How to impute missing values?

Genevieve Robin, Aude Sportisse 08 August 2019

Contents

| softImpute | 2 |
|--------------|---|
| mice | 4 |
| Session info | 5 |
| References | 6 |

If you have a dataset which contains missing values, it is relevant to impute the missing values, mainly for two reasons: (i) these values may be particularly interesting in themselves or (ii) the fully completed data is required to perform some estimation method that does not handle the missing data.

In this section we provide, for some of the main packages (the list is of course not thorough) to impute missing values, links to vignettes and tutorials, as well as a description of their main functionalities and reusable code. The goal is not to describe all the methods precisely, as many resources are already available, but rather to provide an overview of several imputation options. The methods we focus on are gathered in the table below.

| | | | | Computational | |
|--------------------------|----------------------------|--|-----------------|---------------|--|
| Package | Data Types | Underlying Method | Imputation | Time | Comments |
| Amelia | quantitative and binary | multivariate gaussian model | multiple | + | Binary variables modeled as Gaussians |
| mice | mixed | multivariate imputation by chained equations | multiple | - | Very flexible to data types, no parameter to tune |
| missForest | mixed | random forests | single | - | Requires large sample sizes, no parameter to tune |
| $\operatorname{missMDA}$ | mixed | component methods | single/multiple | + | Rank parameter to tune |
| softImpute | quantitative | low-rank matrix completion | single | + | Very fast, strong theoretical guarantees, regularization parameter to tune |

library(Amelia)

library(mice)

library(missForest)

```
library(missMDA)
library(softImpute)
```

Consider the Los Angeles ozone pollution data in 1976, available in R using the function data.

This dataset already contains some missing values.

```
##
        max03
                             T9
                                             T12
                                                               T15
##
    Min.
            : 42.00
                      Min.
                              :11.30
                                        Min.
                                                :14.00
                                                         Min.
                                                                 :14.90
    1st Qu.: 70.00
                       1st Qu.:16.20
                                        1st Qu.:18.48
                                                         1st Qu.:19.10
##
    Median: 81.00
                      Median :18.10
                                        Median :20.30
                                                         Median :22.10
##
    Mean
            : 89.89
                      Mean
                              :18.45
                                        Mean
                                                :21.38
                                                         Mean
                                                                 :22.75
##
    3rd Qu.:107.00
                       3rd Qu.:20.05
                                        3rd Qu.:23.73
                                                         3rd Qu.:26.00
##
            :166.00
                              :27.00
                                                :32.70
                                                                 :33.70
    Max.
                                        Max.
                                                         Max.
                      Max.
##
    NA's
            :13
                       NA's
                              :9
                                        NA's
                                                :16
                                                         NA's
                                                                 :19
##
                                            Ne15
         Ne9
                                                              Vx9
                           Ne12
##
    Min.
            :0.000
                     Min.
                             :0.000
                                       Min.
                                               :0.000
                                                        Min.
                                                                :-6.5778
##
    1st Qu.:3.000
                     1st Qu.:4.000
                                       1st Qu.:3.000
                                                        1st Qu.:-3.4015
##
    Median :6.000
                     Median :5.000
                                       Median :5.000
                                                        Median :-0.9040
##
            :4.887
                             :5.119
                                               :4.889
    Mean
                     Mean
                                       Mean
                                                        Mean
                                                                :-1.2315
##
    3rd Qu.:7.000
                     3rd Qu.:7.000
                                       3rd Qu.:7.000
                                                        3rd Qu.: 0.6919
##
    Max.
            :8.000
                     Max.
                             :8.000
                                       Max.
                                               :8.000
                                                        Max.
                                                                : 5.1962
##
    NA's
            :6
                     NA's
                             :11
                                       NA's
                                               :13
                                                        NA's
                                                                :6
##
         Vx12
                             Vx15
                                              max03v
                                                                vent
                                                                           pluie
##
            :-7.8785
                               :-9.000
                                                  : 42.00
                                                                  : 9
                                                                         Pluie:41
    Min.
                       Min.
                                          Min.
                                                             Est
##
    1st Qu.:-3.6941
                       1st Qu.:-3.939
                                          1st Qu.: 70.50
                                                             Nord:29
                                                                         Sec :63
##
    Median :-1.9039
                       Median :-1.830
                                          Median: 81.00
                                                                         NA's : 8
                                                             Ouest:44
##
    Mean
            :-1.6552
                       Mean
                               :-1.745
                                                  : 89.91
                                                             Sud :19
                                          Mean
##
    3rd Qu.:-0.5209
                       3rd Qu.: 0.000
                                          3rd Qu.:103.50
                                                             NA's :11
##
    Max.
            : 6.5778
                               : 5.000
                                                  :166.00
                       Max.
                                          Max.
##
    NA's
                       NA's
                                          NA's
            :14
                               :14
                                                  :5
```

softImpute

The softImpute package can be used to impute quantitative data. It fits a low-rank matrix approximation to a matrix with missing values via nuclear-norm regularization. A vignette is available online, as well as the original article (Hastie et al. 2015).

The softImpute function computes, based on an incomplete data set, a low-dimensional factorization which can be used to impute the missing values. The function is used as follows:

```
# keep only quantitative variables
dat_miss_quanti <- as.matrix(ozone[, 1:11])
# perform softImpute
sft <- softImpute(x=dat_miss_quanti, rank.max=2, lambda=0, type=c("als", "svd"))</pre>
```

The main arguments are the following (more details can be found on the help page).

- x: the data set with missing values (matrix).
- rank.max: the restricted rank of the solution, which should not be bigger than min(dim(x))-1.
- lambda: the nuclear-norm regularization parameter.
- type: indicates the algorithm which should be used, among "svd" and "als". "svd" returns an exact solution, while "als" returns an approximate solution (in exchange for a faster computation time).

To compute the imputed data set based on the softImpute results, one may use the following code:

```
# compute the factorization
dat_imp_sft <- sft$u%*%diag(sft$d)%*%t(sft$v)
# replace missing values by computed values
dat_imp_sft[which(!is.na(dat_miss_quanti))] <- dat_miss_quanti[which(!is.na(dat_miss_quanti))]</pre>
```

To calibrate the parameter lambda, one may perform cross-validation, the code is given below. One uses the function produce_NA detailed in "amputation.R" available in the related R source code of "How to generate missing values?".

```
source('amputation.R')
cv_sft <- function(y,</pre>
                     N = 10,
                    len = 20) {
  y <- as.matrix(y)</pre>
  Y2 <- y
  Y2[is.na(Y2)] \leftarrow 0
  d \leftarrow dim(y)
  n < -d[1]
  p \leftarrow d[2]
  m <- sum(!is.na(y))</pre>
  lambda1.max <- max(svd(Y2)$d)</pre>
  lambda1.min <- 1e-3*lambda1.max</pre>
  grid.lambda1 <-
    exp(seq(log(lambda1.min), log(lambda1.max), length.out = len))
  ylist <-
    lapply(1:N, function(k)
      produce_NA(as.matrix(y),perc.missing = 0.2))$data.incomp
  res.cv <- lapply(1:N, function(k) {
    sapply(1:len,
            function(i) {
              yy <-produce_NA(as.matrix(y),perc.missing = 0.2)$data.incomp
              res <-
                softImpute(as.matrix(yy),
                             lambda = grid.lambda1[i])
              u <- res$u
              d <- res$d
              v <- res$v
              if (is.null(dim(u))) {
                res <- d * u %*% t(v)
              } else {
                res <- u %*% diag(d) %*% t(v)
              imp <- as.matrix(yy)</pre>
              imp[is.na(yy)] <- res[is.na(yy)]</pre>
              return(sqrt(sum((res - y) ^ 2, na.rm = T)))
            })
  })
  res.cv <- colMeans(do.call(rbind, res.cv))
  1 <- which.min(res.cv)</pre>
  lambda <- grid.lambda1[1]</pre>
  return(lambda)
```

```
}
lambda_sft <- cv_sft(dat_miss_quanti)</pre>
```

Then, the imputation procedure can be performed using the value of lambda computed with cross-validation (the other parameters are set to their default value):

```
sft <- softImpute(x=dat_miss_quanti, lambda=lambda_sft)</pre>
dat_imp_sft <- sft$u%*%diag(sft$d)%*%t(sft$v)</pre>
dat_imp_sft[which(!is.na(dat_miss_quanti))] <- dat_miss_quanti[which(!is.na(dat_miss_quanti))]</pre>
head(dat_imp_sft)
##
            [,1] [,2] [,3] [,4] [,5]
                                           [,6] [,7]
                                                        [,8]
                                                                    [,9]
## [1,]
         87.0000 15.6 18.5 18.4
                                    4 4.000000
                                                   8
                                                      0.6946 -1.7101000
## [2,]
         64.4358 17.0 18.4 17.7
                                    5 5.000000
                                                   7 -4.3301 -4.0000000
## [3,]
         92.0000 15.3 17.6 19.5
                                    2 5.000000
                                                      2.9544 1.8794000
## [4,] 114.0000 16.2 19.7 22.5
                                    1 4.126458
                                                      0.9848 -0.8363165
## [5,]
         94.0000 17.4 20.5 20.4
                                    8 8.000000
                                                   7 -0.5000 -2.9544000
## [6,]
         80.0000 17.7 19.8 18.3
                                    6 6.000000
                                                   7 -5.6382 -5.0000000
##
             [,10]
                        [,11]
## [1,] -0.6946000
                    84.00000
## [2,] -3.0000000 87.00000
## [3,]
        0.5209000 82.00000
## [4,] -0.8555628 92.00000
## [5,] -4.3301000 114.00000
## [6,] -6.0000000 79.17323
```

mice

The mice package implements a multiple imputation methods for multivariate missing data. It can impute mixes of continuous, binary, unordered categorical and ordered categorical data, as well as two-level data. The original article describing the software, as well as the source package and example code are available online (Buuren and Groothuis-Oudshoorn 2011).

The mice function computes, based on an incomplete data set, multiple imputations by chained equations and thus returns m imputed data sets.

The main arguments are the following (more details can be found on the help page).

- data: the data set with missing values (matrix).
- m: number of multiple imputations.
- method: the imputation method to use.

In this case the predictive mean matching method is performed. Other imputation methods can be used, type methods (mice) for a list of the available imputation methods.

```
mice_mice <- mice(ozone,m=5,method="pmm") #contains m=5 completed datasets.
#get back the first completed dataset of the five available in mice_res
mice::complete(mice_mice,1)</pre>
```

The pool function combines all the results together based on Rubin's rules.

```
mice_with <- with(mice_mice, exp = lm(max03 ~ T9 + Ne9))
pool(mice_with)</pre>
```

```
## Class: mipo m = 5
```

```
estimate
                                ubar
                                               b
                                                           t dfcom
## (Intercept) 29.345511 196.0331948 60.3606744 268.4660041
                                                               109 32.26749
                                                   0.5533562
                                                               109 31.44310
                4.460013
                           0.4011372 0.1268492
               -4.324619
                                                               109 44.63210
## Ne9
                           0.5916524 0.1281289
                                                   0.7454072
                     riv
                            lambda
## (Intercept) 0.3694926 0.2698025 0.3112116
               0.3794687 0.2750832 0.3171768
## T9
               0.2598734 0.2062695 0.2395970
## Ne9
```

Session info

sessionInfo()

```
## R version 3.5.1 (2018-07-02)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS 10.14.6
##
## Matrix products: default
## BLAS: /Library/Frameworks/R.framework/Versions/3.5/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/3.5/Resources/lib/libRlapack.dylib
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
## attached base packages:
                 graphics grDevices utils
## [1] stats
                                               datasets methods
                                                                    base
##
## other attached packages:
## [1] mltools_0.3.5
                            gdata_2.18.0
                                                 softImpute_1.4
                                                 missForest 1.4
## [4] Matrix_1.2-17
                            missMDA_1.14
## [7] itertools 0.1-3
                            iterators 1.0.10
                                                 foreach 1.4.4
## [10] randomForest_4.6-14 mice_3.5.0
                                                 lattice 0.20-38
## [13] Amelia_1.7.5
                            Rcpp_1.0.1
##
## loaded via a namespace (and not attached):
## [1] gtools 3.8.1
                             tidyselect 0.2.5
                                                  xfun 0.8
## [4] purrr_0.3.2
                             splines_3.5.1
                                                   generics_0.0.2
## [7] htmltools_0.3.6
                             yaml_2.2.0
                                                  pan_1.6
## [10] survival_2.44-1.1
                             rlang_0.4.0
                                                   jomo_2.6-8
## [13] pillar_1.4.2
                             nloptr_1.2.1
                                                  foreign_0.8-71
                             stringr_1.4.0
## [16] glue_1.3.1
                                                   mvtnorm_1.0-11
## [19] codetools_0.2-16
                             leaps_3.0
                                                   evaluate_0.14
## [22] knitr_1.23
                             doParallel_1.0.14
                                                  parallel_3.5.1
## [25] broom_0.5.2
                             flashClust_1.01-2
                                                  backports_1.1.4
## [28] scatterplot3d_0.3-41 lme4_1.1-21
                                                   digest_0.6.19
## [31] stringi_1.4.3
                             dplyr_0.8.2
                                                   grid_3.5.1
## [34] tools_3.5.1
                             magrittr_1.5
                                                  tibble_2.1.3
## [37] cluster 2.1.0
                                                  tidyr 0.8.3
                             crayon_1.3.4
## [40] FactoMineR_1.42
                             pkgconfig_2.0.2
                                                  MASS_7.3-51.4
## [43] data.table_1.12.2
                             assertthat_0.2.1
                                                  minqa_1.2.4
## [46] rmarkdown_1.13
                             mitml_0.3-7
                                                  R6_2.4.0
## [49] boot_1.3-22
                             rpart_4.1-15
                                                  nnet_7.3-12
```

[52] nlme_3.1-140

compiler_3.5.1

References

Buuren, Stef van, and Karin Groothuis-Oudshoorn. 2011. "mice: Multivariate Imputation by Chained Equations in R." *Journal of Statistical Software* 45 (3): 1–67. http://www.jstatsoft.org/v45/i03/.

Hastie, Trevor, Rahul Mazumder, Jason D Lee, and Reza Zadeh. 2015. "Matrix Completion and Low-Rank Svd via Fast Alternating Least Squares." *The Journal of Machine Learning Research* 16 (1). JMLR. org: 3367–3402.