Master Program in *Data Science and Business Informatics*

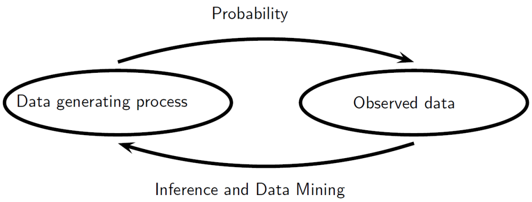
Statistics for Data Science

Lesson 16 - Numerical summaries

Salvatore Ruggieri

Department of Computer Science
University of Pisa, Italy
salvatore.ruggieri@unipi.it

Condensed observations: numerical summaries



- Probability models governs some random phenomena
- Confronted with a new phenomenon, we want to learn about the randomness associated with it
  - Parametric (efficient) vs non-parameteric (general) methods
- Record observations $x_1, \ldots, x_n$ (a dataset)
- n can be large: need to condense for easy comprehension and processing
- Numerical summaries:
  - Univariate: sample/empirical mean, median, standard deviation, quantiles, MAD
  - Multi-variate: Pearson's, Spearman's, Kendall's correlation coefficients

Sample summaries

Main idea (plug-in method): translate summaries of empirical distribution (sample) F_n to estimate summaries of the generating distribution F

- Measures of centrality
  - *Sample mean*:

$$\bar{x}_n = \frac{x_1 + \ldots + x_n}{n} \qquad\qquad E[X],\ \mu$$

  - *Median* for sorted $x_1, \ldots, x_n$:

$$Med(x_1, \ldots, x_n) = \begin{cases} x_{\frac{n}{2}+1} & \text{if } n \text{ is odd} \\ (x_{\frac{n}{2}} + x_{\frac{n}{2}+1})/2 & \text{if } n \text{ is even} \end{cases} \qquad\qquad F^{-1}(0.5)$$

    E.g., $Med(2,3,4) = 3$ and $Med(2,3,4,5) = 3.5$

Measures of variability

- *Sample variance*:

$$s_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x}_n)^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} x_i^2 - n \cdot \bar{x}_n^2\right) \qquad Var(X),\ \sigma^2$$

  Divide by $n-1$ for a sample, and by n for a population! *[Bessel's correction]*

- *Sample standard deviation*:

$$s_n = \sqrt{s_n^2} \qquad \sqrt{Var(X)},\ \sigma$$

- Median of absolute deviations (MAD):

$$MAD(x_1, \ldots, x_n) = Med(|x_1 - Med(x_1, \ldots, x_n)|, \ldots, |x_n - Med(x_1, \ldots, x_n)|)$$

  - For $X \sim F$, the population MAD is $Md = G^{-1}(0.5)$ where $|X - F^{-1}(0.5)| \sim G$
  - For F symmetric, $Md = F^{-1}(0.75) - F^{-1}(0.5)$.
  - Md is a more robust-to-outlier measure of scale than standard deviation

Order statistics and empirical quantiles

- Let $x_{\langle 1\rangle}, \ldots, x_{\langle n\rangle}$ be `sort`$(x_1, \ldots, x_n)$. We call $x_{\langle i\rangle}$ the i-th order statistics.
  - The order statistics consist of the same elements in the dataset, but in ascending order
- Distribution quantiles $q_p = \inf_x\{P(X \leq x) \geq p\} = \inf_x\{F(x) \geq p\}$ *[See Lesson 08]*
- Empirical quantiles: $q(p) = \inf_x\{F_n(x) \geq p\} = \inf_x\{|\{i \mid x_i \leq x\}|/n \geq p\}$
  - Type 6 (book [T]): for $p = i/(n+1)$ *[There are 9 variants, see `help(quantile)`]*

$$q(p) = x_{\langle p\cdot(n+1)\rangle} = x_{\langle i\rangle}$$

    - E.g., for $2, 3, 4, 5, 6$, $q(.167) = 2$, $q(.333) = 3$, $q(0.5) = 4$, $q(0.667) = 5$, $q(.833) = 6$
  - Type 7 (default in `R`): for $p = (i-1)/(n-1)$

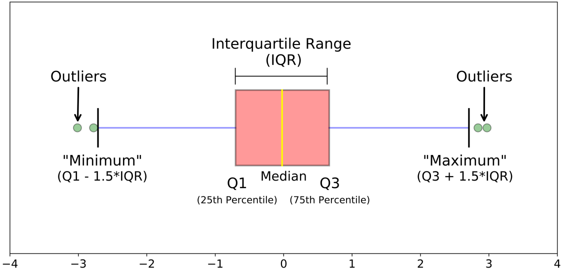
$$q(p) = x_{\langle p\cdot(n-1)+1\rangle} = x_{\langle i\rangle}$$

    - E.g., for $2, 3, 4, 5, 6$, $q(0) = 2$, $q(0.25) = 3$, $q(0.5) = 4$, $q(0.75) = 5$, $q(1) = 6$
- What is $q(p)$ when $p \cdot (n+1)$ is not an integer?

$$q(p) = x_{\langle k\rangle} + \alpha(x_{\langle k+1\rangle} - x_{\langle k\rangle})$$

where $k = \lfloor p \cdot (n+1)\rfloor$ and $\alpha = p \cdot (n+1) - k$ (remainder)

The box-and-whisker plot

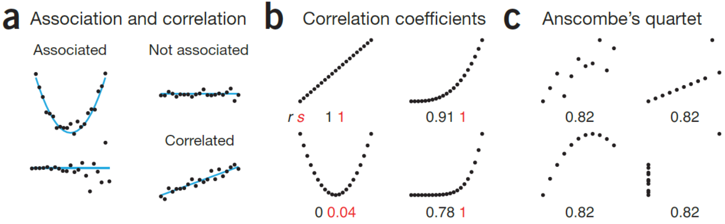


- Axis here is with reference to a standard Normal distribution
- **See John Tukey** (designed FFT, coined 'bit' & 'software', and visionary of **data science**)

See R script

Association and correlation

- Bivariate analysis of joint distribution of X and Y or of a sample $(x_1, y_1), \ldots, (x_n, y_n)$
- *Association*: one variable provides information on the other
  - $X \perp\!\!\!\perp Y$ independent, i.e., $P(X|Y) = P(X)$: zero information
  - $Y = f(X)$ deterministic association with f invertible: maximum information
- *Correlation*: the two variables show an increasing/decreasing trend
  - $X \perp\!\!\!\perp Y$ implies $Cov(X, Y) = 0$
  - the converse is not always true
- *Coefficient or measure of association/correlation*: determine the strength of association/correlation between two variables and the direction of the relationship



Measures of association

	Variable X		
Variable Y	Nominal	Ordinal	Continuous
Nominal	φ or λ	Rank biserial	Point biserial
Ordinal	Rank biserial	τ_b or Spearman	τ_b or Spearman
Continuous	Point biserial	τ_b or Spearman	Pearson or Spearman

φ = phi coefficient, λ = Goodman and Kruskal's lambda, τ_b = Kendall's τ_b.

- Dimension: level of measurement
  - Ordinal: discrete but ordered, e.g., 0, 1, 2 for "low", "medium", "severe" risks
  - Nominal: discrete without any order, e.g., 0, 1, 2 for "bus", "car", "train" transportation
- See [Khamis, 2008] for a guide to the selection
- See [Berry et al., 2018] for extensive introduction
- See **mhahsler.github.io** for a list of measures in association rule mining $X \Rightarrow Y$

Linear correlation of continuous r.v.: Pearson's r

- Bivariate analysis of joint distribution of X and Y or of a sample $(x_1, y_1), \ldots, (x_n, y_n)$
- Sample covariance:

$$s_{xy} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y}) \qquad\qquad Cov(X, Y) = E[(X - \mu_X) \cdot (Y - \mu_Y)]$$

- Apply plug-in method to correlation between X and Y:

$$\rho = \frac{Cov(X, Y)}{\sqrt{Var(X) \cdot Var(Y)}} = \frac{E[(X - \mu_X) \cdot (Y - \mu_Y)]}{\sigma_X \cdot \sigma_Y}$$

- Pearson's (linear/product-moment) correlation coefficient:

$$r = \frac{s_{xy}}{s_x \cdot s_y} = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2 \cdot \sum_{i=1}^{n} (y_i - \bar{y})^2}}$$

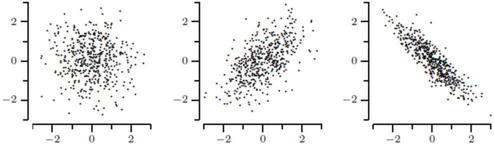
- Support in $[-1, 1]$ due to Schwarz's inequality: $|s_{xy}| \leq s_x \cdot s_y$
- Computational cost is $O(n)$

Linear correlation of continuous r.v.: Pearson's r

$$\rho = \frac{Cov(X,Y)}{\sqrt{Var(X)\cdot Var(Y)}} = \frac{E[(X-\mu_X)\cdot(Y-\mu_Y)]}{\sigma_X \cdot \sigma_Y}$$

- Pearson's (linear/product-moment) correlation coefficient: *[support in $[-1,1]$]*

$$r = \frac{s_{xy}}{s_x \cdot s_y} = \frac{\sum_{i=1}^{n}(x_i-\bar{x})\cdot(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2\cdot\sum_{i=1}^{n}(y_i-\bar{y})^2}}$$



Uncorrelated **Positively correlated** **Negatively correlated**

r	Interpretation of Linear Relationship
0.8	Strong positive
0.5	Moderate positive
0.2	Weak positive
0.0	No relationship
–0.2	Weak negative
–0.5	Moderate negative
–0.8	Strong negative

Rank correlation of continuous/ordinal r.v.: Spearman's ρ

- Pearsons's r asseses *linear relationships* over continuous values
- Let $rank(x)$ be the ranks of x_i's
  - For $x = 7, 3, 5$, $rank(x) = 3, 1, 2$
- Spearman's correlation coefficient is the Pearson's coefficient over the ranks:

$$\rho = r(rank(x), rank(y)) \qquad \frac{Cov(rank(X), rank(Y))}{\sqrt{Var(rank(X)) \cdot Var(rank(Y))}}$$

  - In case of no ties in x and y:

$$\rho = 1 - \frac{6 \sum_{i=1}^{n} (rank(x)_i - rank(y)_i)^2}{n \cdot (n^2 - 1)}$$

- Spearman's correlation assesses monotonic relationships (whether linear or not)
- Computational cost is $O(n \cdot \log n)$

Rank correlation of continuous/ordinal r.v.: Kendall's τ

- Spearman's applies when Y (or also X) is ordinal
  - Association between age and fraction of exams passed (“0-5”, “6-10”, “11-15”, “+15”)
- Kendall's τ_a is another (more robust) rank measure: *[support in $[-1, 1]$]*

$$\tau_{xy} = \frac{2 \sum_{i<j} sgn(x_i - x_j) \cdot sgn(y_i - y_j)}{n \cdot (n-1)} \qquad E_{X_1, X_2 \sim F_X, Y_1, Y_2 \sim F_Y}[sgn(X_1 - X_2) \cdot sgn(Y_1 - Y_2)]$$

  Fraction of concordant pairs minus discordant pairs, i.e., probability of observing a difference between concordant and discordant pairs.

- Correction τ_b accounting for ties, i.e., $x_i = x_j$ or $y_i = y_j$ *[implemented by `cor` in R]*
  - Correction to divide by the number of pairs for which $sgn(x_i - x_j) \cdot sgn(y_i - y_j) \neq 0$
- Computational cost is $O(n^2)$

See R script

Rank correlation of continuous and binary r.v.: Somers' D

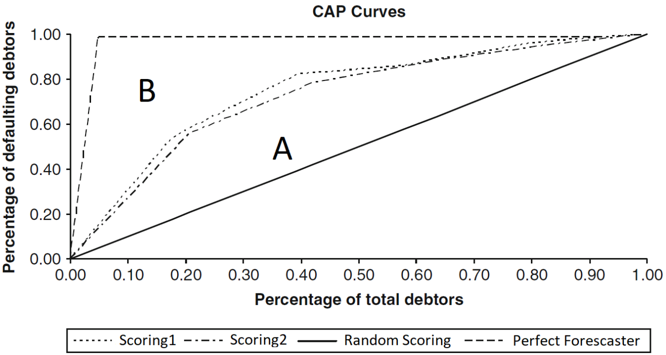
- X continuous and Y binary.
- An asymmetric Kendall's:

$$D = \frac{\tau_{xy}}{\tau_{yy}} = \frac{\sum_{i<j} sgn(x_i - x_j) \cdot sgn(y_i - y_j)}{\sum_{i<j} sgn(y_i - y_j)^2}$$

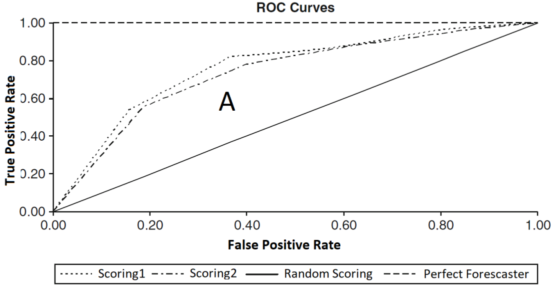
  i.e., fraction of concordand pairs minus discordant pairs conditional to unequal values of y
- Example with probabilistic classifiers
  - $x =$ positive prediction confidence, i.e., `predict_proba(...)[,1]` in Python
  - y true class
  - D is the Gini index of classifier performances
  - related to AUC of ROC curve:

$$D = 2 \cdot AUC - 1 \qquad AUC = \frac{D}{2} + 0.5 = \frac{\tau_{xy}}{2 \cdot \tau_{yy}} + 0.5$$

See R script



$$Gini = D = A/(A + B)$$



$$AUC = A + 1/2$$

Association between nominal variables: Thiel's U

- Recall from Lesson 11

Mutual information and NMI

$$I(X,Y) = \sum_{a,b} p_{XY}(a,b) \log \frac{p_{XY}(a,b)}{p_X(a)p_Y(b)} \qquad NMI = \frac{I(X,Y)}{\min\{H(X),H(Y)\}} \in [0,1]$$

- Uncertainty coefficient (also called entropy coefficient or Thiel's U) :

$$U_{sym} = \frac{I(X,Y)}{(H(X)+H(Y))/2} \qquad U_{asym} = \frac{I(X,Y)}{H(X)}$$

where p_{XY} is the *empirical joint p.m.f.*, and p_X, p_Y are *the empirical marginal p.m.f.'s*

- U_{asym} what fraction of X can be predicted by Y

Association between nominal variables: χ^2-based

- Several other measures based on Pearson χ^2 (introduced later)
  - Contingency coefficient C
  - Cramer's V
  - ϕ coefficient (or MCC, Matthews correlation coefficient)
  - Tschuprov's T
  - ...

See R script

Optional references

Harry Khamis (2008)
Measures of Association: How to Choose?
J. of Diagnostic Medical Sonography, Vol. 24, Issue 3, pages 155–162.

Kenneth J. Berry, Janis E. JohnstonPaul, and W. Mielke, Jr. (2018)
The Measurement of Association: A Permutation Statistical Approach.
Springer.