TNO report PG/VGZ/00.038

Multivariate Imputation by Chained Equations

MICE V1.14 User's manual

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September 2005

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Project number

011.40684/01.01

ISBN-number

90-6743-677-1

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1 Introduction

Multiple imputation (Rubin, 1987, 1996) is the method of choice for complex incomplete data problems. Schafer (1999) contains introductory material about the use of multiple imputation (MI). Other information about MI can be found in *Multiple Imputation Online* at

www.multiple-imputation.com

This document describes the mice library, which runs under S-Plus V4.5 and S-Plus 2000 for Windows. The library assists in performing the steps required in a full multiple imputation (MI) analysis: generation of imputations, repeated analyses on the imputed data, and pooling of the results.

Specific features of the software are:

- columnwise specification of the imputation model;
- arbitrary patterns of missing data;
- transformations and index variables;
- subset selection of predictors;
- supports standard lm and glm complete-data methods;
- automated pooling using the Barnard-Rubin adjustment;
- callable user-written imputation functions;
- online help files.

This document describes how the tools of the mice library can be used. The software was programmed in the S-Plus programming language.

The intended audience of the software consists of S-Plus users with S-Plus programming experience and with sound statistical capabilities who wish to solve incomplete data problems in a principled way. This document does not discuss problems of incomplete data in general (see the books by Little & Rubin, 1987 or Schafer, 1997), the technique of multiple imputation (see the book by Rubin, 1987 and the 1996-article) or Gibbs sampling methodology (see Gelfand and Smith, 1990).

2 Installation

The mice library runs under S-Plus 4.5 and S-Plus 2000. The simplest way to install mice is to copy the mice directory into the standard library directory, under Windows NT typically something like C:/Program Files/sp2000/library. The following S-plus command makes the functions available to the current session:

```
> library(mice)
```

It is also possible to install mice outside the standard S-Plus library, which might be useful for example if S-Plus runs on a network. The library can then be attached with a statement like

```
> library(mice, lib.loc = "C:\\mylib")
```

where the distributed mice directory is assumed to be located in the directory C:\mylib.

The library is 'pure S-Plus' and does not use any compiled code. It should therefore also work on other systems, but this has not been tested. Check the documentation of your local system on attaching libraries.

3 A simple example

The data frame nhanes in the mice library contains example data from Schafer (1997, page 237). Suppose that the incomplete data are collected in either a matrix or data frame, where missing values are coded as NA's.

```
> nhanes
  age bmi hyp chl
1
    1
        NA NA NA
2
    2 22.7
            1 187
3
             1 187
        NA
 4
    3
        NA NA NA
 5
    1 20.4
             1 113
```

The number of the NA's can be counted and visualized as follows:

```
> md.pattern(nhanes)
   age hyp bmi chl
13
    1
         1
             1
                 1
                     0
 1
     1
         1
              0
                  1
                     1
 3
     1
             1
                  0 1
         1
 1
     1
             0
                  1
                     2
         0
 7
     1
         0
              0
                 0
                    3
                 10 27
     0
         8
              9
```

There are 13 (out of 25) rows that are complete, there is one for which only bmi is missing, and there are seven cases for which only age is known. The total number of missing values is equal to (7*3)+(1*2)+(3*1)+(1*1)=27. Most missing values (10) occur in chl.

The imputation algorithm is implemented in a function called mice. The function is invoked as

```
> imp <- mice(nhanes)
...</pre>
```

which results in the object imp of a special class mids for storing multiple imputations. To see the results of the imputation, type

```
> imp
Multiply imputed data set
Call:
mice(data = nhanes)
Number of multiple imputations: 5
Missing cells per column:
   age bmi hyp chl
    0 9 8 10
```

```
Imputation methods:
     bmi
            hyp
"" "pmm" "pmm" "pmm"
VisitSequence:
bmi hyp chl
   2
       3
PredictorMatrix:
    age bmi hyp chl
     0
          0
              0
age
      1
          0
               1
                   1
bmi
               0
                   1
hyp
      1
          1
chl
      1
          1
               1
                   0
Random generator seed value:
```

Imputations are generated according to the default method, which is predictive mean matching (pmm) here. Entries VisitSequence and PredictorMatrix are algorithmic options that will be discusses later. Imputations for bmi are stored in

Each row corresponds to a missing entry in the bmi variable. The columns contain the different, multiple imputations. The default number of multiple imputations is equal to five. The first completed data set can be obtained as

```
> complete(imp,1)
   age bmi hyp chl
     1 29.6
               1 187
 2
     2 22.7
               1 187
 3
     1 30.1
               1 187
 4
     3 24.9
               1 184
 5
     1 20.4
               1 113
```

Note that the missing entries in nhanes have now been filled by the values from the first imputation.

Suppose that our complete-data analysis involves a linear regression of chl on age and hyp. For this purpose, an adapted function lm.mids is available that works on the imputed data:

```
> fit<-lm.mids(chl~age+hyp, imp)</pre>
```

which repeatedly calls the standard regression function lm. The fit object contains the results of five complete-data analyses. These can be pooled as follows:

More extensive output can be obtained, as usual, with the summary function, i.e.,

```
> summary(pool(fit))
                                                 df
                                                        Pr(>|t|)
                  est
                                       t
                            se
(Intercept) 136.28021 28.12605 4.8453373 13.551184 0.0002844227
            18.32603 12.45221 1.4717092 11.131217 0.1687990086
        hyp 20.59693 27.84369 0.7397343
                                          7.302421 0.4825601408
                 lo 95
                           hi 95 missing
                                                fmi
(Intercept)
             75.767847 196.79257
                                     NA 0.2504597
        age -9.041727
                        45.69378
                                       0 0.3239345
                        85.88807
                                      8 0.4771509
        hyp -44.694201
```

This completes the full multiple imputation analysis.

4 Specification of the imputation model

4.1 Elementary imputation methods

Data sets typically contain variables with various coding types, e.g., numerical, categorical or binary. Some authors (Brand, 1999; Van Buuren *et al.*, 1993, 1999; Raghunathan *et al.*, 1998) have proposed to specify an *elementary imputation method* for each variable that is to be imputed. Given the availability of these, some form of iteration can be used for obtaining imputations. Attractive aspects of this strategy are that model specification takes place on a level that is typically well understood by the user (i.e. the individual variable), and that many methods for creating univariate imputations are available. A disadvantage is that the properties of the combined multivariate distribution of the resulting imputations may not be known, which complicates the assessment of convergence. See Appendix A for more details.

In mice, the user can specify an elementary imputation method for each incomplete data column. The elementary imputation method takes a set of (at that moment) complete predictors, and returns a single imputation for each missing entry in the incomplete target column. Multiple imputations are created by repeated calls to the function. The mice library supplies a number of built-in elementary imputation models, which are are given in Table 4.4.1.

Table 4.4.1Built-in	elementary	imputation	methods in mice
1 uvie 4.4.1 Duiii-iii	eiememarv	imbuianon	memous in mice.

Method	Description	Type of target
impute.norm	Bayesian linear regression	Numeric
impute.pmm	Predictive mean matching	Numeric
impute.mean	Unconditional mean imputation	Numeric
impute.logreg	Logistic regression	2 categories
impute.logreg2	Logistic regression (direct minimization)	2 categories
impute.polyreg	Polytomous logistic regression	>= 2 categories
impute.lda	Linear discriminant analysis	>= 2 categories
impute.sample	Random sample from the available observed values	Any

The default methods used in the mice function are impute.pmm for numeric data, impute.logreg for binary data (=factors with two categories), and impute.polyreg for categorical variables (=factors with more than two categories). These defaults can be changed by the defaultImputationMethod argument to the mice function. For example

```
> mice(nhanes, defaultImp = c("norm", "logreg", "polyreg"))
```

changes the default method for numerical data to impute.norm, while leaving the defaults for binary and categorical data unchanged. The imputationMethod argument specifies the imputation method per column and overides the default. This argument can be either a

string or a vector of strings with length ncol (data). If imputationMethod is specified as one string, then all visited columns will be imputed by the technique specified by this string. So

```
> mice(nhanes, imputationMethod = "norm")
```

specifies that impute.norm is to be applied on all columns. If imputationMethod is vector of strings of length ncol (data), then each column will be imputed by the method indicated by the position in the vector. Columns that need not be imputed have method "". For example,

```
> mice(nhanes, imputationMethod = c("", "norm", "pmm", "mean"))
```

uses different methods for different columns. The nhanes 2 data frame contains one polytomous, one binary and two numeric variables. Imputations might be created as

```
> imp <- mice(nhanes2, im=c("polyreg", "pmm", "logreg", "norm"))</pre>
```

where polyreg is used for the first (categorical) variable, ppm for the second (numeric), logreg for the third (binary) and norm for the fourth variable (numeric). The imparameter is a legal S-plus abbreviation of the imputationMethod argument. Note: Running this example produces a list of warning messages because the sample size of 25 is actually too small relative to the number of parameters.

If the data contains factors that are used for imputing other variables, the algorithm creates dummy variables and fills these from the corresponding factor variable. The dummy variables are created automatically (and discarded) within the main algorithm, and are automatically imputed where necessary.

Appendix B describes the arguments of the major functions of the mice library.

4.2 Adding your own imputation functions

It is possible to write one's own elementary imputation function, and call this function from within the Gibbs sampling algorithm. The easiest way to write such a function is to copy and modify an existing impute function, for example impute.norm. Note that this only works if the argument list is kept intact. For more information about the proper function arguments, see the help on impute.norm or other impute functions, e.g. by typing

```
> ?impute.norm
```

The new function can be called by the Gibbs sampler by the imputationMethod argument. For example, calling the function impute.myfunc for each column can be done by typing

```
> mice(nhanes, imputationMethod="myfunc").
```

4.3 Transformations and index variables

There is often a need for transformed, combined or recoded versions of the data. In the case of incomplete data, one could 1) impute the original, and transform the completed original afterwards, or 2) transform the incomplete original and impute the transformed version. If, however, both the original and the transform are needed within the imputation algorithm, neither of these approaches work because one cannot be sure that the transformation holds between the imputed values of the original and transformed versions.

The mice function uses a special mechanism, called 'passive imputation', to deal with such situations. Passive imputation maintains the consistency among different transformations of the same data. The method can be used to ensure that the transform always depends on the most recently generated imputations in the original untransformed data. Passive imputation is invoked by specifying a "~" as the first character of the imputation method. The entire string, including the "~" is interpreted as the formula argument in a call to model.frame (formula, data[!r[,j],]). This provides a simple method for specifying a large variety of dependencies among the variables, such as transformed variables, recodes, interactions, sum scores, and so on, that may themselves be needed in other parts of the algorithm. As an example,

```
> imp <- mice(nhanes, imp=c("", "pmm", "pmm", "~log(bmi)"))</pre>
```

replaces the missing values in the fourth column by the log of bmi, the second column. The result is

```
> complete(imp)
   age bmi hyp
                        chl
                  3.387774
     1 29.6 1
 2
     2 22.7
              1 187.000000
 3
     1 30.1
              1 187.000000
     3 24.9
                  3.214868
> complete(imp,2)
   age bmi hyp
                        chl
                  3.387774
     1 29.6
             1
 2
     2 22.7
              1 187.000000
 3
              1 187.000000
     1 30.1
 4
     3 25.5
              2
                  3.238678
```

Missing entries 1 and 4 in chl were replaced by the log of bmi. Note that entry 4 takes the imputed values of bmi into account. Note also that the nonmissing values in chl are simply copied from the data, so as a whole, the column now contains nonsensical data. One easy way

to create consistency is by coding all entries in chl as NA, but for large data sets, this can be inefficient. Another way is to apply the log transform using available cases beforehand, followed by coding the remainder as NA.

An index of more variables can be specified by means of the I () operator, e.g. " \sim I (0.5*log(age) +hyp)" computes the sum of half log(age) and hypertension status:

```
imp <- mice(cbind(nhanes,index=NA),imp=c("","pmm","pmm","pmm",
"~I(0.5*log(age)+hyp)"))</pre>
```

a discretized version of the imputed variable can be obtained by

```
> imp_mice(cbind(nhanes,obese=NA),imp=c("","pmm","pmm","pmm",
"~cut(bmi,breaks=c(0,30,35,100))")).
```

and an interaction term of two variables can be created as

```
> imp_mice(cbind(nhanes,int=NA),imp=c("","pmm","pmm","pmm",
"~I((bmi-25)*hyp)"))
```

so that it is available for imputation.

There are two specific points that need attention when defining transformations through the "~" mechanism. First, deterministic relations between columns remain synchronized if the target variable is updated immediately after any of its predictors are imputed. So in the last example above, column int should then be updated each time after bmi or hyp is imputed. This can be done by changing the sequence in which the algorithm visits the columns. See section 4.4 for more details. Second, the "~" mechanism may easily lead to linear dependencies among predictors, which produces in a fatal error if both the original and the transformed variables are simultaneously used for imputation. One can circumvent this problem by defining the set of predictors such that original and transformed do not jointly occur. Section 4.5 described how to do this.

In S-Plus 4.5, the mice function will error if any column consists entirely of NA's. The cbind (nhanes, index=NA) arguments creates such a data set. A workaround to the problem is to compute the values of index for the nonmissing cases before entering the mice function.

4.4 Visiting scheme

The standard algorithm imputes each incomplete column in the data from left to right. The visitation scheme of the Gibbs sampler is essentially irrelevant as long as each column is visited often enough, but some schemes are more efficient than others. Also, as indicated in sec-

tion 4.3, the visiting scheme plays a role in keeping relations between variables synchronised and consistent with the current set of imputations.

It is possible to alter the default visiting scheme by the visitSequence argument of the mice function. This is a vector of integers of arbitrary length, specifying the visiting sequence, that is, the column order that is used to impute the data during one iteration of the algorithm. Note that a given column may be visited more than once within the same iteration. All columns with missing data that are used as predictors should be visited, or else the function will stop with an error.

Continuing the interaction example of section 4.3, we can take care that the interaction term is always up to date by the following command:

```
> imp_mice(cbind(nhanes,int=NA),imp=c("","pmm","pmm","pmm",
"~I((bmi-25)*hyp)"),visitSequence=c(2,5,3,5,4))
```

Using the statement, the algorithm will visits column 5 immediately after column 2 or column 3.

4.5 Choice of predictors

The argument predictorMatrix of the mice function is a square matrix of size ncol (data) containing 0/1 data. This matrix specifying the set of predictors to be used for each incomplete column. If diagnostics=T, then the object returned by mice contains the predictor matrix used for imputation, e.g.

<pre>> imp\$predictorMatrix</pre>				
	age	bmi	hyp	chl
age	0	0	0	0
bmi	1	0	1	1
hyp	1	1	0	1
chl	1	1	1	0

Rows correspond to incomplete target variables, in the sequence as they appear in data. A value of '1' indicates that the column variable is used as a predictor for the target (row) variable. Thus, in the above example, age, hyp and chl are predictors for imputing bmi. The diagonal of predictorMatrix is zero. The default setting implies that for every incomplete column all other columns are used as predictors. However, for variables that are complete (age in the above example) predictors are automatically removed.

The user can specify a predictorMatrix, thereby effectively limiting the number of predictors per variable. For example, suppose that bmi is not needed as a predictor. Setting all entries in the bmi column to zero removes it from the predictor set of all other variables, e.g.

> my	.pred	ictor	Matri	X
	age	bmi	hyp	chl
age	0	0	0	0
bmi	1	0	1	1
hyp	1	0	0	1
chl	1	0	1	0

will not use bmi as a predictor, but still impute it. The predictorMatrix argument is especially useful when dealing with data sets with a large number of variables. The next section contains some advice regarding the selection of predictors.

4.6 General advice in choosing predictors

As a general rule, using every available bit of available information yields multiple imputations that have minimal bias and maximal certainty. This principle implies that the number of predictors in should be chosen as large as possible. Some authors observed that including as many predictors as possible tends to make the MAR assumption more plausible, thus reducing the need to make special adjustments for NMAR mechanisms.

However, data sets often contain several hundreds of variables, all of which can potentially be used to generate imputations. It is not feasible (because of multicollinearity and computational problems) to include all these variables. It is also not necessary. In our experience, the increase in explained variance in linear regression is typically negligible after the best, say, 15 variables have been included. For imputation purposes, it is expedient to select a suitable subset of data that contains no more than 15 to 25 variables. Van Buuren et al (1999) provide the following strategy for selecting predictor variables from a large data base:

- 1. Include all variables that appear in the complete-data model. Failure to do so may bias the complete-data analysis, especially if the complete-data model contains strong predictive relations. Note that this step is somewhat counter-intuitive, as it may seem that imputation would artificially strengthen the relations of the complete-data model, which is clearly undesirable. If done properly however, this is not the case. On the contrary, not including the complete-data model variables will tend to bias the results towards zero.
- 2. In addition, include the variables that appear in the response model. Factors that are known to have influenced the occurrence of missing data (stratification, reasons for nonresponse) are to be included on substantive grounds. Others variables of interest are those for which the distributions differ between the response and nonresponse groups. These can be found by inspecting their correlations with the response indicator of the target variable (i.e. the variable to be imputed). If the magnitude of this correlation exceeds a certain level, then the variable is included.

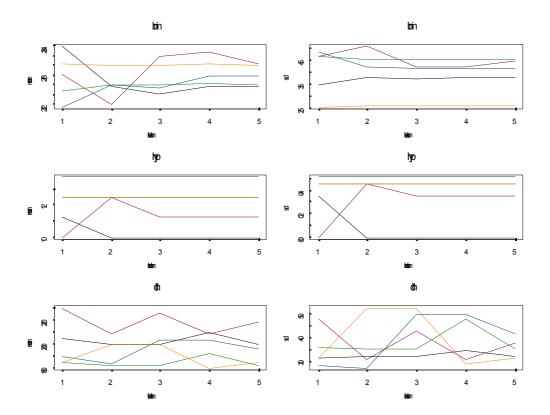
- 3. In addition, include variables that explain a considerable amount of variance of the target variable. Such predictors help to reduce the uncertainty of the imputations. They are crudely identified by their correlation with the target variable.
- 4. Remove from the variables selected in steps 2 and 3 those variables that have too many missing values within the subgroup of incomplete cases. A simple indicator is the percentage of observed cases within this subgroup, the percentage of usable cases.

Typically, many predictors used for imputation are incomplete themselves. In principle, one could apply the above modelling steps for each incomplete predictor in turn, but this may lead to a cascade of auxiliary imputation problems. In doing so, one runs the risk that every variable needs to be included after all. In practice, there is often a small set of key variables, for which imputations are needed, which suggests that steps 1 through 4 are to be performed for key variables only. This was the approach taken in Van Buuren, Boshuizen and Knook (1999), but it may miss important second level predictors in the data. A safer and more efficient, though more laborious, strategy is to perform the modeling steps for all incomplete level-1 predictors. This is done in Oudshoorn et al. (1999). We expect that it is rarely necessary to go beyond this level.

5 Running mice

5.1 Studying convergence

There is no clear-cut method for determining whether the Gibbs sampling algorithm has converged. Plotting the mids object (as produced by mice) yields a graphic display of the mean and standard deviation of the *imputations*. On convergence, the traces should be intermingled with each other, without showing any definite trends. Stated more precisely: convergence is diagnosed when the variance between different sequences is no larger than the variance with each individual sequence. Here is an example of the display that mice produces after 5 iterations:



The means (of the imputed values only) per iteration-imputation combination are plotted on the left, the standard deviations of the imputations (within the same replication) on the right. The plots are a bit crude because the number of missing entries is small (9, 11 and 10). It is somewhat hard to assess convergence in this case. Plotting longer iteration sequences of more missing entries will generally convey a better idea whether the between-imputation variability has stabilized and whether the estimates are free of trend.

Note that one iteration of the algorithm involves a lot of work, e.g. for each variable and each mutiple imputation a statistical model is fitted, imputations are drawn and data are updated. The needed number of main iterations in mice is typically much lower than is common in modern Markov Chain simulation techniques, that often require thousands of iterations. No iterations need to be wasted for achieving independence in the imputations themselves, since elementary imputation procedures create imputations that are already statistically independent for a given value of the regression parameters. Thus, the primary function of the Gibbs sampler as implemented here, is to create independence between the posterior distributions of the regression coefficients. The main question is whether the number of iterations is enough to stabilize the distributions of the parameters. Brand's simulation was based on moderate amounts of missing data and was done with just 5 iterations with satisfactory performance. (Brand, 1999). For large amounts of missing data, convergence can be slower though. In general, we obtained good results with as few as 5 or 10 iterations.

Note that the plot focuses on the mean and variance of the imputations. This may not correspond to the parameter of most interest. Section 5.2 describes a more refined method for studying convergence.

5.2 Step by step

This mice.mids function enables the user to split up the computations of the Gibbs sampler into smaller parts by providing a stopping point after every full iteration. There are various circumstances in which this might be useful:

- Due to the way in which S-Plus handles loops, RAM memory may become easily
 exhausted if the number of iterations is large. Returning to prompt/session level may
 alleviate these problems;
- The user may want to compute special convergence statistics at specific points, e.g. after each iteration, for monitoring convergence;
- For computing a 'few extra iterations'.

The imputation model itself is specified in the mice () function and cannot be changed with mice.mids. The state of the random generator is saved with the mids-object.

As a simple example, the statements

```
> imp1 <- mice(nhanes, maxit=1)
> ... anything you like to do here
> imp2 <- mice.mids(imp1)

yield the same result as
> imp <- mice(nhanes, maxit=2)</pre>
```

To check convergence of an arbitrary parameter of interest, one could write a function that loops over mice.mids, and that extracts imputed data with the complete function, and that recomputes the parameter after each iteration using the current imputations. More in particular, one could set maxit to 1, generate imputations, compute the statistic of interest on the completed data, save the result, compute the second iteration using mice.mids, and so on.

5.3 Running problems

The mice function was programmed for flexibility, and not to minimise the use of time or resources. Combined with the greedy nature of S-Plus in general and that fact that method does not used compiled functions, this poses some limits to the size of the data sets and the type of data that can be analysed. The time that mice needs depends primarily on the choice of the elementary imputation methods. Methods like impute.norm or impute.pmm are fairly fast, while others, impute.polyreg in particular, can be slow. To give an idea of the time needed, we successfully imputed a 4000 by 20 matrix containing a variety of levels in about 15 minutes on a 400 MHz processor.

Collinearity and instability problems occur in the impute-functions if the predictors are (almost) linearly related. For example, if one predictor can be written as a linear combination of some others, then this results in messages like Error in solve.qr(a): apparently singular matrix and Length of longer object is not a multiple of the length of the shorter object in: beta + rv %*% rnorm(ncol(rv)). The solution is eliminate duplicate information, for example by specifying a reduced set of predictors. Finding the pair of nearly dependent variables can prove to be difficult and laborious. One trick that we use in practice is to study the last eigenvector of the covariance matrix of the incomplete data. Variables with high values on that factor often cause the problems. Alternatively, one could revert to collinearity diagnostics like the VIF (Kleinbaum et al, 1988) or graphical displays (Cook and Weisburg, 1999). Pedhazur (1973) provides a good discussion on multicollinearity. The ambitious user might like to write elementary imputation functions that are less sensitive to collinearity, for example, based on ridge regression.

5.4 Studying the initial solution

It is possible to create a mice object without doing any Gibbs sampling. Simply specify maxit=0 as an argument to the mice function. This allows you to get hold of the initial imputations (starting values).

5.5 Using (starting) imputations created by other software

It is possible to transform data from other imputation software into a mids object. First create a mids object by calling mice on the incomplete data using maxit=0. Then, manually replace the starting imputations in the mids object by the values generated by the other software. It is essential that external imputations are stored in the proper format of the mids object. The altered mids object can then be used as input for the Gibbs sampler by calling the mice.mids function. Note that this requires all empty cells to be imputed, otherwise the sampler will error on empty cells. Alternatively, the altered mids object can be used for repeated complete data analyses (by calling the lm.mids or glm.mids functions). For this use, it is allowed that only a subset of empty cells is imputed, and that the complete data software handles the remaining incomplete records.

6 After mice

6.1 Overview

The mice library defines three data classes:

- mids: multiply imputed data set (= result of imputation)
- mira: multiply imputed repeated analyses (= results of repeated complete data analyses)
- mipo: multiple imputed pooled analysis (= result of pooling the repeated analyses)

The table below contains a short description of the key functions in the mice library.

Function	Input	Output	Description
md.pattern	data.frame	matrix	summarizes the pattern of the missing data
mice	data.frame	mids	creates a multiply imputed data set
complete	mids	data.frame	converts mids into completed data
lm.mids	mids	mira	linear regression for imputed data
glm.mids	mids	mira	generalized linear model for imputed data
pool	mira	mipo	pools the repeated analyses

6.2 Extracting imputed data

The complete function extracts imputed data sets from a mids object, and returns the completed data as a data frame. For example,

```
> complete(imp, 3)
```

extracts the third complete data set from a multiply imputed data in imp. Specifying

```
> complete(imp, "long")
```

produces a long matrix where the *m* completed data matrices are vertically stacked and padded with the imputation number. This form is convenient for making point estimates and for exporting multiply imputed data to other software. Other options are "broad" and "repeated", which produce complete data in formats that are convenient for investigating between-imputation patterns.

6.3 Complete data analysis

The mice library provides two functions for complete-data analysis on a mids object: lm.mids and glm.mids. These functions are analogues to the standard lm and glm functions. Their main contribution is that they repeated call the complete data function, and store the resulting fits in an object of class mira, which stands for multiply imputed repeated analyses. So

```
> fit5<-lm.mids(chl~age+hyp, imp)</pre>
```

repeatedly calls the standard regression function lm. The fit5 object contains the results of five complete-data analyses. The expression

```
> fit5$analyses[[1]]
```

returns the fit object of the first repeated analysis. It is easy to adapt the lm.mids function to other types of complete data analysis.

6.4 Pooling

The function averages the estimates of the complete data model, computes the total variance over the repeated analyses, and computes the relative increase in variance due to nonresponse and the fraction of missing information.

The function takes an object of class mira, and returns an object of class mipo, which stands for *multiply imputed pooled analysis*. For example,

produces an object result of class mira, which contains the pooling results. The command summary (result) provides a more extensive overview of the results.

The function pool implements the method based on the adjusted degrees of freedom as in Barnard & Rubin (1999). The function relies on the availability of

- the estimates of the model, typically present as 'coefficients' in the fit object;
- an appropriate estimate of the variance-covariance matrix of the estimates per analysis.

The latter is estimated from the fit-object by the Varcov function taken from Harrell's design library (Alzola & Harrell, 1999). Currently, Varcov functions exists for the S-Plus standard lm and glm function, as well as for design's specific analysis functions. For other complete data methods, the user should define an appropriate Varcov function.

Note that not all information from the analyses is pooled. If one wants, for example, a combined estimate of the residual variance around the regression line, this cannot be computed by the pool function. It is however easy to adapt the pool function to other measures of interest.

Meng & Rubin (1992) describe a procedure for calculating the pooled log-likelihood ratio test and corresponding p-value for statistical analyses on multiply imputed data. This procedure can be used for modelling purposes in the context of generalized linear models. Appendix C contains a worked-out example that one may adapt to apply the procedure.

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Appendix A Imputation algorithm

Let $X = (X_1, X_2, ..., X_k)$ be a set of k random variables, where each variable $X_j = (X_j^{\text{obs}}, X_j^{\text{mis}})$ may be partially observed, with j = 1, ..., k. The imputation problem is to draw from P(X), the unconditional multivariate density of X. Let t denote an iteration counter. Assuming that data are missing at random, one may repeat the following sequence of Gibbs sampler iterations:

```
For X_1: draw imputations X_1^{t+1} from P(X_1 | X_2^t, X_3^t, ..., X_k^t)
For X_2: draw imputations X_2^{t+1} from P(X_2 | X_1^{t+1}, X_3^t, ..., X_k^t)
:
For X_k: draw imputations X_k^{t+1} from P(X_k | X_1^{t+1}, X_2^{t+1}, ..., X_{k-t}^t),
```

i.e., condition each time on the most recently drawn values of all other variables. Properties of this general iteration scheme have been described by Gelfand and Smith (1990). Rubin and Schafer (1990) show that if P(X) is multivariate normal, then iterating linear regression models like $X_1 = X_2'\beta_{12} + X_3'\beta_{13} + ... + X_k'\beta_{1k} + \varepsilon_1$ with $\varepsilon_1 \sim N(0, \sigma_1^2)$ will produce a random draw from the desired distribution. Schafer (1997) generalizes this results to other multivariate distributions.

The implemented algorithm differs slightly from Schafer's approach in that the conditional models can be specified directly, thus without the need to choose an encompassing multivariate model for the entire data set. It is *assumed* that a multivariate distribution exists, and that draws from it can be generated by iteratively sampling from the conditional distributions. In this way, the multivariate problem is split into a series of univariate problems. Similar ideas have been applied by Kennickell (1991), Brand (1999), Van Buuren *et al* (1993, 1999) and Raghunathan *et al*. (1998). Rubin coined the term 'incompatible Gibbs' to refer to these kinds of algorithms.

It is not always certain whether the multivariate distribution actually exists. It is possible that the specification of two conditional distributions $P(X_1|X_2)$ and $P(X_2|X_1)$ are incompatible, so that no joint distribution $P(X_1, X_2)$ exists. Arnold *et al.* (1999) deal with this problem from a mathematical-statistical point of view. Very little is known about the properties of the Gibbs sampler under a given incompatible specification. It could be that, since there is no distribution to converge to, the algorithm will alternate between isolated conditional distributions. In that case, the final result will depend on the precise stopping point, which is clearly undesirable. Things may be worse if variables are related in a nonlinear way. Brand (1999) studied the performance of a variety of actual algorithms based on possibly incompatible conditionals, with quite encouraging results. By and large, the subject of incompatible Gibbs is still somewhat of an open research problem, and more work is needed to establish its properties.

Appendix B Function arguments

This appendix describes the arguments of the major functions of the mice library. For more details on a specific function, use the standard help mechanism, e.g. by typing ?complete.

FUNCTIONS

```
Produces imputed flat files from multiply imputed data set (mids)
complete
DESCRIPTION:
Takes an object of type mids, fills in the missing data, and
returns the completed data in a specified format.
data.frame <- complete(x, action=1)</pre>
REQUIRED ARGUMENTS:
        An object of class 'mids' (created by the function mice()).
OPTIONAL ARGUMENTS:
If action is a scalar between 1 and x$m, the function returns the data with the ac-
tion's imputation filled in. Thus, action=1 returns the first completed data set.
The can also be one of the following strings: "long", "broad", "repeated". This
has the following meaning:
action="long" produces a long matrix with n*m rows, containing all imputed data plus
two additional variables " ID " (containing the row names) and " IMP " (containing the
imputation number).
action="broad"
                 produces a broad matrix with m times the number of columns in the
original data. The first ncol(x$data) columns contain the first imputed data matrix.
Column names are changed to reflect the imputation number.
action="repeated" produces a broad matrix with m times ncol(x$data) columns. The first
m columns give the filled-in first variable. Column names are changed to reflect the
imputation number.
VALUE:
A data frame with the imputed values filled in.
```

```
response ~ predictors. See the documentation of lm and formula for details.
data
         An object of type 'mids', which stands for 'multiply imputed data set',
         typically created by function mice().
OPTIONAL ARGUMENTS:
family
                 see glm
weights
subset
na.action
start
control
method
model
y
contrasts
VALUE:
         An objects of class 'mira', which stands for 'multiply imputed repeated
         analysis'.
         This object contains m glm.objects, plus some descriptive information.
                  Elementary imputation method: Linear Discriminant Analysis
impute.lda
DESCRIPTION:
         Imputes univariate missing data using linear discriminant analysis
USAGE:
         imp <- impute.lda(y, ry, x)</pre>
REQUIRED ARGUMENTS:
         Incomplete data vector of length n
ry
         Vector of missing data pattern (F=missing, T=observed)
         Matrix (n \times p) of complete covariates.
VALUE:
         A vector of length nmis with imputations.
impute.logreg
                Elementary imputation method: Logistic Regression
DESCRIPTION:
         Imputes univariate missing data using logistic regression.
USAGE:
         imp <- impute.logreg(y, ry, x)</pre>
REQUIRED ARGUMENTS:
         Incomplete data vector of length n
ry
         Vector of missing data pattern of length n (F=missing, T=observed)
         Matrix (n x p) of complete covariates.
```

VALUE:

imp A vector of length nmis with imputations (0 or 1).

DESCRIPTION:

Imputes univariate missing data using logistic regression.

USAGE:

imp <- impute.logreg2(y, ry, x)

REQUIRED ARGUMENTS:

y Incomplete data vector of length n

ry Vector of missing data pattern of length n (F=missing, T=observed)

x Matrix (n x p) of complete covariates.

VALUE:

imp A vector of length nmis with imputations (0 or 1).

DESCRIPTION:

Imputes the arithmetic mean of the observed data $% \left(1\right) =\left(1\right) \left(1\right)$

USAGE:

 $\verb|imp <- impute.mean(y, ry, x=NULL)| \\$

REQUIRED ARGUMENTS:

y Incomplete data vector of length ${\bf n}$

ry Vector of missing data pattern (F=missing, T=observed)

OPTIONAL ARGUMENTS:

Matrix (n x p) of complete covariates.

VALUE:

imp A vector of length nmis with imputations.

DESCRIPTION:

 ${\tt Imputes \ univariate \ missing \ data \ using \ linear \ regression \ analysis}$

USAGE:

```
imp <- impute.norm(y, ry, x)</pre>
REQUIRED ARGUMENTS:
        Incomplete data vector of length n
        Vector of missing data pattern (F=missing, T=observed)
ry
        Matrix (n x p) of complete covariates.
VALUE:
        A vector of length nmis with imputations.
imp
impute.pmm
               Elementary imputation method: Linear Regression Analysis
DESCRIPTION:
        Imputes univariate missing data using predictive mean matching
USAGE:
        imp <- impute.pmm(y, ry, x)</pre>
REQUIRED ARGUMENTS:
        Incomplete data vector of length n
ry
        Vector of missing data pattern (F=missing, T=observed)
        Matrix (n \times p) of complete covariates.
VALUE:
imp
        A vector of length nmis with imputations.
DESCRIPTION:
        Imputes missing data in a categorical variable using polytomous regression
USAGE:
        imp <- impute.polyreg(y, ry, x)</pre>
REQUIRED ARGUMENTS:
        Incomplete data vector of length n
        Vector of missing data pattern (F=missing, T=observed)
ry
        Matrix (n x p) of complete covariates.
VALUE:
        A vector of length nmis with imputations.
imp
```

```
impute.sample
                 Elementary imputation method: Simple random sample
DESCRIPTION:
         Imputes a random sample from the observed y data
USAGE:
         imp <- impute.sample(y, ry, x=NULL)</pre>
REQUIRED ARGUMENTS:
         Incomplete data vector of length n
         Vector of missing data pattern (F=missing, T=observed)
ry
OPTIONAL ARGUMENTS:
        Matrix (n x p) of complete covariates.
VALUE:
        A vector of length nmis with imputations.
imp
lm.mids Linear regression on multiply imputed data
DESCRIPTION:
         Performs repeated linear regression on multiply imputed data set
USAGE:
         fit <- lm.mids(formula, data, weights, subset, na.action, method="qr",
model=F,
                  x=F, y=F, contrasts=NULL, ...)
REQUIRED ARGUMENTS:
         a formula object, with the response on the left of a \sim operator, and the
         terms, separated by + operators, on the right.
data
         An object of type 'mids', which stands for 'multiply imputed data set',
         typically, created by function mice().
OPTIONAL ARGUMENTS:
weights
                 see lm
subset
                 see lm
na.action
                 see lm
                 see lm
method
model
                 see lm
                 see lm
Х
                 see lm
V
                 see lm
contrasts
VALUE:
         An objects of class 'mira', which stands for 'multiply imputed repeated
         analysis'.
         This object contains m lm.objects, plus some descriptive information.
```

md.pattern Missing data pattern

DESCRIPTION:

Computes the missing data pattern of a matrix or data.frame.

USAGE:

pat <- md.pattern(x)</pre>

REQUIRED ARGUMENTS:

A data frame or a matrix containing the incomplete data. Missing values are coded as NA's.

VALUE:

A matrix with ncol(x)+1 columns, in which each row corresponds to a missing data pattern (1=observed, 0=missing). Rows and columns are sorted in increasing amounts of missing information. The last column and row contain row and column counts, respectively.

mice.mids Multivariate Imputation by Chained Equations (iteration step)

DESCRIPTION:

Takes a "mids"-object, and produces an new object of class "mids".

USAGE:

mice.mids(obj, maxit=1, diagnostics=T, printFlag=T)

REQUIRED ARGUMENTS:

obj

An object of class "mids", typically produces by a previous call to mice() or mice.mids()

OPTIONAL ARGUMENTS:

maxit

The number of additional Gibbs sampling iterations.

diagnostics

A Boolean flag. If TRUE, diagnostic information will be appended to the value of the function. If FALSE, only the imputed data are saved. The default is TRUE.

printFlag

A Boolean flag. If TRUE, diagnostic information during the Gibbs sampling iterations will be written to the command window. The default is TRUE.

VALUE:

An object of class mids, which stands for 'multiply imputed data set'.

mice Multivariate Imputation by Chained Equations

DESCRIPTION:

Produces an object of class "mids", which stands for 'multiply imputed data set'.

REQUIRED ARGUMENTS:

data

A data frame or a matrix containing the incomplete data. Missing values are coded as ${\tt NA's.}$

OPTIONAL ARGUMENTS:

m

Number of multiple imputations. If omitted, m=5 is used.

$\verb"imputationMethod"$

Can be either a string, or a vector of strings with length ncol(data), specifying the elementary imputation method to be used for each column in data. If specified as a single string, the given method will be used for all columns. The default imputation method (when no argument is specified) depends on the measurement level of the target column and are specified by the defaultImputationMethod argument.

Columns that need not be imputed have method "". Built-in methods are:

```
Bayesian linear regression
         Predictive mean matching
pmm
                                                      Numeric
         Unconditional mean imputation
                                                      Numeric
mean
         Logistic regression
                                                      2 categories
         Logistic regression (direct minimization)
loarea2
                                                      2 categories
         Polytomous logistic regression
polyreg
                                                      >= 2 categories
lda
         Linear discriminant analysis
        Random sample from the observed values
sample
                                                      Anv
```

For example, for the j'th column, the impute.norm function that implements the Bayesian linear regression method can be called by specifying the string "norm" as the j'th entry in the vector of strings.

The user can write his or her own imputation function, say impute.myfunc, and call it for all columns by specifying imputationMethod="myfunc", or for specific columns by specifying imputationMethod=c("norm", "myfunc",...).

Special method: If the first character of the elementary method is a "~", then the string is interpreted as the formula argument in a call to model.frame(formula, data [!r[,j],]). This provides a simple mechanism for specifying a large variety of dependencies among the variables, for example transformed versions of imputed variables, recodes, interactions, sum scores, and so on, that may themselves be needed in other parts of the algoritm. Note that the "~" mechanism works only on those entries which have missing values in the target column. The user should make sure that the combined observed and imputed parts of the target column make sense. One easy way to create consistency is by coding all entries in the target as NA, but for large data sets, this could be inefficient.

Though not strictly needed, it is often useful to specify visitSequence such that the column that is imputed by the " \sim " mechanism is visited each time after one of its predictors was visited. In that way, deterministic relation between columns will always be synchronized.

predictorMatrix

A square matrix of size ncol(data) containing 0/1 data specifying the set of predictors to be used for each target column. Rows correspond to target variables (i.e. variables to be imputed), in the sequence as they appear in data. A value of 'l' means that the column variable is used as a predictor for the target variable (in the rows). The diagonal of predictorMatrix must be zero. The default for predictorMatrix is that all other columns are used as predictors (sometimes called massive imputation).

visitSequence

A vector of integers of arbitrary length, specifying the column indices of the visiting sequence. The visiting sequence is the column order that is used to impute the data during one iteration of the algorithm. A column may be visited more than once. All incomplete columns that are used as predictors should be visited, or else the function will stop with an error. The default sequence 1:ncol(data) implies that columns are imputed from left to right.

defaultImputationMethod=c("pmm","logreg","polyreg")

A vector of three strings containing the default imputation methods for numerical columns, factor columns with 2 levels, and factor columns with more than two levels, respectively. If nothing is specified, the following defaults will be used:

pmm predictive mean matching numeric data logreg logistic regression imputation binary data (

logreg logistic regression imputation binary data (factor with 2 levels) polyreg polytomous regression imputation categorical data (factor >= 2 levels)

maxit

A scalar giving the number of iterations. The default is 5.

diagnostics

A Boolean flag. If TRUE, diagnostic information will be appended to the value of the function. If FALSE, only the imputed data are saved. The default is TRUE.

0000

An integer between 0 and 1000 that is used by the set.seed function for ofsetting the random number generator. Default is to leave the random number generator alone.

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An object of class mids, which stands for 'multiply imputed data set'. For a description of the object, see the documentation on "mids.object".

DESCRIPTION:

Pools the results of m repeated complete data analysis

USAGE:

y <- pool(x, dfmethod="smallsample")

REOUIRED ARGUMENTS:

object

An object of class 'mira', produced by functions like lm.mids or glm.mids.

OPTIONAL ARGUMENTS:

dfmethod

A string describing the method to compute the degrees of freedom. The default value is "smallsample", which specifies the is Barnard-Rubin adjusted degrees of freedom (Barnard& Rubin, 1999) for small samples. Specifying a different string produces the conventional degrees of freedom as in Rubin (1987).

VALUE:

An object of class 'mipo', which stands for 'multiple imputation pooled'.

DATA OBJECTS

mids multiply imputed data set

DESCRIPTION

An object containing a multiply imputed data set

GENERATION

The "mids" object is generated by the mice and mice.mids functions.

METHODS

The "mids" class of objects has methods for the following generic functions: print, summary, plot.

STRUCTURE

An object of class mids is a list of the following components:

call The call that created the object.

data A copy of the incomplete data set.

m The number of imputations.

nmis An array containing the number of missing observations per column.

imp A list of nvar components with the generated multiple imputations.
Each part of the list is a nmis[j] by m matrix of imputed values for
variable j.

imputationMethod

A vector of strings of length(nvar) specifying the elementary imputation method per column.

predictorMatrix

A square matrix of size $\operatorname{ncol}(\operatorname{data})$ containing 0/1 data specifying the predictor set.

visitSequence

The sequence in which columns are visited.

seed

The seed value of the solution.

iteration

Last Gibbs sampling iteration number.

${\tt lastSeedValue}$

The most recent seed value.

chainMean

A list of m components. Each component is a length(visitSequence) by maxit matrix containing the mean of the generated multiple imputations. The array can be used for monitoring convergence. Note that observed data are not present in this mean.

chainCov

A list with similar structure of itermean, containing the covariances of the imputed values.

pad A list containing various settings of the padded imputation model, i.e. the imputation model after creating dummy variables. Normally, this array is only useful for error checking.

mipo multiply imputed pooled analysis

DESCRIPTION

An object containing the m fit objects of a complete data analysis, plus some additional information.

GENERATION

The "mipo" object is generated by the lm.mids and glm.mids functions.

METHODS

The "mipo" class of objects has methods for the following generic functions: print, summary.

STRUCTURE

An object of class mipo is a list of the following components:

- call The call that created the mipo object.
- call1 The call that created the mira object that was used in 'call'.
- call2 The call that created the mids object that was used in 'call1'.
- nmis An array containing the number of missing observations per column.
- m Number of multiple imputations.
- qhat $\;\;$ An m x npar matrix containing the complete data estimates for the npar paremeters of the m complete data analyses.
- u An m \times npar \times npar array containing the variance-covariance matrices of the m complete data analyses.
- qbar The average of complete data estimates.
- ubar The average of the variance-covariance matrix of the complete data estimes.
- b The between imputation variance-covariance matrix.
- t The total variance-covariance matrix.
- r Relative increases in variance due to missing data
- df Degrees of freedom associated with the t-statistics.
- f Fractions of missing information.

mira multiply imputed repeated analysis

DESCRIPTION

An object containing the m fit objects of a complete data analysis, plus some additional information.

GENERATION

The "mira" object is generated by the lm.mids and glm.mids functions.

METHODS

The "mira" class of objects has methods for the following generic functions: print, summary.

STRUCTURE

An object of class mira is a list of the following components:

- call The call that created the object.
- call1 The call that created the mids object that was used in 'call'.

nmis An array containing the number of missing observations per column.

analyses

A list of m components containing the individual fit objects from each of the m complete data analyses.

Appendix C Likelihood ratio test

```
## Reference: (1992) Meng, X., Rubin, D.B., Performing likelihood ratio tests with
multiply-imputed datasets
## Biometrika, 79, pp 103-111.
imp mice(nhanes2)
\label{eq:fit1_glm.mids}  \mbox{(hyp~chl+age+bmi,data=imp)} 
fit0_glm.mids(hyp~age+bmi,data=imp)
formula1_hyp~chl+age+bmi
formula0 hyp~age+bmi
\#\#\# Calculate for each imputed dataset the deviance for the model
#### with and without the variable (this example: chl). #### devM is the mean of these deviances (mean(d)'_m from the article of Meng).
deviance_0
for (i in (1:(imp$m))){
         data.i_complete(imp,i)
         model.\overline{0} model.matrix(formula0,data=data.i)%*%coef(fit0$analyses[[i]])
         model.1_model.matrix(formula1,data=data.i)%*%coef(fit1$analyses[[i]])
         deviance <- deviance + deviance.logistic (data.i$hyp, logistic (model.1)) - de-
viance.logistic(data.i$hyp,logistic(model.0))
devM<-deviance/imp$m
#### Calculate the pooled coefficients for the "large" and "small" model.
####
result1 pool(fit1)
result0 pool(fit0)
k<-length (result1$qbar) -length (result0$qbar)
#### Calculate now the deviance for each imputed dataset with the pooled coefficients
#### The five deviances will then be pooled: devL (mean(d) L in the article of Meng).
deviance 0
for (i in (1:(imp$m))){
         data.i complete(imp,i)
         model. model.matrix(formula0,data=data.i)%*%result0$qbar
         model.1 model.matrix(formula1,data=data.i)%*%result1$qbar
         deviance<-deviance+deviance.logistic(data.i$hyp,logistic(model.1))-de-</pre>
viance.logistic(data.i$hyp,logistic(model.0))
devL<-deviance/imp$m
loglikelihoodratio(k,imp$m,devL,devM) ## The pooled loglikelihoodratio
pooled.p.deviance(k,imp$m,devL,devM)
                                       ## The pooled p-value of the loglikelihoodra-
tio.
############ functions needed
deviance.logistic<-function(yvector, fittedprobs) {</pre>
         yvector<-as.numeric(yvector)-1
         term1 term2 rep(0,length(yvector))
         term1[yvector!=0] <-yvector[yvector!=0]*log(yvector[yvector!=0]/fittedprobs
[yvector!=0])
         term2[yvector==0]<-(1-yvector[yvector==0])*log((1-yvector[yvector==0])/(1-
fittedprobs[yvector==0]))
         return(-(2*sum(term1+term2)))}
logistic<-function(mu) exp(mu)/(1+exp(mu))</pre>
\#\#\# Calculation teststatistic D L .
```

```
loglikelihoodratio<-function(k,nimp,devL,devM) {
    r.L<-((nimp+1)/(k*(nimp-1)))*(devM-devL)
    return(devL/(k*(1+r.L))) }

pooled.p.deviance<-function(k,nimp,devL,devM) {
    r.L<-((nimp+1)/(k*(nimp-1)))*(devM-devL)
    D.L<-devL/(k*(1+r.L))
    nu<-k*(nimp-1)
    if (nu>4) w<-4+(nu-4)*((1+(1-nu/2)*(1/r.L))^2) else w<-nu*(1+1/k)*((1+1/r.L))^2)
    return(p.value<-1-pf(D.L,k,w)) }</pre>
```