

Model of the Dataset (types, semantic,...)

- Missing Data (none or partial value)
- Non relevant
- Duplicated

Give potential explanations



PRE-PROCESSING OF DATA (2)

Distributions of Data Problems

Analyse the position of missing values in the Dataset

- ► MCAR, Missing Completely at random (unpredictable missing)
- ► MAR, Missing at random (predictable values : model)
- MNAR, Non missing at random



PRE-PROCESSING OF DATA (2)

Distributions of Data Problems

Analyse the position of missing values in the Dataset

- ► MCAR, Missing Completely at random (unpredictable missing)
- MAR, Missing at random (predictable values : model)
- MNAR, Non missing at random

Processing Missing Data

- Do nothing
- Remove samples with missing values
- Weighted analysis
- Value imputation (central tendency, EM, regression, random hot deck, neighbouring,...)

Report the method that has been used

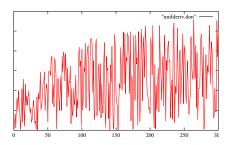


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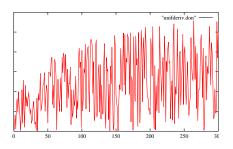


ANALYSIS OF DATASET (1)





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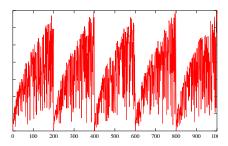
Tendency analysis

non homogeneous experiment

⇒ model the evolution of experiment estimate and compensate tendency explain why



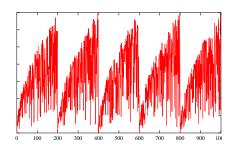
ANALYSIS OF DATASET (2)





CAUSALITY DATA SET DATA PRODUCTION (EXPLORATIONS) SYNTHESIS

ANALYSIS OF DATASET (2)



Periodicity analysis

periodic evolution of the experimental environment?

 \Rightarrow model the evolution of experiment

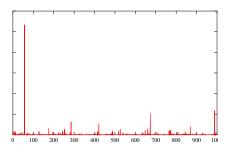
Fourier analysis of the sample

Integration on time (sliding window analysis) Danger: size of the window

Wavelet analysis explain why

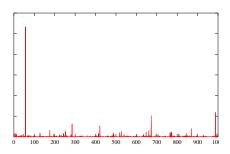


ANALYSIS OF DATASET (3)





ANALYSIS OF DATASET (3)



Non significant values

extraordinary behaviour of experimental environment

rare events with different orders of magnitude

 \Rightarrow threshold by value

Danger: choice of the threshold: indicate the rejection rate

 $\Rightarrow \text{threshold by quantile}$

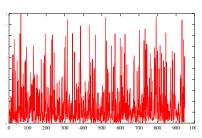
Danger: choice of the percentage: indicate the rejection value

explain why

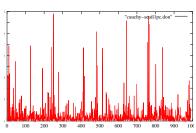


ANALYSIS OF DATASET (4)

Threshold value: 10



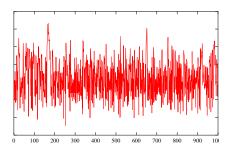
Threshold percentage: 1%





CAUSALITY DATA SET DATA PRODUCTION (EXPLORATIONS) SYNTHESIS

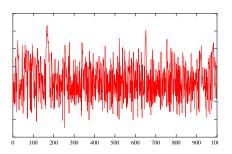
ANALYSIS OF DATASET (5)





CAUSALITY DATA SET DATA PRODUCTION (EXPLORATIONS) SYNTHESIS

ANALYSIS OF DATASET (5)



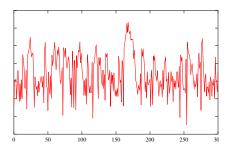
looks like correct experiments

Statistically independent Statistically homogeneous



ANALYSIS OF DATASET (5BIS)

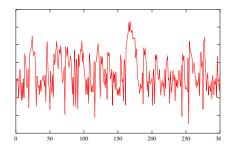
Zooming





ANALYSIS OF DATASET (5BIS)

Zooming



Autocorrelation

Danger time correlation among samples experiments impact on experiments ⇒ stationarity analysis autocorrelation estimation (ARMA)



EXPERIMENTAL RESULTS

After a campain of experiment/surveys

- ► Deterministic (controlled error non significant (white noise))
- ► Statistic (the system is non deterministic)

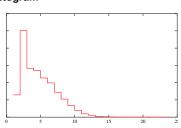
Sample analysis

- ► Identification of the response set
- Structure of the response set (measure)



DISTRIBUTION ANALYSIS

Summarize data in a histogram

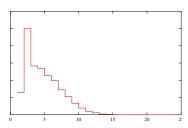


Shape analysis

- ▶ unimodal / multimodal
- variability
- symmetric / dissymmetric (skewness)
- ► flatness (kurtosis)
- **⇒** Central tendency analysis
- ⇒ Variability analysis around the central tendency



MODE VALUE



Mode

- Categorical data
- Most frequent value
- ► highly unstable value
- ▶ for continuous value distribution depends on the histogram step
- ▶ interpretation depends on the flatness of the histogram
- ⇒ Use it carefully
- ⇒ Predictor function



MEDIAN VALUE

Median

- Ordered data
- ► Split the sample in two equal parts

$$\sum_{i \leqslant \textit{Median}} f_i \leqslant \frac{1}{2} \leqslant \sum_{i \leqslant \textit{Median}+1} f_i.$$

- ► more stable value
- does not depends on the histogram step
- ► difficult to combine (two samples)
- ⇒ Randomized algorithms



MEAN VALUE

Mean

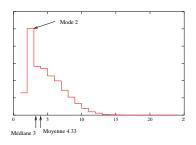
- ► Vector space
- Average of values

$$\textit{Mean} = \frac{1}{\textit{Sample_Size}} \sum x_i = \sum_x x.f_x.$$

- ► stable value
- ▶ does not depends on the histogram step
- ► easy to combine (two samples ⇒ weighted mean)
- ⇒ Additive problems (cost, durations, length,...)



CENTRAL TENDENCY



Complementarity

- ► Valid if the sample is "Well-formed"
- ► Semantic of the observation
- ► Goal of analysis
- ⇒ Additive problems (cost, durations, length,...)



CENTRAL TENDENCY (2)

Summary of Means

- Avoid means if possible Loses information
- Arithmetic mean
 When sum of raw values has physical meaning
 Use for summarizing times (not rates)
- ► Harmonic mean
 Use for summarizing rates (not times)
- Geometric mean
 Not useful when time is best measure of perf Useful when multiplicative effects are in play



VARIABILITY

Categorical data (finite set)

 f_i : empirical frequency of element i Empirical entropy

$$H(f) = \sum_{i} f_i \log f_i.$$

Measure the empirical distance with the uniform distribution

- $ightharpoonup H(f) \geqslant 0$
- ightharpoonup H(f) = 0 iff the observations are reduced to a unique value
- \blacktriangleright H(f) is maximal for the uniform distribution



VARIABILITY (2)

Ordered data

Quantiles: quartiles, deciles, etc

Sort the sample:

$$(x_1, x_2, \cdots, x_n) \longrightarrow (x_{(1)}, x_{(2)}, \cdots, x_{(n)});$$

 $Q_1 = x_{(n/4)}; \ Q_2 = x_{(n/2)} = Median; \ Q_3 = x_{(3n/4)}.$

For deciles

$$d_i = argmax_i \{ \sum_{i \le i} f_i \leqslant \frac{i}{10} \}.$$

Utilization as quantile/quantile plots to compare distributions



VARIABILITY (3)

Vectorial data

Quadratic error for the mean

$$Var(X) = \frac{1}{n} \sum_{1}^{n} (x_i - \bar{x}_n)^2.$$

Properties:

$$Var(X) \geqslant 0;$$

 $Var(X) = \overline{x^2} - (\overline{x})^2, \text{ où } \overline{x^2} = \frac{1}{n} \sum_{i=1}^n x_i^2.$
 $Var(X + cste) = Var(X);$
 $Var(\lambda X) = \lambda^2 Var(X).$



PRE-PROCESSING OF DATA (3)

Variability Model of Data

Analyse the variability of the variables Establish an hypothesis for the variability

- ► Deterministic properties
- ► Gaussian noise (parametric approach)
- Quantiles (non-parametric approach)



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Analysis of Outliers

Assumption : the outliers of the observed phenomena are not frequent

- Do nothing
- Remove outliers
- Weighted analysis
- ▶ Value imputation (central tendency, EM, regression, random hot deck, neighbouring,...)

Report the method that has been used

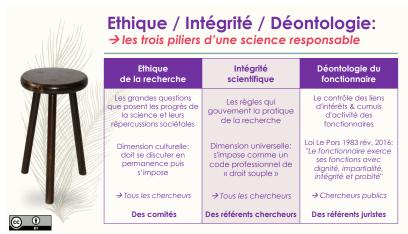


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TO GO FURTHER



by Olivier Le Gall Inra Bordeaux

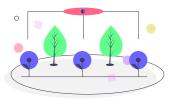


REFERENCES



Vers une recherche reproductible

Faire évoluer ses pratiques



Loïc Desquilbet, Sabrina Granger, Boris Hejblum, Arnaud Legrand, Pascal Pernot, Nicolas Rougier

