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Missing Data: Empirical Comparison between Imputation and Nearest Neighbors Algorithms

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To the *R* community and *ESS* developers for their contribution.

Abstract

Incomplete or missing data are common in scientific works, and the most common solution to cope with them is the simply to discard them. However, this might lead to bias in the conclusion. This semester paper summaries modern methods and offers an empirical comparison of the packages *amelia*, *imputeknn*, *mi*, *mice*, *softimpute* with the statistical software R.

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Notation

Explain your symbols and abbreviations.

Chapter 1

Theoretical Background

This chapter provides an overview and an intuition on the field of missing data. It follows mainly Schafer and Graham (2002), Little and Rubin (2002), Van Buuren (2012), with some impute from Wikipedia (2015), Matloff (2015), Gelman and Hill (2006), Troyanskaya, Cantor, Sherlock, Brown, Hastie, Tibshirani, Botstein, and Altman (2001).

This chapter begins with a short description on the nature missingness, then describes several procedures in order to handle missing data.

1.1 Mechanism of missingness

Van Buuren (2012) describes two concepts helping us to understand how to solve the problem of missing data: intentional and unintentional missingness, as well as unit and item missingness. The experimenter can decide to not measures all possible variable in an experiment and encode his decisions as missing observations. This is a reasonable decision if the cost of measuring variables is material and unnecessary for some experimental case, such as in medical experimentation. However, it might also happen that the experimenter could not measure some variable, e.g. when a respondent to a survey refuse to answer to some question. In this case, the missingness is named unintentional. The second concept is often missingness is about unit and items: one says a unit is missing when none of the variables of interest could be measured, whereas item refers to some variable missing.

In order to complete missing data, assumptions need to be taken about the underlying mechanism creating missing observations: missing completely at random (MCAR), missing at random (MAR) and missing not at random (MNAR).

Notation Let $Y \in \mathbb{R}^{n \times p}$ be the data matrix containing missing data for n observations with p variables, $R = (r_{ij})_{i=1,j=1}^{n,p} \in \{0,1\}^{n \times p}$ denotes the response y_{ij} (i.e. $r_{ij} = 1$ is y_{ij} is observed, and is 0 otherwise). Y_{obs} and Y_{mis} denote the observation that is observed, respectively, missing, such that $Y = (Y_{obs}, Y_{mis})$. Note that we always observed R whereas we usually do not have Y_{mis}.

MCAR The data are said to be *MCAR* if

$$P(R = 0 \mid Y_{obs}, Y_{mis}) = P(R = 0),$$

or equivalently

$$P(Y = y \mid R = i) = P(Y = y),\ i \in \{0, 1\},\ y \in \mathbb{R}^{n \times p}.$$

It means the probability of being missing depends does not depends on the actual value of Y.

MAR For multiple imputation, one requires only $R \perp Y_{mis}$, that is

$$P(R = 0 \mid Y_{obs}, Y_{mis}) = P(R = 0 \mid Y_{obs}),$$

that is other observed variables impact of the probability of missingness but the missing mechanism only depends on the observed variables and not the actual missing value. In this case, we say the data Y are *MAR*.

MNAR The data are MNAR if

$$P(R = 0 \mid Y_{obs}, Y_{mis})$$

can not be simplified. It essentially means that the rate of response depends on the actual value of the missing observations. The standard example is the survey about salary where people with extremely high salary tends to hide their earnings.

Modern statistical technique can handle MNAR and MAR cases, whereas simple technique only MCAR, which is quite restrictive.

1.2 Statistical completion

Complete case analysis Unfortunately, One of the most used technique to cope with missing data: the researcher only keeps observation that are complete. This might lead to valid analysis, as the method does not introduce any bias if the missing values are uniformly distributed. Nevertheless, this methodology can not work in modern settings where the probability of one missing variable is quite high: Many data points would be discarded.

Pairwise deletion This methods improve from the previous one by deleting observations only if the variable which is missing must be used in the model. This is typically relevant for computing correlation for example, although some care must be taken in this case.

Single imputation The data matrix is sorted according to some order, *last observation carried forward* is the method of replacing the missing value with last valid value. The missing value can also be replaced with the mean of the other observations, however, correlations are attenuated. Regression imputation use the other variables as predictors to replace the missing value, although precision is misleadingly augmented, hence does not reflect the statistical errors of the missing data. This problem is partially solved by multiple imputation.

Multiple imputation Under the MAR assumption, the multiple imputation (MI) is similar to bootstrapping method: the distribution of each variable conditional and the others is fitted, then in case of missing value, a sample is drawn from this distribution. The desired statistics are averaged except for the standard error which is constructed by adding the variance of the imputed data and the within variance of each data set. The last step solves the problem of understating uncertainty. Standard errors reflect missing-data uncertainty and finite-sample variation.

More precisely, in the one-dimensional case, if the sample is large enough so that the estimator Q follows a Gaussian distribution, then the estimate $\hat{Q}$ and the standard error T can be computed from the estimates of $(Q^j, U^j)_{j=1}^m$, Q^j, respectively, U^j being the fitted value of Q, respectively the standard error, for data sets j:

$$\begin{aligned}
\hat{Q} &= m^{-1} \sum_{j=1}^{m} Q^j, \\
\hat{U} &= m^{-1} \sum_{j=1}^{m} U^j, \\
B &= (m-1)^{-1} \sum_{j=1}^{m} (Q^j - \hat{Q})^2, \\
T &= \hat{U} + (1 + m^{-1})B.
\end{aligned}$$

For confidence interval, the Student's t approximation can be used with the degree of freedom given by

$$\nu = (m-1)\Big[1 + \frac{\hat{U}}{(1+m^{-1})B}\Big]^2.$$

The estimated rate of missing information for Q is approximately $\tau/(\tau+1)$ where $\tau = (1+m^{-1})B/\hat{U}$, the relative increase in variance due to non-response. See Schafer (1997) for more cases.

An advantage of MI is the number of need imputation: the efficiency based on m samples relative o an infinite number is $(1+\lambda/m)^{-1}$, where λ is the rate of missing information, which measures the increase in the large-sample variance of a parameter estimate due to missing values. $m = 20$ is often good in practice.

Obviously, the missing values problem is dealt before the analysis with MI, in contrast with maximum likelihood estimation. The danger from MI is the ability to use different models for imputation and analysis, which might lead to inconsistency.

1.3 Algorithmic completion

Singular value decomposition

Soft-impute completion

K-nearest neighbors completion Finally, one should not forget why these technique exists:

> With or without missing data, the goal of a statistical procedure should be to make valid and efficient inferences about a population of interest – not to estimate, predict, or recover missing observations nor to obtain the same results that we would have seen with complete data. Schafer and Graham (2002)

Chapter 2

Empirical Comparison of Imputation Methods

2.1 Data set and imputation methods

2.2 Methodology

Let $\mathcal{M}$ denote the set of imputation methods and let $Y \in \mathbb{R}^{n \times p}$ be a complete data matrix.

2.2.1 Simulation of missingness

Two types of missing were implemented: MCAR and MAR. The former is quit straightforward to implement: For a given missingness rate $p \in (0, 1)$, the response[1] r_{ij} of the value Y_{ij} follows a binomial distribution with probability p. Implementation of MAR usually make assumptions on the underlying multivariate distribution is a little more involved. Nevertheless, a mechanism based of the empirical distribution of the missingnes pattern can also been used.

The original data set contained pattern of missingness and for a missing rate q, one could sample the patterns from it with the multinomial distribution until the desired rate q is reached. The patterns are then randomly assigned to our completed data set. This method has the disadvantage that it can not attain any missingness rate $q \in (0, 1)$, as one can only assign one pattern per observation.

For our study, it implies that for the MAR method, only data set with a missingness rate below 30% were analyzed.

2.2.2 Ranking methods

For a simulated data matrix Y^l with values y_{ij}, $i \in \{1, \dots, n\}$, $j \in \{1, \dots, p\}$ and for an imputation method $m \in \mathcal{M}$ with predicted values $\hat{y}_{ij}$ if y_{ij} is missing, the scaled mean

[1] Recall that r_{ij} is 0 if y_{ij} is missing and 1 otherwise.

squared error (SMSE)

$$\text{SMSE}_{l,j}^{m} = \Big\{ \sum_{i=1}^{n} 1(r_{ij} = 1) \Big\}^{-1} \sum_{i=1}^{n} \frac{(\hat{y}_{ij} - y_{ij})^2}{\mu_j} \cdot 1(r_{ij} = 0),$$

where $\mu_j = n^{-1} \sum_{i=1}^{n} Y_{ij}$, is used to assess the quality of imputation methods. To aggregate it across the columns of the data matrix, for each column, the methods are ranked by SMSE, then thes ranks are summed by imputation method. More precisely, the score s_l^m of the imputation methods m

$$s_l^m = \sum_{j=1}^{p} \sum_{\nu \in \mathcal{M}} 1(\text{SMSE}_{l,j}^{m} \leq \text{SMSE}_{l,j}^{\nu}) \tag{2.1}$$

The scores s_l^m are then used to assess the performance of the imputation methods.

2.3 Implementation constraints

Nearest neighbors imputation It appears that the `impute.knn` method from the `impute` package from the *bioconductor* repository causes *segmentation fault* (with the underlying FORTRAN code) when the number of neighbors is either to high with respect to the available data.

Colinear dimensions If the data matrix Y has colinear variables, then some challenges might occur when variables are colinear. More precisely, although multiple imputation techniques try to estimate

$$Y_j \mid Y_{k_1}, \ldots, Y_{k_j},$$

using regression models, their results might be unstable if Y_{k_i}, $i \in \{1, \ldots, k_j\}$ are linearly dependent. Said differently, as regression parameters depends on the quality of the inversion the data matrix, but a matrix with colinear columns has an unstable inverse[2]. The `Amelia` package is the most prone to this issue, although `MICE` and `mi` algorithms fail to converge at some point when Y_{k_i} exhibit high colinearity.

Timing Usually, CPU time, i.e. time spent by the processor on the *R* process, is measured to evaluate the speed performance. Nonetheless, a trend has emerged for packages implement pretty good parallelism, i.e. packages implement the parallelism procedures themselves. It leads to underestimated human elapsed time as most of the computational burden is performed by sub-process.

Tuning parameters For the packages `softImpute` and `impute`, some defaults parameters for the imputation methods are provided. For the `impute.knn` function, the quality of the inference grows with the number of neighbors. The `softImpute` function unexpectedly has offers good default parameters, even if some restrain should be kept when the missing rate is high.

[2] The matrix is so-called *ill conditioned*.

2.4 Results

`softImpute` and `MICE` were the only package able to cope with a quite high missing rate ($p \geq 0.7$).

`impute.knn` from the `impute` package, when it works, is almost always the method with the best score (as defined in Equation (2.1)).

`MICE` offers a good balance between speed, robustness and quality of imputations, but the methods depends on the linear dependence of the columns of the data matrix.

Although `softImpute` can cope with almost any type of data matrix, its inferences are subpar with the other methods. Some further analysis might be needed to confirm this results.

`Amelia` is the package which is the least able to cope with a random impute matrix: routines failed without exception with any missing rate above $p \geq 0.3$.

The `Amelia` and `mi` packages use by default parallel backends to perform their computations. However, they are the slowest methods in terms of elapsed time. This might be overcome by setting the number of iteration to a lower threshold. Nonetheless, this is not recommended as convergence is not guaranteed with data with dimensions having a strong linear dependence.

2.5 Open questions

Heuristically, the quality of models output normally depends on the amount of available data. In the missing data framework, precision are needed for this notion: Is it the number of complete observations, the number of non-missing values, or a mixture of both? Interactions between the number of observation n, the number of dimensions p and imputation methods with their optimal parameters are left unanswered with this work. In order to answer this question, a multivariate sampling mechanism should be devised and tested.

Moreover, are there any reasonable solutions which can be applied to overcome colinearity? One could cluster the similar dimension and then pick one randomly to create an imputed value. Nevertheless, such solutions were not yet implemented.

Additionally, this small simulation study has been applied to certain data set and it should be interesting to repeat the experience with other real data.

Finally, the concern of this work has been to apply imputation methods to retrieve potential candidate values for inference, it would have been interesting to verify the quality of inferences performed with the imputed data set, for example multiple imputation against nearest neighbors.

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