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Imputation of Incomplete Multilevel Data with R

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Abstract

This tutorial illustrates the imputation of incomplete multilevel data with the R package **mice**. Our scope is only simple multilevel models, to show how imputation can yield less biased estimates from incomplete clustered data. More complex models can be accomodated, but are outside the scope of this paper. Incomplete multilevel data requires careful consideration of the missing data problem and analysis strategy. In this tutorial, we focus on a popular strategy for accommodating missingness in multilevel data: replacing the missing data with one or more plausible values, i.e., imputation.Imputation separates the missing data problem from the main analysis and the completed data can be analyzed as if it has been fully observed.This tutorial illustrates the imputation of incomplete multilevel data with the statistical programming language R. We aim to show how imputation can yield less biased estimates from incomplete clustered data. We provide practical guidelines and code snippets for different missing data situations, including non-ignorable missingness mechanisms. For brevity, we focus on multilevel imputation using chained equations with the R mice package and its adjacent packages.

Keywords: missing data, multilevel, clustering, **mice**, R.

1. Introduction

1.1. Multilevel data

Many datasets include individuals that are clustered together, for example in geographic regions, or even different studies. In the simplest case, individuals (e.g., students) are nested within a single cluster (e.g., school classes). More complex clustered structures may occur when there are multiple hierarchical levels (e.g., students in different schools or patients within hospitals within regions across countries), or when the clustering is non-nested (e.g., electronic health record data from diverse settings and populations within large databases). With clustered data we generally assume that individuals from the same cluster tend to be more similar than individuals from other clusters. In statistical terms, this implies that observations from the same cluster are not independent and may in fact be correlated. If this correlation is left unaddressed, estimates of p values, confidence intervals even model parameters are prone to bias (Localio, Berlin, Ten Have, and Kimmel 2001). Statistical methods for clustered data typically adopt hierarchical models that explicitly describe the grouping of observations. These models are also known as 'multilevel models', 'hierarchical models', 'mixed effect models', 'random effect models', and in the context of time-to-event data as 'frailty models'. Table **??** provides an overview of some key concepts in multilevel modeling.

Table 1: Concepts in multilevel methods

1.2. Missingness in multilevel data

As with any other dataset, clustered datasets may be impacted by missingness in much the same way. Several strategies can be used to handle missing data, including complete case analysis and imputation. We focus on the latter approach and discuss statistical methods for replacing the missing data with one or more plausible values. Imputation separates the missing data problem from the analysis and the completed data can be analyzed as if it were completely observed. It is generally recommended to impute the missing values more than once to preserve uncertainty due to missingness and to allow for valid inferences (c.f. Rubin 1976).

With incomplete clustered datasets we can distinguish between two types of missing data: sporadic missingness and systematic missingness (**?**). Sporadic missingness arises when variables are missing for some but not all of the units in a cluster (Van Buuren 2018; Jolani 2018). For example, it is possible that test results are missing for several students in one or more classes. When all observations are missing within one or more clusters, data are said to be systematically missing. Sporadic missingness is visualized in Figure XYZ.

Imputation of missing data requires consideration of the mechanism behind the missingness. Rubin proposed to distinguish between data that are missing completely at random (MCAR), data that are missing at random (MAR) and data that are missing not at random (MNAR; see Table **??**). For each of these three missingness generating mechanisms, different imputation strategies are warranted (Yucel (2008) and Hox, van Buuren, and Jolani (2015)). We here consider the general case that data are MAR, and expand on certain MNAR situations.

Table 2: Concepts in missing data methods

Concept	Details
MCAR	Missing Completely At Random, where the probability to be missing is equal

Concept	Details
	across all data entries
MAR	Missing At Random, where the probability to be missing depends on observed information
MNAR	Missing Not At Random (MNAR), where the probability to be missing depends on unrecorded information, making the missingness non-ignorable (Rubin 1976; Meng 1994).

1.3. Aim of this paper

This papers serves as a tutorial for imputing incomplete multilevel data with **mice** in R. **mice** has become the de-facto standard for imputation by chained equations, which iteratively solves the missingness on a variable-by-variable basis. **mice** is known to yield valid inferences under many different missing data circumstances (Van Buuren 2018).

We provide practical guidelines and code snippets for different missing data situations, including non-ignorable mechanisms. For reasons of brevity, we focus on multilevel imputation by chained equations with **mice** exclusively; other imputation methods and packages (see e.g. **?**, and Grund, Lüdtke, and Robitzsch (2018)) are outside the scope of this tutorial. Assumed knowledge includes basic familiarity with the **lme4** notation for multilevel models (see Table **??**).

We illustrate imputation of incomplete multilevel data using three case studies:

- `popmis` from the **mice** package (simulated data on perceived popularity, $n = 2,000$ pupils across $N = 100$ schools with data that are MAR, van Buuren and Groothuis-Oudshoorn 2021);
- `impact` from the **metamisc** package (empirical data on traumatic brain injuries, $n = 11,022$ patients across $N = 15$ studies with data that are MAR, Debray and de Jong 2021);
- `obesity` from the **micemd** package [simulated data on obesity, $n = 2,111$ patients across $N = 5$ regions with data that are MNAR].

For each of these datasets, we discuss the nature of the missingness, choose one or more imputation models and evaluate the imputed data, but we will also highlight one specific aspect of the imputation workflow.

This tutorial is dedicated to readers who are unfamiliar with multiple imputation. More experienced readers can skip the introduction (case study 1) and directly head to practical applications of multilevel imputation under MAR conditions (case study 2) or under MNAR conditions (case study 3).

1.4. Imputation workflow

Below we provide a imputation workflow that can be used in general to impute cluster data.

Table 1: Concepts in multilevel methods

Concept	Details
Sample units	Units of the population from which measurements are taken in a sample, e.g., students.
Cluster	Variable that specify the cluster or agruppation, e.g., Classroom
Hierarchical data	Data are grouped into clusters at different levels, observations belonging to the same cluster are expected to share certain characteristics.
Level-1	Variable that varies within a cluster, eg. Test score
Level-2	Variable that does not vary within a cluster but between, e.g. teacher experience.
Hierarchical model	Model accounting for dependant observations relying on certain parameters (within cluster) which in turn depend on other parameters (between cluster)
Fixed effect	Effects that are constant across all sample units, e.g. something that researchers control for and can repeat, such as a teaching strategy (tutoring after class)
Random effect	Effects that are a source of random variation in the data, and whose levels are not fully sampled. e.g. test score tendency during academic year between students due to no controlled factors such as genetic,family history
Mixed effect	Includes fixed and random effects, e.g. the fixed effect would be the treatment effect of a drug and the random effect would be the ID of the hospital where the patient is treated. Multilevel models typically accommodate for variability by including a separate group mean for each cluster e.g random intercept on hospitals. In addition to random intercepts, multilevel models can also include random coefficients and heterogeneous residual error variances across clusters (see e.g. @gelm06, @hox17 and @jong21).
ICC	The variability due to clustering is often measured by means of the intraclass coefficient (ICC). The ICC can be seen as the percentage of variance that can be attributed to the cluster-level, where a high ICC would indicate that a lot of variability is due to the cluster structure.
Stratified intercept	

	cluster	X_1	X_2	X_3	...	X_p
1	1			NA		
2	1					
3	2		NA			
4	2		NA	NA		
5	3					
...						
n	N					

Figure 1: Sporadic missingness in multilevel data

Focus on the Main Analysis

When imputing clustered data, we initially focus on the research question and the intended analysis, assuming the presence of non-incomplete values. This assessment sheds light on research hypotheses and the contemplated main(s) statistical model(s) and it provides insights into the data's structure (refer to the level table), variable types (e.g., confounders, auxiliary variables), and other considerations about variables relationships such as interactions or polynomial terms.

Exploration of Available Data

Next, it is necessary to explore the information available in the data. Exploring individual variables using tools such as histograms or QQ plots can help to delineate variable distributions and plausible ranges of values and also identify input errors or outliers. Evaluating interactions between predictors using scatter plots or conditional plots, assessing collinearity using VIF or correlations, can help to glimpse nonlinear relationships that may affect the original formulation of the main model. Further testing of assumptions related to the response variable, including variance (homogeneity using conditional box plots), independence (e.g., ACF, variograms) and response vs. predictor relationships (conditional plots - x vs. y), may serve to choose an imputation model more suitable to the data. In addition, the intraclass correlation coefficient (ICC) can be examined to assess cluster differences, aiding in the choice between the 2l and 1l methods for imputation.

One can also explore missingness, specifically missing patterns at the cluster level to identify types of patterns (e.g., non-monotonic, systematic) to guide the selection of an appropriate imputation approach in terms of computational efficiency (e.g., simpler regression imputation versus FCS in univariate patterns). Similarly, these missing patterns can also be used to identify potential predictors in individual imputation models by means of inflow criteria (quantifying the connections between missing data in one variable and other observed variables) and outflow criteria (determining the connections between observed values in one variable and missing data in other variables). Although several packages exist for visualizing missing data, this tutorial focuses on the recently implemented ggmice package.

Assess Estimation Procedure Robustness to Missing Data

Prior to implementing multiple imputation, it is critical to assess the robustness of the estimation model when confronted with missing data. **?** highlighted scenarios in which specific Maximum Likelihood (ML) estimation methods outperform Multiple Imputation (MI) methods. Notably, when the response variable is the sole incomplete variable, mixed models demonstrate robustness to missing data under the Missing at Random (MAR) assumption and with a correct variance-covariance specification.**?**. Furthermore, depending on the proportion of missingness (usually is <5%), opting for a simpler complete case analysis might be sufficient.

Pre-imputation

Before proceeding with the imputation model, it is necessary to filter the dataset to include only the minimal variables required for the main model. If additional procedures are conducted during the analysis, it is essential to include variables associated with these procedures, such as confounders in the case of balancing techniques. Other relevant variables, like instrumental variables or auxiliary variables, may enhance parameter estimates even if not included in the main model, as they could be linked to the probability of missingness for some incomplete variables.

Furthermore, at the variable level, it is crucial to assess whether proxy variables should be considered or if deterministic imputation alone is adequate for imputing missing values. For instance, certain incomplete variables may not necessitate stochastic imputation methods like MICE. Instead, they can be effectively addressed through deductive imputation, where incomplete values are inferred from logical and deterministic relationships between variables. This approach is especially beneficial for variables that are functions of others, such as deriving a person's BMI from their weight and height. It also proves valuable for determining values for one-level variables from two-level ones, as seen in the context of Individual Participant Data (IPD). In such cases, incomplete information can be deduced from metadata, like inferring incomplete data about abortion in a country where abortion is illegal, or through cross-temporal or protocol-based deduction, such as imputing missing test values for deceased patients.

Setting Imputation Model

Clustering Inclusion Various strategies can be employed in the imputation process to account for clustering, including the inclusion of a cluster indicator variable, conducting a separate imputation process for each cluster, or employing a simultaneous imputation method that considers clustering (Stata: Clustering and MI Impute) TODO: Replace ref.

The choice of strategy depends primarily on the assumptions made in the main analysis and the constraints imposed by the analyzed data.Concerning data restrictions, if there are few clusters with many observations per cluster, the cluster indicator or imputation separated by groups may be appropriate **?**. Conversely, an imputation model that simultaneously imputes all clusters using a hierarchical model can be employed when there are more clusters or fewer observations per cluster **?**.

In a hierarchical imputation model, correlations between observations within clusters are modeled by a random effect, allowing estimation even with a limited number of observations per cluster. Multiple imputation models based on hierarchical models have been proposed, each with different assumptions.

Before choosing a particular strategy, it is crucial to verify if the assumptions of the imputation model align with those of the main analysis. For example, using the cluster indicator strategy may introduce bias estimates when the model is based on a hierarchical structure **?**. Even if an imputation strategy congruent with the main model is preferred, it is essential to assess its appropriateness for the data, considering that less complex imputation strategies may lead to unbiased estimates in certain scenarios \cite(Bailey_2020).

Choice of Individual Imputation Methods The initial step involves selecting the individual imputation model for each incomplete variable in the dataset. The mice package automatically proposes imputation methods based on the variable type for 1l variables. For 2l level variables, the micemd package's () function can be utilized. This function selects among the 2l imputation methods based on the size of the clusters and the proportion of missingness in each cluster.

In addition to the package-defined imputation methods, users can specify custom methods using the "I formula". This flexibility allows for the calculation of derived variables internally or adjustments to imputation methods based on specific conditions, such as conditioning the imputation model on the level of an incomplete covariate (e.g., pregnancy test on females).

Model Specification The imputation model must be congenial with the main model **?**. Congeniality issues arise when the imputation model and the main model make different assumptions, often due to the omission of a polynomial or interaction term or the use of transformed variables.

The imputation model can include additional terms than the main model terms that do not lead to uncongeniality. For instance, it is advisable to include the outcome variable in the imputation model for prediction variables **?**. In cases where the outcome is time-to-event, the Nelson-Aalen estimate of the time to the event should be included as a covariate in the imputation model [REF]. Furthermore, the inclusion of auxiliary variables, even if not part of the main model, can be associated with the probability of missingness, enhancing the likelihood of satisfying the Missing at Random (MAR) assumption and improving estimation efficiency **?**.

The specification of imputation models is done on a variable basis, either using a prediction matrix where the type of prediction variable should be specified accordingly (see table) or through a list of formulas in the formula parameter. The latter option proves useful in formulating imputation models with polynomial terms or interactions compared to the prediction matrix specification, which requires the inclusion of additional terms as Just Another Variable (JAV).

However, even when considering an interaction term, depending on the adapted individual imputation model, it has been suggested, for instance, for treatment interaction effects, to conduct separated imputation by treatment group **?**. Additionally, there are imputation models based on random forest or deep learning that can handle interaction and non-linear terms that do not require the explicit inclusion of the non-linear terms.

Post-Imputation

During the imputation process, certain issues may arise that halt the process. In hierarchical model imputations, many issues are linked to methods based on parametric hierarchical models, which may struggle to estimate a model midway through the process. In such cases, it is advisable to examine the imputation log file to identify variables with imputation issues. Subsequently, reducing the number of predictors in the imputation model could be explored, either by using functions like quickpred or by considering variable transformations, such as scaling. Adjusting the level of the hierarchical model (e.g., using a homogenous variance model or a 1l model) can also be beneficial. Additionally, checking the range of imputed variables is crucial, as excessively large imputed values for one predictor could lead to convergence issues in other variables. This can be mitigated by including post-processing specifications on problematic variables or by using imputation models like Predicted Mean Matching (PMM), ensuring imputed values align with the observable values. In certain cases, a separate imputation strategy may be considered. For instance, in analyses involving multiple endpoints, conducting separate imputation processes for each endpoint might be preferable to a unified imputation process.

Convergence and Sensitivity Analysis

Before commencing the analysis, it is imperative to verify the convergence of the imputation process. This is typically achieved through trace plots or by evaluating prediction plots.

While the majority of Multiple Imputation by Chained Equations (MICE) methods are based on Missing at Random (MAR) assumptions, field expert input may suggest that the Missing Not at Random (MNAR) mechanism could be plausible for certain variables. An MNAR variable is one in which the probability of missingness depends on an unobservable variable. This can occur when missingness is associated with the incomplete value itself (self-marking) or when there is an unobserved variable linked to both the value and the probability of missingness of the incomplete value (indirectly non-informative). Specifically, for the indirectly non-informative case in hierarchical datasets, imputation methods based on the Heckman method, such as those proposed by Hammon (2021) and Munoz (2023), can be considered.

1.5. Setup

Set up the R environment and load the necessary packages:

```
R> set.seed(123)          # for reproducibility
R> library(mice)          # for imputation
R> library(miceadds)      # for additional imputation routines
R> library(ggmice)        # for incomplete/imputed data visualization
R> library(ggplot2)       # for visualization
R> library(dplyr)         # for data wrangling
R> library(lme4)          # for multilevel modeling
R> library(mitml)         # for multilevel parameter pooling
R> library(micemd)        # for case study data and imputation cf. heckman models
R> library(metamisc)      # for case study data
R> library(broom.mixed)   # for multilevel estimates
```

TODO: add table with predictor matrix values

- -2 = cluster variable

- 1 = overall effect
- 3 = overall + group-level effect
- 4 = individual-level (random) and group-level (fixed) effect

2. Case study I: popularity data

In this section we will go over the different steps involved with imputing incomplete multilevel data with the R package mice. We consider the simulated `popmis` dataset, which included pupils ($n = 2000$) clustered within schools ($N = 100$). The following variables are of primary interest:

- `school`, school identification number (clustering variable);
- `popular`, pupil popularity (self-rating between 0 and 10; unit-level);
- `sex`, pupil sex (0=boy, 1=girl; unit-level);
- `texp`, teacher experience (in years; cluster-level).

The research objective of the `popmis` dataset is to predict the pupils' popularity based on their gender and the experience of the teacher. The analysis model corresponding to this dataset is multilevel regression with random intercepts, random slopes and a cross-level interaction. The outcome variable is `popular`, which is predicted from the unit-level variable `sex` and the cluster-level variable `texp`:

```
R> mod <- popular ~ 1 + sex + (1 | school)
```

The estimated effects in the complete data are presented in Table XYZ. We consider the associations in the full data set to be the true associations.

Load the data into the environment and select the relevant variables:

```
R> popmis <- popmis[, c("school", "popular", "sex")]
```

First we plot the pattern of missing data within categories of the relevant variables. Plot the missing data pattern:

```
R> plot_pattern(popmis)
```

The missingness is univariate and sporadic, which is illustrated in the missing data pattern in Figure 2.

The ICC in the incomplete data is `round(icc(popular ~ as.factor(school), data = na.omit(popmis)), 2)`. This tells us that the multilevel structure of the data should probably be taken into account. If we don't, we'll may end up with incorrect imputations, biasing the effect of the clusters towards zero.

To develop the best imputation model for the incomplete variable `popular`, we need to know whether the observed values of `popular` are related to observed values of other variables. Plot the pair-wise complete correlations in the incomplete data:

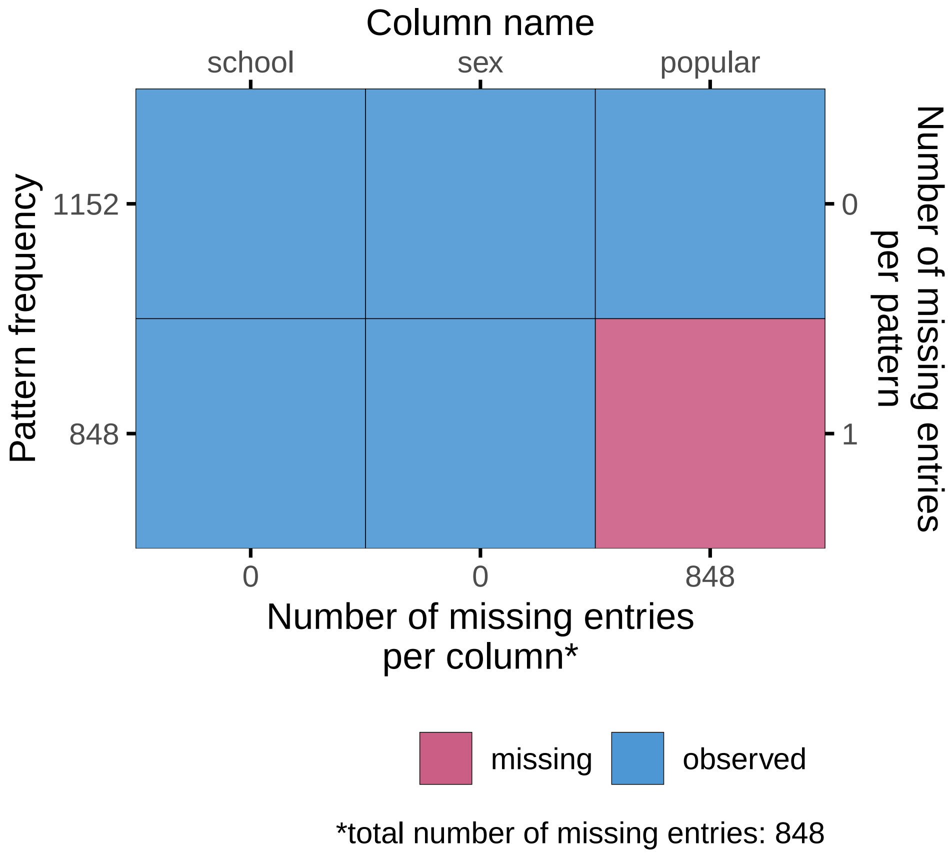
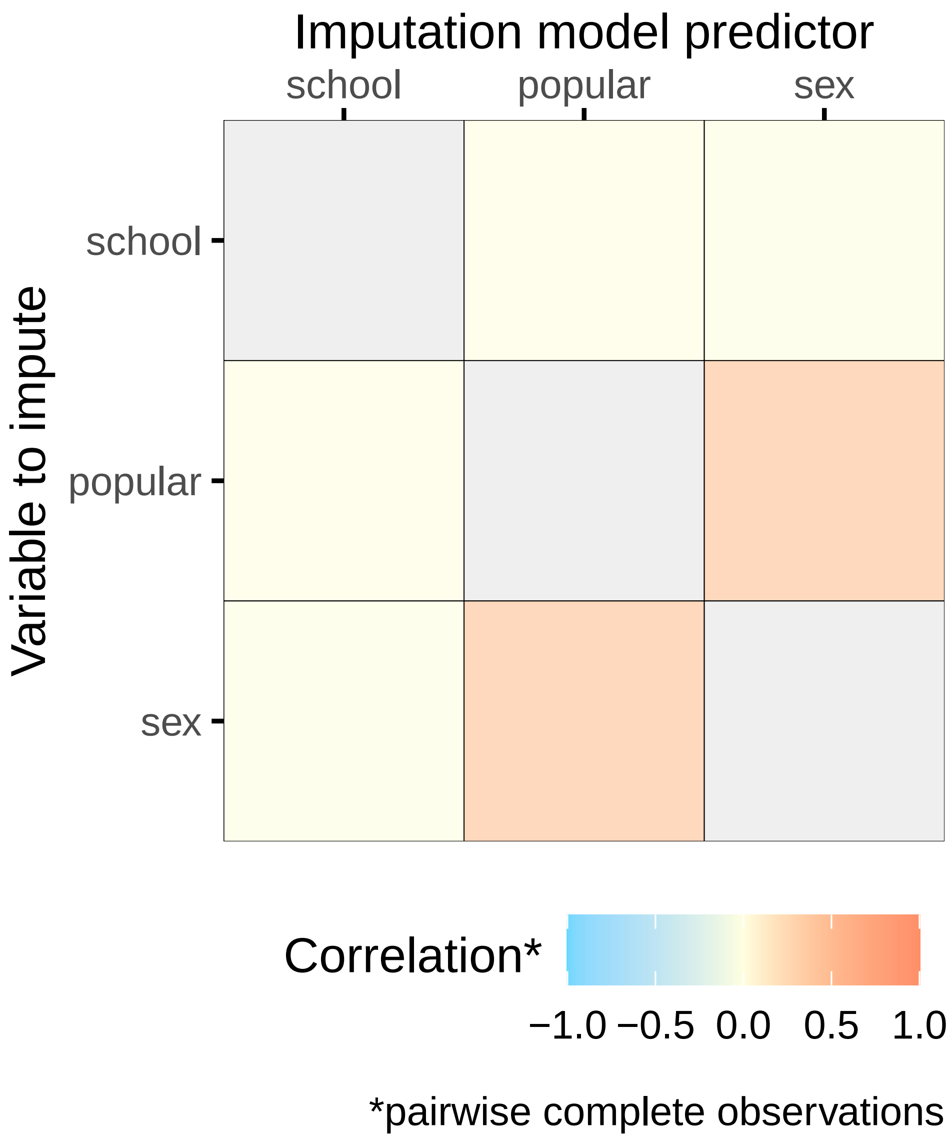


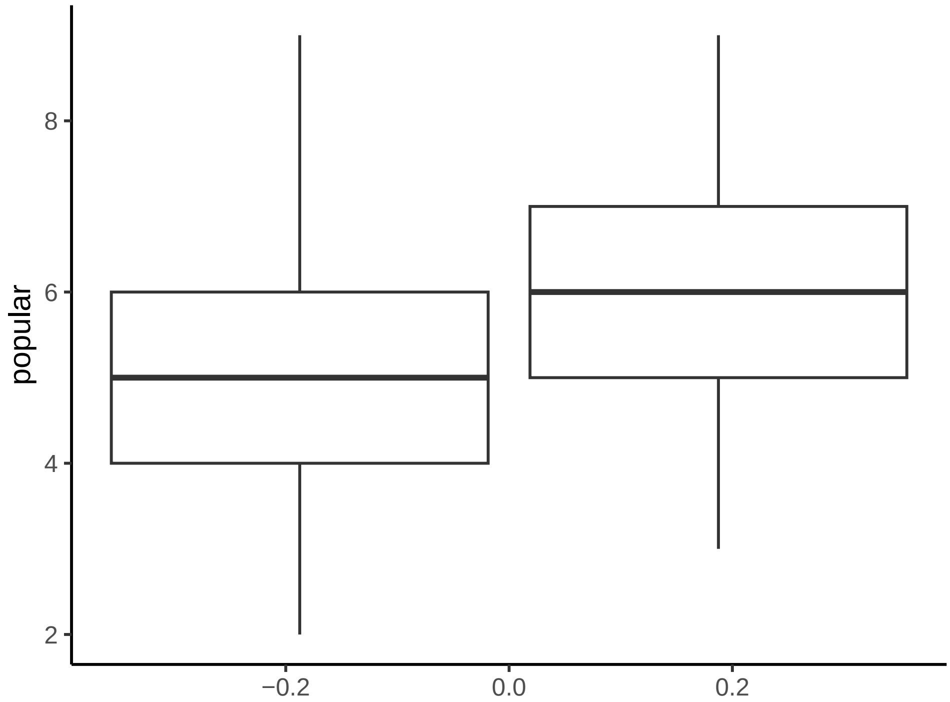
Figure 2: Missing data pattern in the popularity data

```
R> plot_corr(popmis)
```



This shows us that `sex` may be a useful imputation model predictor. Moreover, the missingness in `popular` may depend on the observed values of other variables.

```
R> # ggmice(popmis, aes(sex)) +
R> #   geom_histogram(fill = "white") +
R> #   facet_grid(. ~ is.na(popular), scales = "free", labeller = label_both)
R>
R> ggplot(popmis, aes(y = popular, group = sex)) +
+   geom_boxplot() +
+   theme_classic()
```

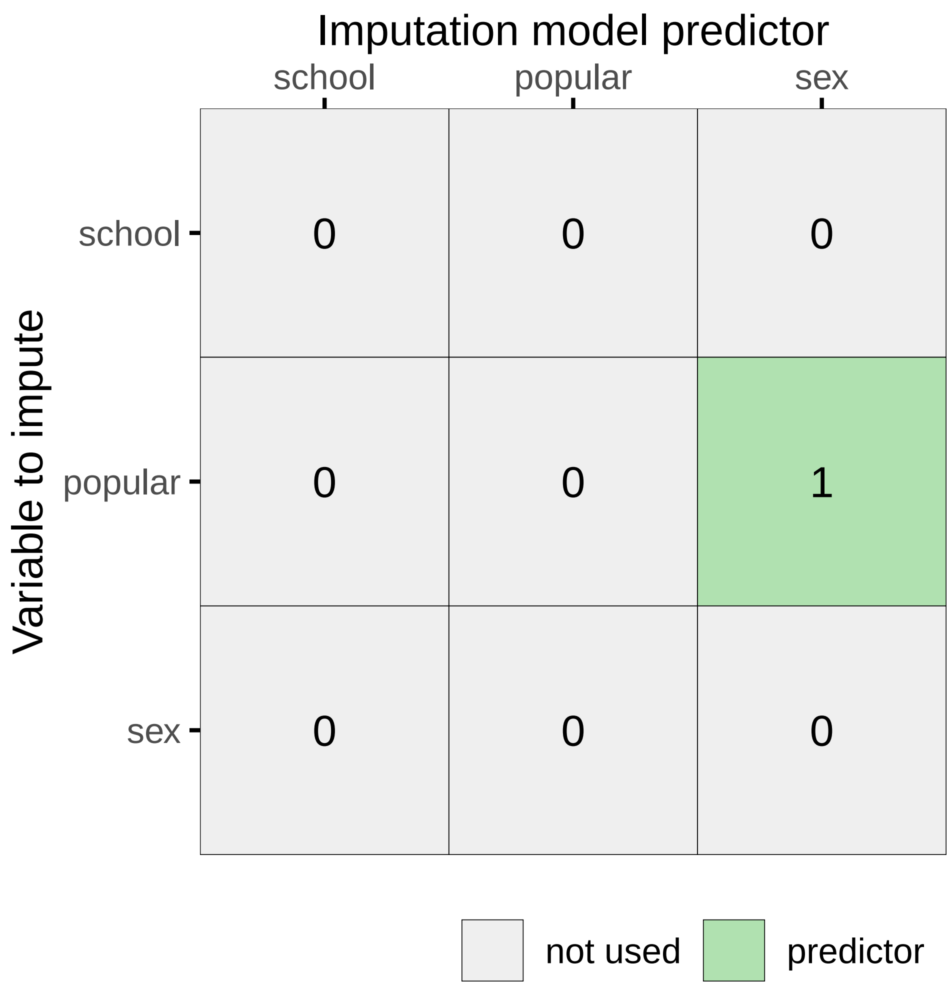


Imputation ignoring the cluster variable (not recommended)

The first imputation model that we'll use is likely to be invalid. We do not use the cluster identifier `school` as imputation model predictor. With this model, we ignore the multilevel structure of the data, despite the high ICC. This assumes exchangeability between units. We include it purely to illustrate the effects of ignoring the clustering in our imputation effort.

Create a methods vector and predictor matrix for `popular`, and make sure `school` is not included as predictor:

```
R> meth <- make.method(popmis) # methods vector
R> pred <- quickpred(popmis)   # predictor matrix
R> plot_pred(pred)
```

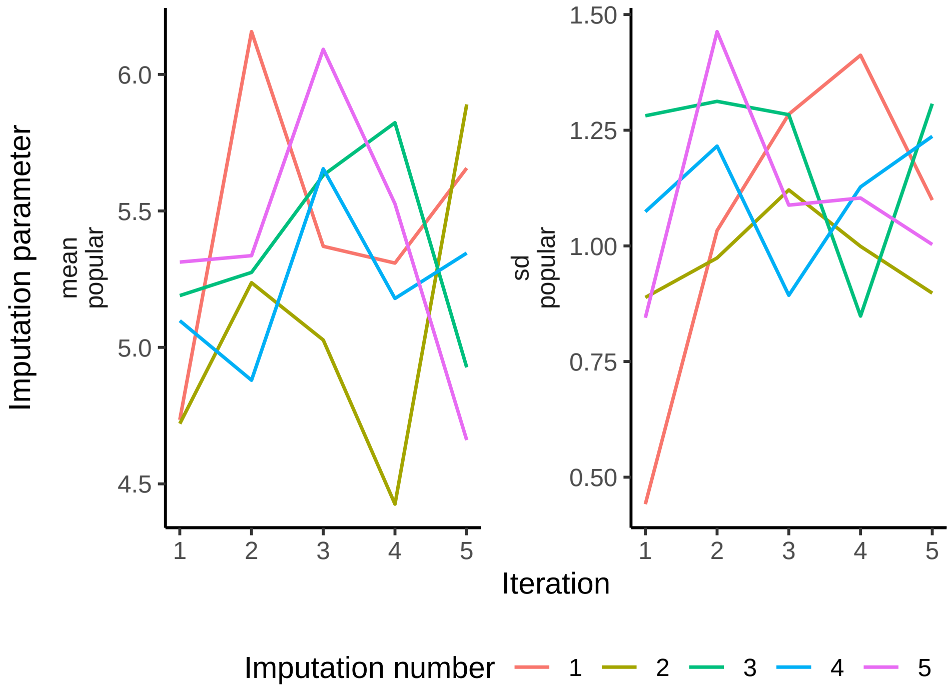


Impute the data, ignoring the cluster structure:

```
R> imp <- mice(popmis, pred = pred, print = FALSE)
```

Evaluate the convergence of the algorithm:

```
R> plot_trace(imp)
```



Analyze the imputations:

```
R> fit <- with(imp,
+              lmer(popular ~ 1 + sex  + (1 | school)))
```

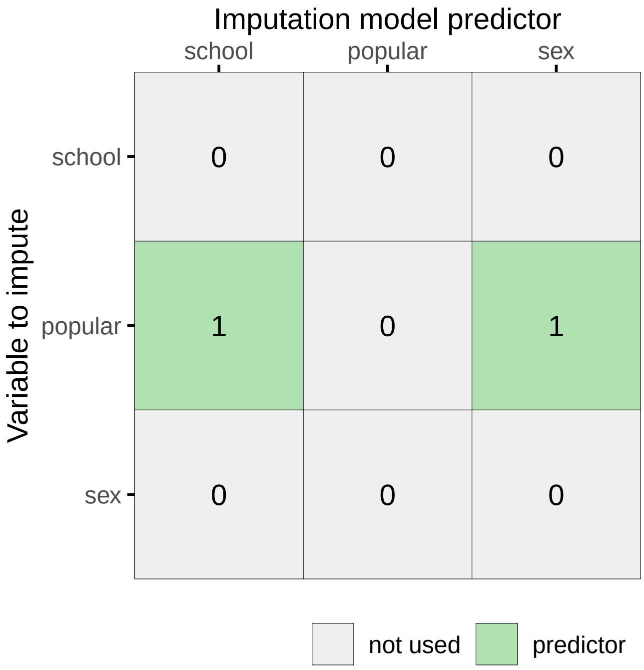
Print the estimates:

```
R> testEstimates(as.mitml.result(fit), extra.pars = TRUE)
```

Imputation with the cluster variable as predictor (not recommended)

We will now use `school` as a predictor to impute all other variables. This is still not recommended practice, since it only works under certain circumstances and results may be biased (Drechsler 2015; Enders, Mistler, and Keller 2016). But at least, it includes some multilevel aspect. This method is also called 'fixed cluster imputation', and uses N-1 indicator variables representing allocation of N clusters as a fixed factor in the model (Reiter, Raghunathan, and Kinney 2006; Enders et al. 2016). Colloquially, this is 'multilevel imputation for dummies'.

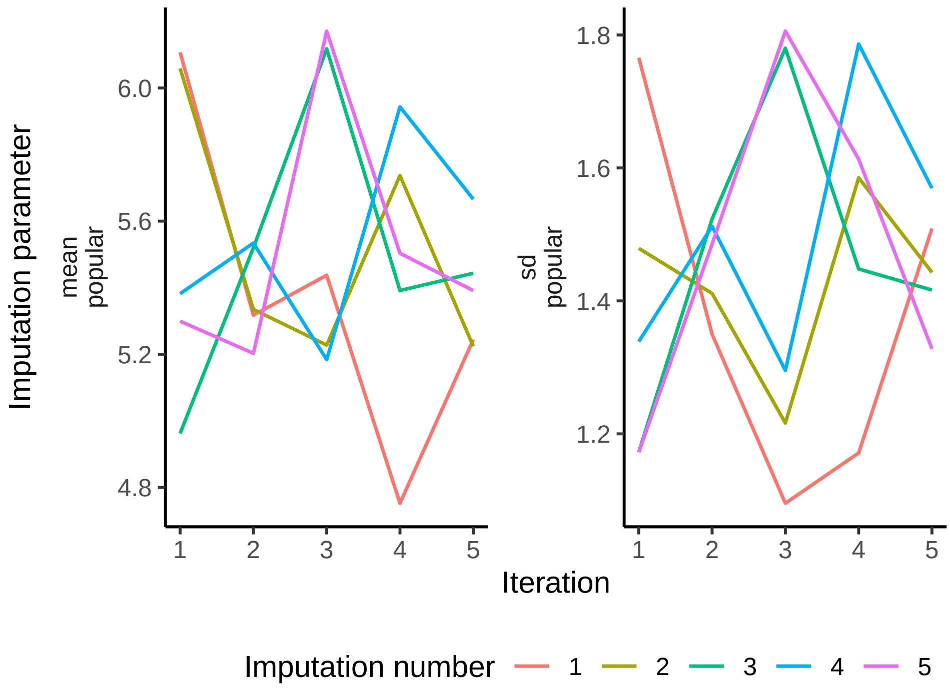
```
R> # adjust the predictor matrix
R> pred["popular", "school"] <- 1
R> plot_pred(pred)
```




```
R> # impute the data, cluster as predictor
R> imp <- mice(popmis, pred = pred, print = FALSE)
```

Evaluate the convergence of the algorithm:

```
R> plot_trace(imp)
```



Analyze the imputations:

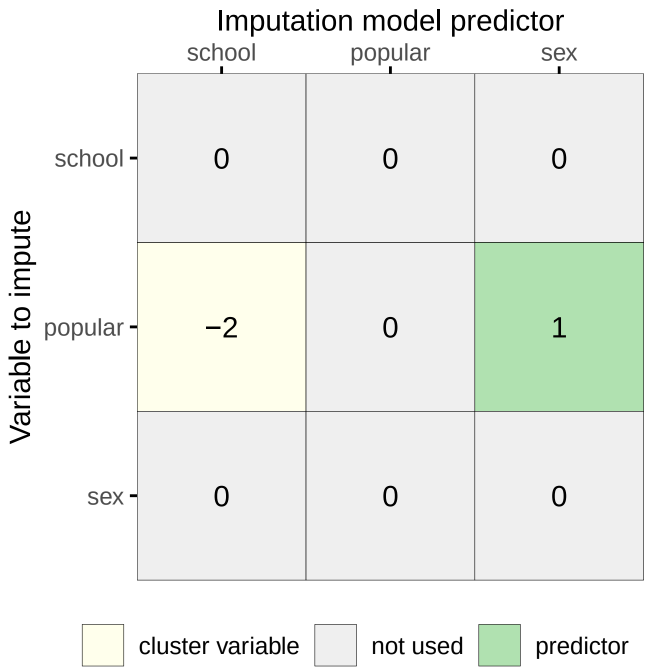
```
R> fit <- with(imp,
+              lmer(popular ~ 1 + sex + (1 | school)))
```

Print the estimates:

```
R> testEstimates(as.mitml.result(fit), extra.pars = TRUE)
```

Imputation with multilevel model

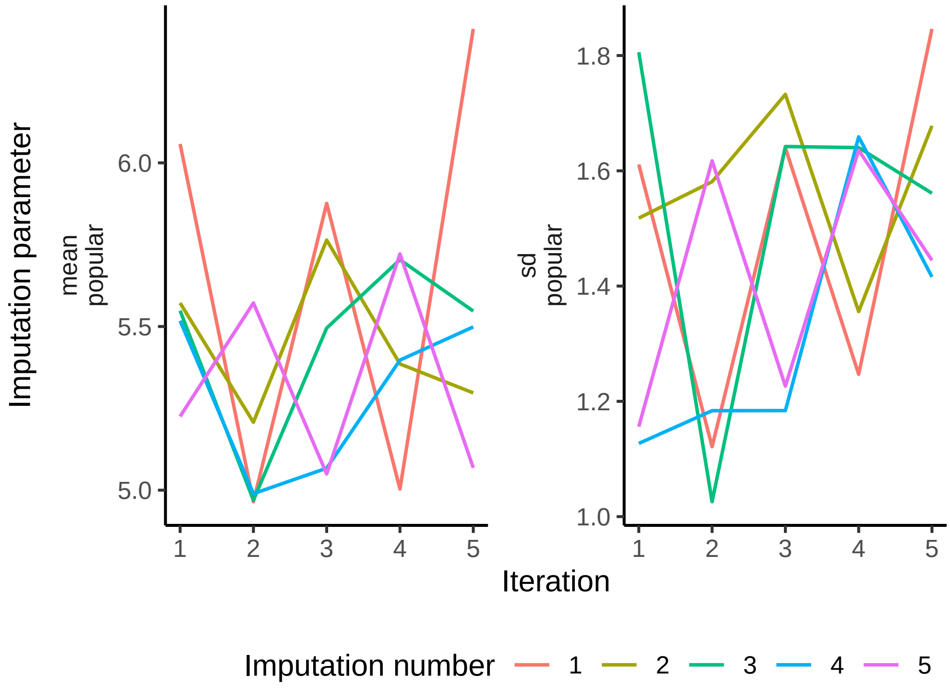
```
R> # adjust the predictor matrix
R> pred["popular", "school"] <- -2
R> plot_pred(pred)
```




```
R> # impute the data, cluster as predictor
R> imp <- mice(popmis, pred = pred, print = FALSE)
```

Evaluate the convergence of the algorithm:

```
R> plot_trace(imp)
```



Analyze the imputations:

```
R> fit <- with(imp,
+              lmer(popular ~ 1 + sex + (1 | school)))
```

Print the estimates:

```
R> testEstimates(as.mitml.result(fit), extra.pars = TRUE)
```

3. Case study II: IMPACT data (syst missingness, pred matrix)

We illustrate how to impute incomplete multilevel data by means of a case study: `impact` from the **metamisc** package (empirical data on traumatic brain injuries, $n = 11,022$ units across $N = 15$ clusters, Debray and de Jong 2021). The `impact` data set contains traumatic brain injury data on $n = 11022$ patients clustered in $N = 15$ studies with the following 11 variables:

- `name` Name of the study,
- `type` Type of study (RCT: randomized controlled trial, OBS: observational cohort),
- `age` Age of the patient,
- `motor_score` Glasgow Coma Scale motor score,
- `pupil` Pupillary reactivity,
- `ct` Marshall Computerized Tomography classification,
- `hypox` Hypoxia (0=no, 1=yes),
- `hypots` Hypotension (0=no, 1=yes),

- `tsah` Traumatic subarachnoid hemorrhage (0=no, 1=yes),
- `edh` Epidural hematoma (0=no, 1=yes),
- `mort` 6-month mortality (0=alive, 1=dead).

The analysis model for this dataset is a prediction model with `mort` as the outcome. In this tutorial we'll estimate the adjusted prognostic effect of `ct` on mortality outcomes. The estimand is the adjusted odds ratio for `ct`, after including `type`, `age` `motor_score` and `pupil` into the analysis model:

```
R> mod <- mort ~ type + age + motor_score + pupil + ct + (1 | name)
```

Note that variables `hypots`, `hypox`, `tsah` and `edh` are not part of the analysis model, and may thus serve as auxiliary variables for imputation.

The `impact` data included in the **metamisc** package is a complete data set. The original data has already been imputed once (Steyerberg et al, 2008). For the purpose of this tutorial we have induced missingness (mimicking the missing data in the original data set before imputation). The resulting incomplete data can be accessed from zenodo link to be created.

Load the complete and incomplete data into the R workspace:

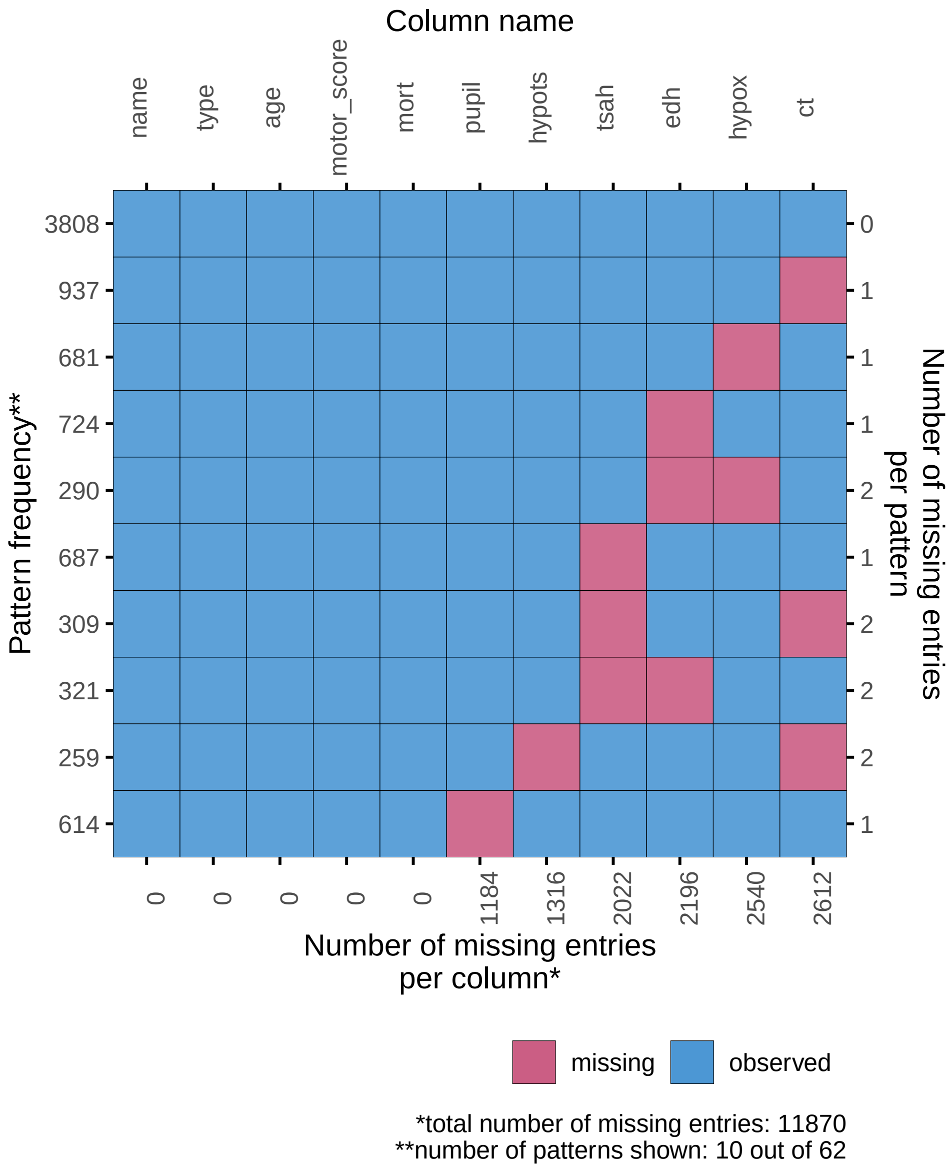
```
R> data("impact", package = "metamisc")      # complete data
R> dat <- read.table("link/to/the/data.txt") # incomplete data
```

We will use the complete data estimates as comparative truth in this tutorial. The estimated effects in the complete data are presented in Table XYZ.

3.1. Missingness

To explore the missingness, it is wise to look at the missing data pattern. The ten most frequent missingness patterns are shown:

```
R> plot_pattern(dat, rotate = TRUE, npat = 10L)  # plot missingness pattern
```

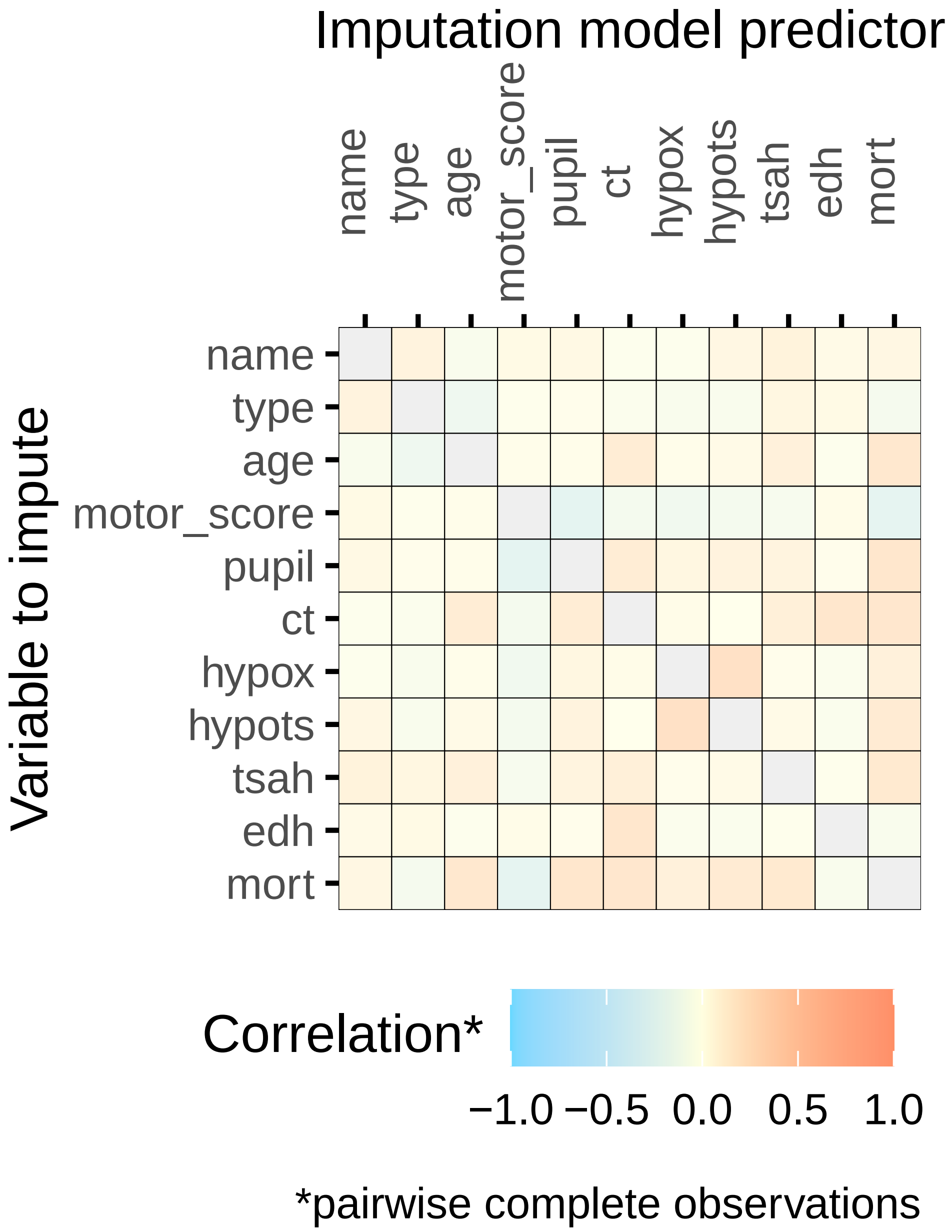


This shows that we need to impute `ct` and `pupil`.

To develop the best imputation model, we need to investigate the relations between the observed values of the incomplete variables and the observed values of other variables, and the relation between the missingness indicators of the incomplete variables and the observed values of the other variables. To see whether the missingness depends on the observed values of other variables, we can test this statistically or use visual inspection (e.g. a histogram faceted by the missingness indicator).

We should impute the variables `ct` and `pupil` and any auxiliary variables we might want to use to impute these incomplete analysis model variables. We can evaluate which variables may be useful auxiliaries by plotting the pairwise complete correlations:

```
R> plot_corr(dat, rotate = TRUE) # plot correlations
```



This shows us that `hypox` and `hypot` would not be useful auxiliary variables for imputing `ct`. Depending on the minimum required correlation, `tsah` could be useful, while `edh` has the strongest correlation with `ct` out of all the variables in the data and should definitely be included in the imputation model. For the imputation of `pupil`, none of the potential auxiliary variables has a very strong relation, but `hypots` could be used. We conclude that we can exclude `hypox` from the data, since this is neither an analysis model variable nor an auxiliary variable for imputation:

```
R> dat <- select(dat, !hypox)  # remove variable
R> dat <- mutate(dat, motor_score = as.factor(motor_score))
```

3.2. Complete case analysis

As previously stated, complete case analysis lowers statistical power and may bias results. The complete case analysis estimates are:

```
R> fit <- glmer(mod, family = "binomial", data = na.omit(dat)) # fit the model
R> tidy(fit, conf.int = TRUE, exponentiate = TRUE)             # print estimates
```

```
# A tibble: 11 x 9
   effect   group term   estimate std.error statistic   p.value conf.low conf.high
   <chr>    <chr> <chr>     <dbl>     <dbl>     <dbl>     <dbl>    <dbl>     <dbl>
 1 fixed    <NA>  (Int~    0.0863   0.0182     -11.6   3.00e-31   0.0571     0.130
 2 fixed    <NA>  type~    0.757    0.137       -1.54  1.22e- 1   0.531      1.08
 3 fixed    <NA>  age      1.03     0.00265     12.9   7.40e-38   1.03       1.04
 4 fixed    <NA>  moto~    0.651    0.0732      -3.82  1.34e- 4   0.522      0.811
 5 fixed    <NA>  moto~    0.489    0.0555      -6.30  2.97e-10   0.391      0.611
 6 fixed    <NA>  moto~    0.274    0.0321     -11.0   2.28e-28   0.218      0.345
 7 fixed    <NA>  pupi~    3.20     0.317       11.7   8.18e-32   2.63       3.88
 8 fixed    <NA>  pupi~    1.75     0.195        5.06  4.27e- 7   1.41       2.18
 9 fixed    <NA>  ctIII    2.41     0.268        7.89  3.05e-15   1.94       2.99
10 fixed    <NA>  ctIV~    2.30     0.214        8.95  3.56e-19   1.92       2.76
11 ran_pa~ name  sd__~    0.230   NA           NA    NA          NA         NA
```

As we can see, a higher `ct` (Marshall Computerized Tomography classification) is associated with a lower odds of 6-month mortality, given by the odds ratio exp(0.42), CI … to …, when controlling for…

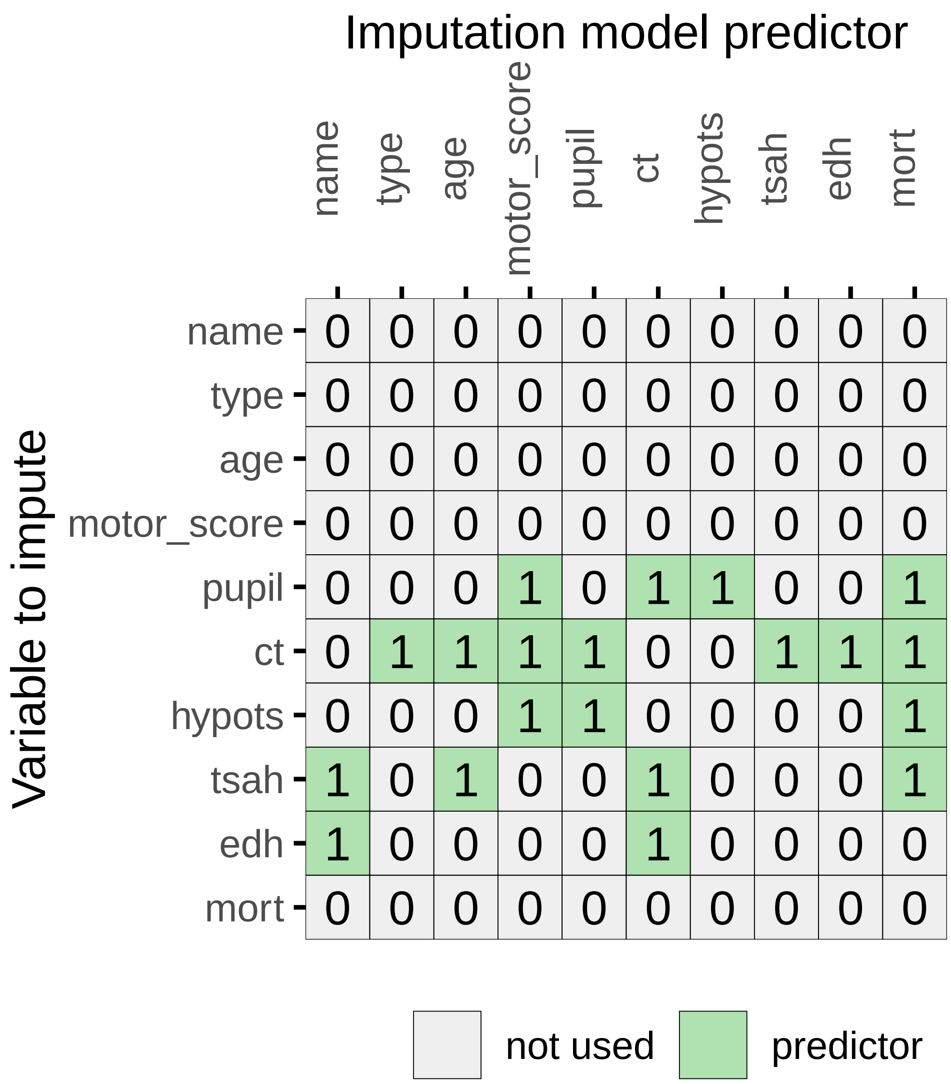
3.3. Imputation model

Mutate data to get the right data types for imputation (e.g. integer for clustering variable).

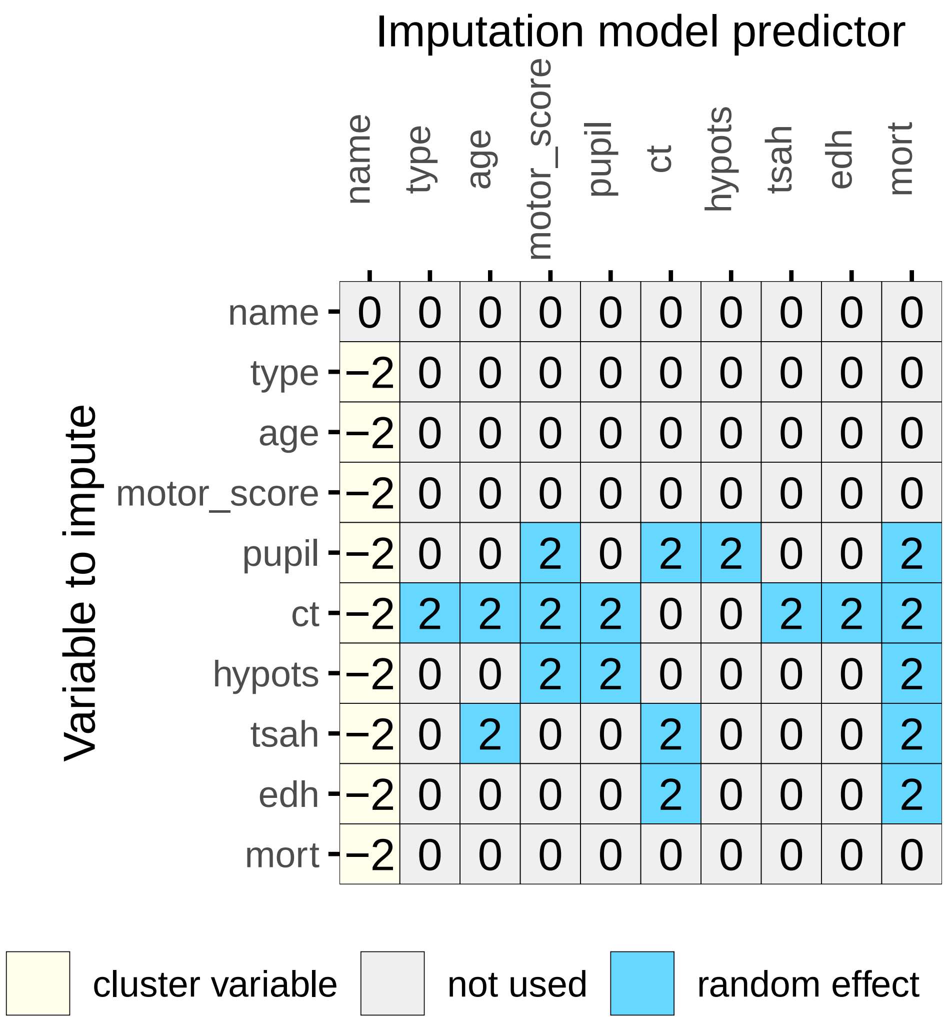
```
R> dat <- dat %>% mutate(across(everything(), as.integer))
```

Create a methods vector and predictor matrix, and make sure `name` is not included as predictor, but as clustering variable:

```
R> meth <- make.method(dat) # methods vector
R> pred <- quickpred(dat)   # predictor matrix
R> plot_pred(pred, rotate = TRUE)
```




```
R> pred[pred == 1] <- 2
R> pred["mort", ] <- 2
R> pred[, "mort"] <- 2
R> pred[c("name", "type", "age", "motor_score", "mort"), ] <- 0
R> pred[, "name"] <- -2
R> diag(pred) <- 0
R> plot_pred(pred, rotate = TRUE)
```




```
R> meth <- make.method(dat)
R> meth
```

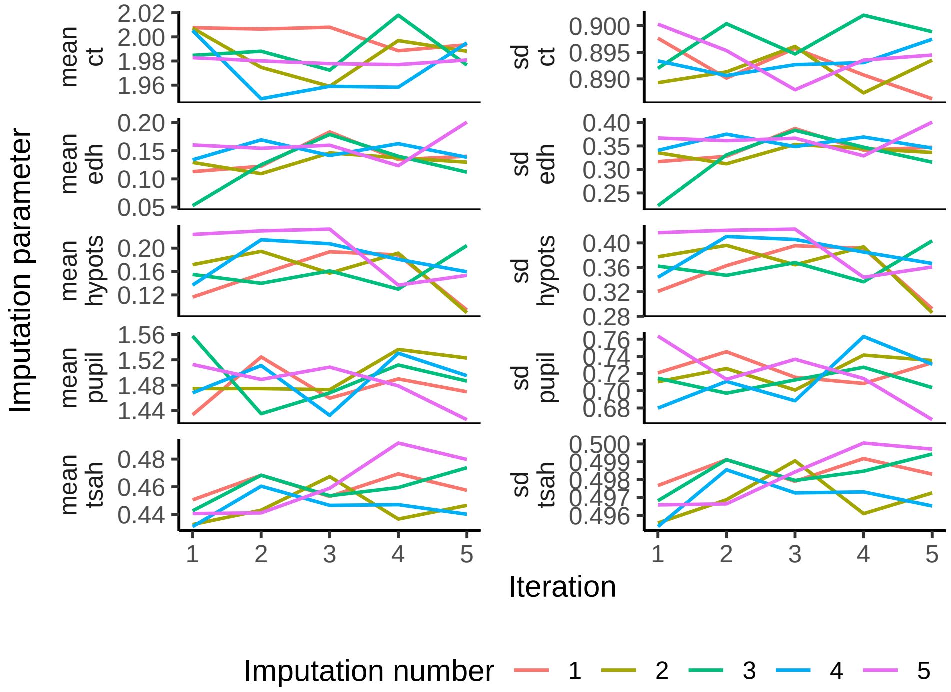
```
       name        type         age motor_score       pupil          ct
         ""          ""          ""          ""       "pmm"       "pmm"
     hypots        tsah         edh        mort
      "pmm"       "pmm"       "pmm"          ""
```

Impute the incomplete data

```
R> imp <- mice(dat, method = meth, predictorMatrix = pred, printFlag = FALSE)
```

Evaluate the convergence of the algorithm:

```
R> plot_trace(imp)
```



Analyze the imputed data:

```
R> fit <- imp %>%
+   with(glmer(
+     mort ~ type + age + as.factor(motor_score) + pupil + ct + (1 | name),
+     family = "binomial"
+     ))
R> # tidy(pool(fit))
R> # as.mitml.result(fit)
R> # testEstimates(as.mitml.result(fit))
```

The estimated effects after imputation are presented in Table XYZ.

4. Case study III: obesity data

In this example, we demonstrate a multilevel imputation of random intercept and random slope model with a continuous response. We utilize the obesity dataset included in the `micemd`@ package, a simulated dataset that emulates an electronic survey in which individuals are asked to provide information about their weight and consumption habits in different countries. We simulate data for 5 clusters so that the true values are known. We use the following variables from the dataset:

- **Cluster:** Region of the patients' healthcare provider (Cluster variable),
- **Gender:** Subjects' Gender (0=male, 1=female),
- **Age:** Subjects' age,
- **Height:** Subjects' height in metres,

- **Weight:** Subjects' weight in kilograms,
- **BMI:** Subjects' body mass index,
- **FamOb:** Family obesity history (yes or no),
- **Time:** Response time in minutes (exclusion-restriction variable).

In this dataset, Age and FamOb are MAR, while the weight variable is affected by selection bias, attributed to an indirect MNAR mechanism. This MNAR mechanism typically arises when an unobserved or omitted variable influences both the value of the incomplete variable (in this case, Weight) and its likelihood of being missing (denoted as R).

In the primary analysis model, BMI serves as the dependent variable, with Age, Gender, and FamOb as predictors. Because of the clustered nature of the data, which is quantified with the Intraclass Correlation Coefficient (ICC) below, we include random intercepts, as well as a random slope for the Age variable. The model is represented as:

$$BMI_{ij} = (\beta_o + b_{oj}) + (\beta_1 + b_{oj}) * Age_{ij} + \beta_2 * FamOb_{ij} + \beta_3 Gender_{ij} + \epsilon_{ij} \qquad (1)$$

We start by loading the data:

```
R> #data("data_heckman", package = "micemd")
R> #dat <- data_heckman
```

Now, let's begin by examining the missing patterns in the data by cluster:

```
R> #ggmice::plot_pattern(data=Obesity,cluster="Cluster") does not work!! bug
R> #ggmice::plot_pattern(data=Obesity,cluster=Obesity$Cluster) does not work!! bug
R> library(ggpubr)
R> myplots <- lapply(1:5, function(i) {
+   ggmice::plot_pattern(setDT(Obesity)[Cluster==i])+
+   ggplot2::ggtitle(paste0("Cluster", i))
+ })
R> ggarrange(myplots[[1]], myplots[[3]], nrow=1,common.legend = TRUE, legend="bottom")
```

We observe that the missing pattern is non-monotonic and quite similar across the clusters. However, regarding the weight variable, we notice that is systematically missing in cluster 3. In order to evaluate if we require a imputation method that accounts for clustering we assess the Intraclass Correlation

```
R> Nulmodel <- lme4::lmer(BMI ~ 1 + (1|Cluster), data = Obesity)
R> performance::icc(Nulmodel)
```

```
# Intraclass Correlation Coefficient

    Adjusted ICC: 0.362
  Unadjusted ICC: 0.362
```

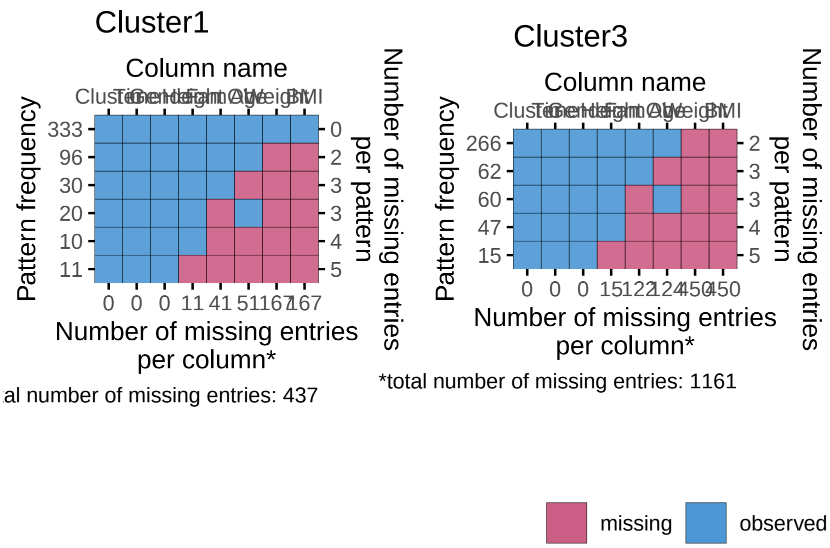


Figure 3: Missing pattern

Since the ICC is above 0.1 and as the main analysis will be use a mixed model, we decide to use two-level (2l) imputation methods. In this imputation process, we include all predictor variables from equation 1 in the main model. However, since BMI is a composite of weight and height, we use deterministic imputation for these, which is described below.

We use the **find.defaultMethodfunction** provided in the **micemd** package, which suggests an appropriate method for MAR variables based on the type of variable, number of observations in the cluster, and number of clusters.

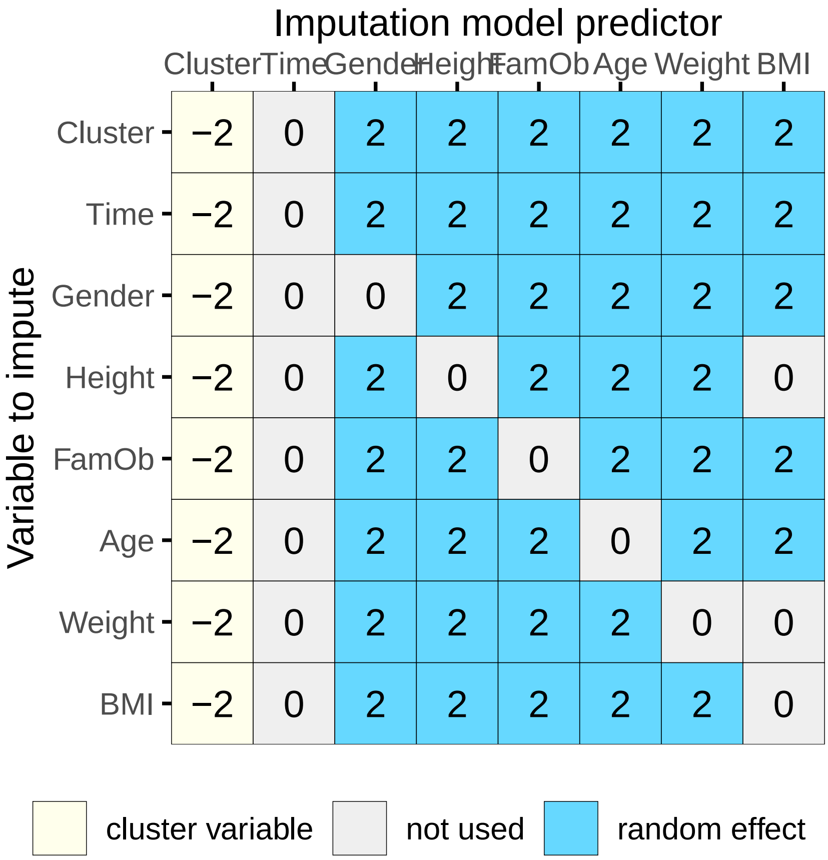
It suggests using '2l.2stage.bin' for the FAV variable and '2l.2stage.norm' for the age variable. However, after inspecting the age density plot, we consider modifying its method to '2l.2stage.pmm'. For the BMI variable, we employ deterministic imputation.

```
R> library(micemd)
R> meth_mar <- micemd::find.defaultMethod(Obesity, ind.clust=1, I.small = 7,
+                                  ni.small = 100, prop.small = 0.4)
R> meth_mar["BMI"]<- "~ I(Weight / (Height)^2)"
R> meth_mar["Age"]<-"2l.2stage.pmm"
```

For these imputation models, it is necessary to specify the prediction matrix, with the cluster variable labelled as -2 and the predictor variable measured within clusters labelled as 2, encompassing all variables. We need to suprime the variable Time as this variable is not specified in the main model. We also modify the relationship between BMI, weight and height in the prediction matrix to avoid circular predictions. Then we proceed to run the imputation model.

```
R> pred_mar <- mice(Obesity, maxit = 0)$pred
R> pred_mar[,"Cluster"] <- -2 # clustering variable
R> pred_mar[,"Time"] <- 0
R> pred_mar[pred_mar==1] <- 2
```

```
R> pred_mar[c("Height", "Weight"), "BMI"] <- 0
R> ggmice::plot_pred(pred_mar)
```




```
R> imp_mar <- mice::mice(data = Obesity, meth = meth_mar, pred = pred_mar,
+                   m=10, seed = 123, printFlag = FALSE)

R> summary(complete(imp_mar,"long")$Weight)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
 -19.48   68.45   81.65   81.28   94.12  160.76
```

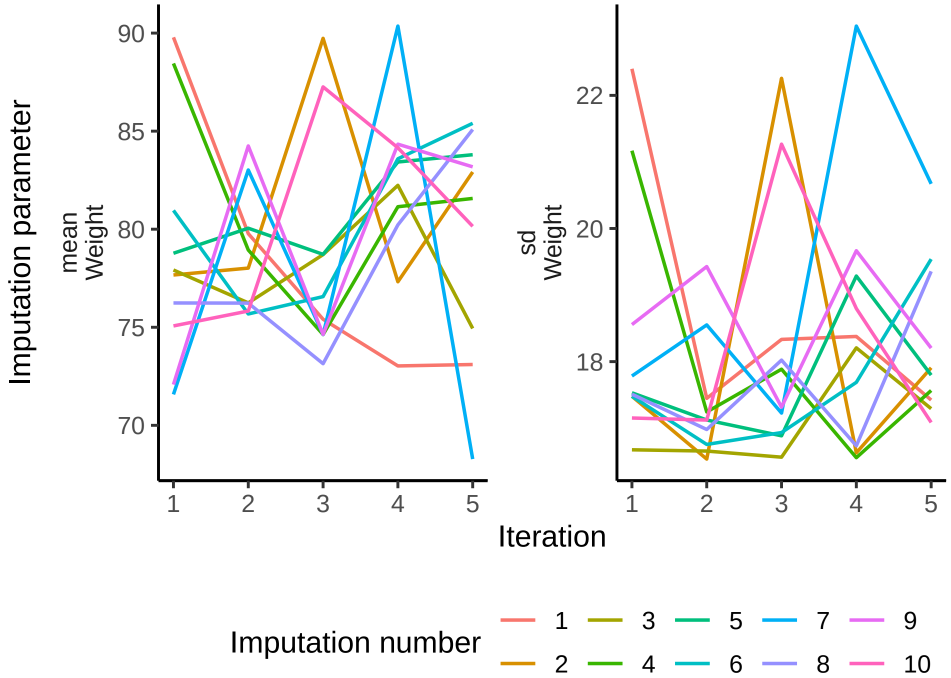
We are also contemplating the utilisation of the ???pmm??? option, as the values imputed using a fully parametric method may be implausibly low for some patients.

```
R> meth_mar["Weight"]<-"2l.2stage.pmm"
R> imp_mar_pmm <- mice(data = Obesity, meth = meth_mar, pred = pred_mar,
+                       m=10, seed = 123, printFlag = FALSE)

R> summary(complete(imp_mar_pmm,"long")$Weight)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  28.35   69.25   82.43   82.41   94.76  134.61
```

```
R> ggmice::plot_trace(imp_mar_pmm, "Weight")
```



After confirming convergence, we proceed to save the results for future use. We consider the possibility that patients may not have been selected randomly, which would then have led to a distribution for weight that does not reflect the weight in the population. It???s likely that an omitted variable, like self-esteem, could influence this selection. For instance, individuals with lower self-esteem might have higher weight values, impacting their willingness to provide honest information due to embarrassment.

To address this situation, two approaches have been proposed for dealing with Missing Not at Random (MNAR) data: pattern-mixed models and selection models. Within pattern-mixed models, methods like the delta method and more advanced ones like NARFS have been suggested. The selection model approach includes methods such as the Heckman model, which can be particularly useful in this case. Several methods, including those by **??**, and the recently a Heckman method designed for two-level data, allow for variations in intercepts and exposure effects (random intercept and slope).

To apply the **2l.2stage.heckman** method, the weight variable should be specified as '2l.2stage.heckman' found in the micemd package. Additionally, the prediction matrix needs modification because this method involves specifying two equations: one for the outcome, describing the incomplete variable in terms of partially observed predictors (in this case, all variables from the main model), and the other for the selection model, explaining the probability of being observed based (R) on certain variables. For the outcome equation we consider the same imputation model that we used for the MAR case (main model).

$$Weight_{ij} = \beta_o^O + \beta_1^O Age_{ij} + \beta_2^O FamOb_{ij} + \beta_3^O Gender_{ij} + \epsilon_{ij}^O$$

Regarding the selection equation, we include the same predictors as those in the main model, as well as a time variable. Here the time variable serves as a restriction exclusion variable specifically explaining the probability of being observed but not affecting the incomplete value (Weight). In this context, we assume that the time a user spends completing the survey serves as a proxy for the barriers they may encounter in survey completion, such as familiarity with the survey content or internet speed. These factors may lead the user to skip specific questions or even the entire survey. Also, we assume the time does not have any influence on the subject???s weight.

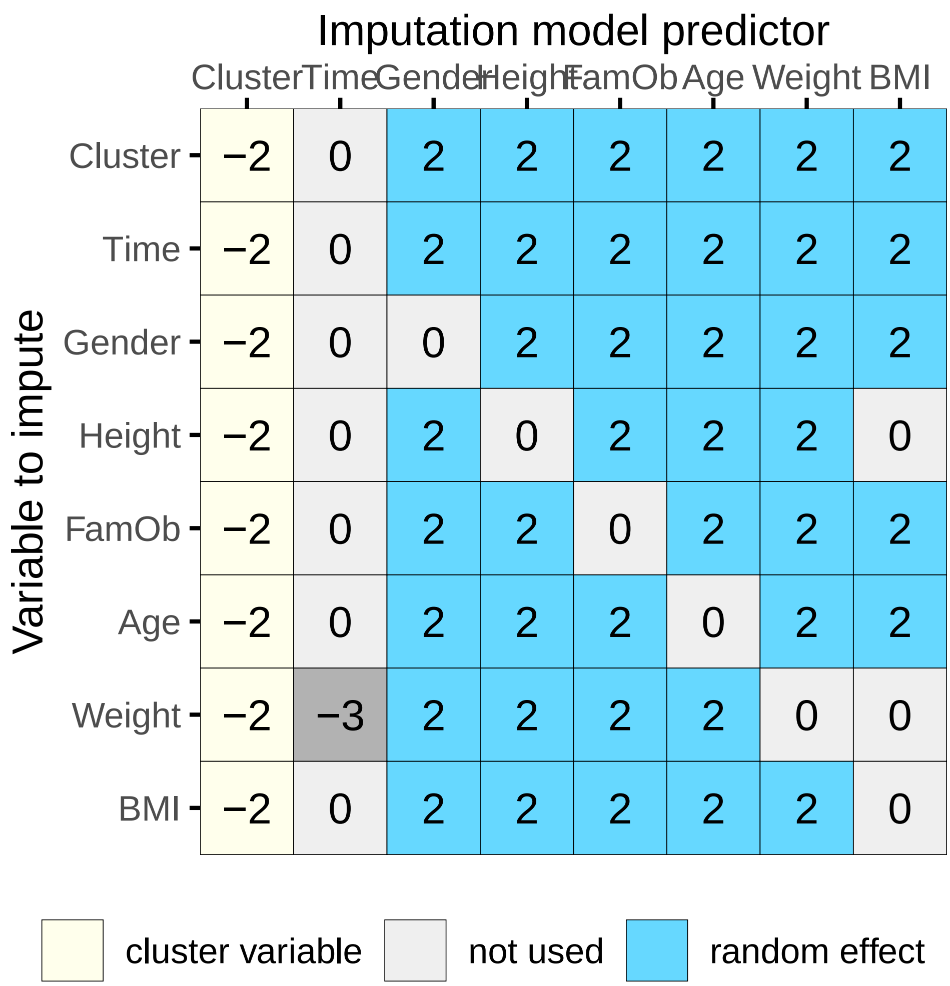
$$R_{ij} = \beta_o^S + \beta_1^S Age_{ij} + \beta_2^S FamOb_{ij} + \beta_3^S Gender_{ij} + \beta_4^S Time_{ij} + \epsilon_{ij}^S$$

These two equations are jointly estimated under the assumption that the error terms are interconnected with a bivariate normal distribution. For a more comprehensive understanding of the model and the exclusion restriction, see **?**.

To use information from both equations, we must adjust the prediction matrix. The cluster variable remains specified as before (-2). In this imputation method, all the variables present in both the selection and outcome equations are included with a random effect.

However, it is essential to distinguish which of these variables appear in each equation. In this framework, when a variable is shared between both equations, it is denoted as (2). Predictors exclusive to the outcome equation are indicated as (-4), while those exclusive to the selection equation are labelled as (-3). Consequently, the only alteration needed in the predictor matrix pertains to the variable ‘Time’.

```
R> pred_mnar <- pred_mar
R> pred_mnar["Weight","Time"]<- -3
R> ggmice::plot_pred(pred_mnar)
```



We also need to modify the method of the weight variable.

```
R> meth_mnar <- meth_mar
R> meth_mnar["Weight"]<- "31.2stage.heckman"
```

Then we proceed to run the imputation model as before, after executing these imputation procedures, it is essential to assess convergence and the coherence of the imputed values.

```
R> imp_mnar<- mice(data = Obesity, meth = meth_mnar, pred = pred_mnar,
+                   m=10, seed = 123, printFlag = FALSE)
R> summary(complete(imp_mnar,"long")$Weight)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  14.09   71.68   85.33   85.79   99.31  186.67
```

Upon examining the weight variable, we noticed that the imputed range falls outside the realm of plausible values (as weight should be positive).

```
R> summary(complete(imp_mnar,"long")$Weight)
```

```
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  14.09   71.68   85.33   85.79   99.31  186.67
```

Consequently, as before we use the 'pmm', option but this time for the Heckman imputation, this approach ensures that the imputed values remain within the range of observable values. We then run the imputation model but this time using the option of pmm, to assure that weight values are in the range of the observable data, this can be implemented by setting the pmm parameter to true.

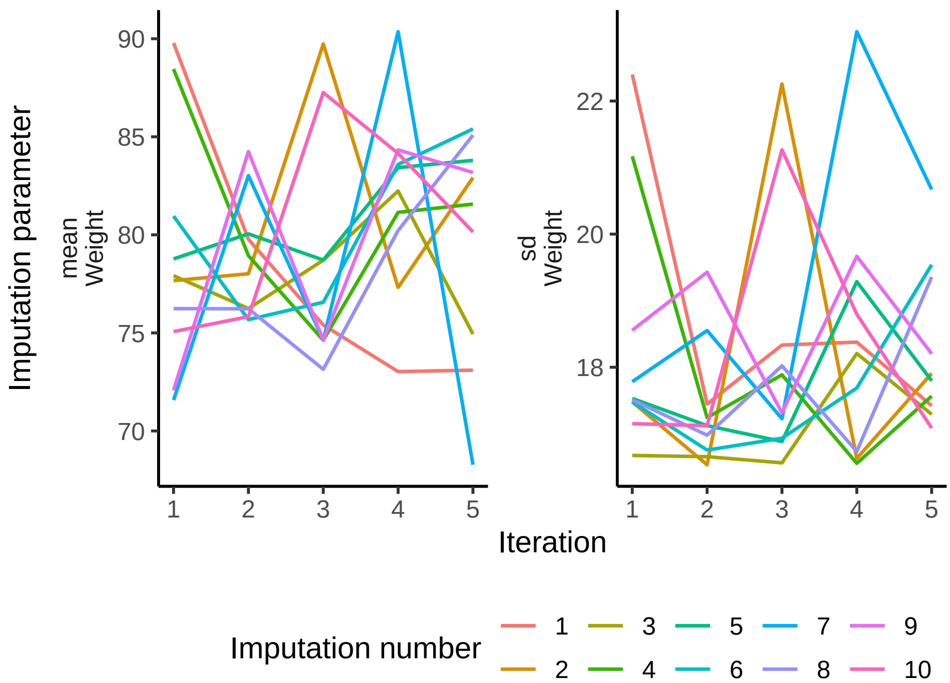
```
R> imp_mnar_pmm <- mice(data = Obesity, meth = meth_mnar, pred = pred_mnar,
+                        m=10, seed = 123, pmm = T,  printFlag = FALSE)
```

We check the convergency of the results

```
R> summary(complete(imp_mnar_pmm,"long")$Weight)
```

```
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  28.35   71.51   85.09   85.64   99.00  134.61
```

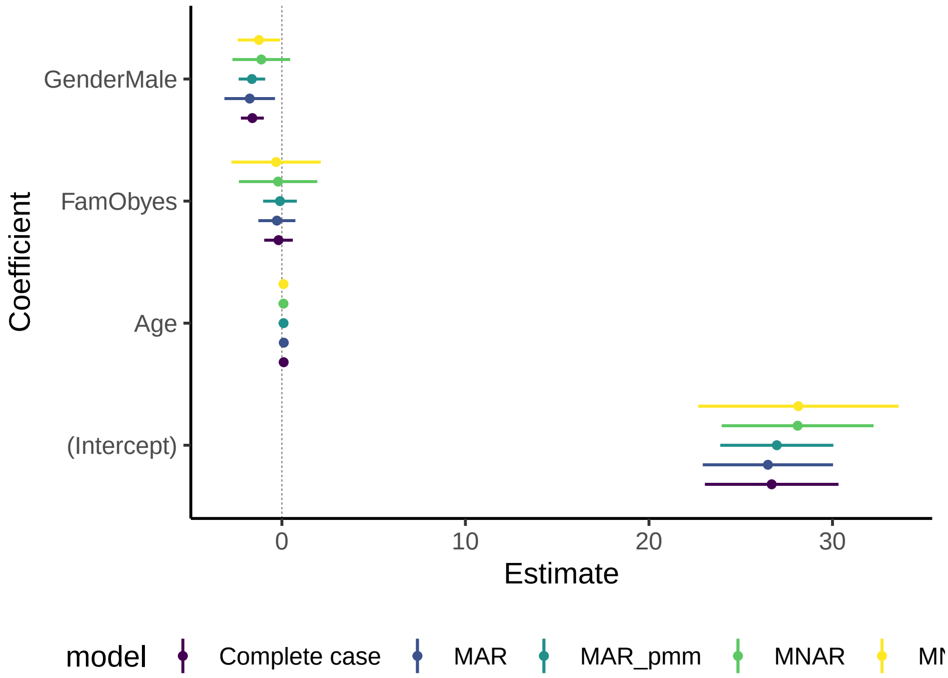
```
R> ggmice::plot_trace(imp_mar_pmm, "Weight")
```



After this modification we proceed to compare the effects on the model. We run the analysis model on each of the completed datasets as well asthe dataset where the incomplete values are removed (Complete Case analysis, CC).

```
R> library(ggplot2)
R> cc_rs<- with(setDT(Obesity)[complete.cases(Obesity),],
```

```
+               lme( BMI ~ Age + FamOb + Gender, random=~1+Age|Cluster))
R> mar_rs <- with(imp_mar,lme( BMI ~ Age + FamOb + Gender,random=~1+Age|Cluster))
R> mar_pmm_rs <- with(imp_mar_pmm,lme( BMI ~ Age + FamOb + Gender,random=~1+Age|Cluster))
R> mnar_rs<- with(imp_mnar,lme(BMI ~ Age + FamOb + Gender,random=~1+Age|Cluster))
R> mnar_pmm_rs<- with(imp_mnar_pmm, lme(BMI ~ Age + FamOb + Gender,random=~1+Age|Cluster))
R> list_models<-list(cc_rs,mar_rs,mar_pmm_rs,mnar_rs,mnar_pmm_rs)
R> plot_models(list_models,
+              mod_name = c("Complete case", "MAR","MAR_pmm", "MNAR", "MNAR_pmm"))
```



We note that there is minimal disparity in the age effect, FamObs, or Gender across the various imputation models under consideration. An analysis of the intercept reveals that, under the MNAR assumption, a higher average BMI is anticipated compared to the MAR assumption. Nonetheless, with respect to precision of estimates, we notice that in general MNAR imputation leads to wider confidence intervals, in this case it does not have any influence on the final result but there could be cases where variation in the assumed missing mechanism could lead also to differences on significant test and therefore lead to contradictory conclusions.

5. Additional

The imputation of these data is based on the IPDMA Heckman Github repo

Visualize missing data pattern:

The matrix only shows the predictors for the main model, not the selection model.

TODO: explain exclusion restriction.

ORDER:

- summary
- congeniality, then in hierarchical models
- look whether we can fit cong. back in the main body
- alt. methods
- conclusion: mice is really easy!
- Additional levels of clustering
- More complex data types: timeseries and polynomial relationship in the clustering.
- FIML vs MI

An alternative approach to missing data is to use Full Information Maximum Likelihood (FIML). This method does not require the imputation of any missing values. Whereas MI consists of imputation, analyses and pooling steps, FIML analyses the data in a single step. When the assumptions are met the two approaches should produce equivalent results. [REF] As FIML requires specialised software, not all analyses can be performed with standard software. [REF]

- Survival / TTE, this could be put in the paragraph on congeniality

When the outcome is time-to-event, the Nelson-Aalen estimate of the time to event should be included as a covariate in the imputation model [REF]

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When the outcome is time-to-event, the Nelson-Aalen estimate of the time to event should be included as a covariate in the imputation model [REF]

In hierarchical datasets, clustering is a concern because the homoscedasticity in the error terms cannot be assumed across clusters and the relationship among variables may vary at different hierarchical levels. When multiple imputation is used to deal with missing data, as the imputation and analysis process is performed separately, it is necessary that imputation model being congenial with the main analysis model (Meng, 1994), e.g. if the main model accounts for the hierarchical structure also imputation model should do it (Audigier, 2021). Not including clustering into the imputation process may lead to effect estimates with smaller standard errors and inflated type I error.

There are different strategies that can be adopted in the imputation process that account for clustering: inclusion of cluster indicator variable, performing a separate imputation process for each cluster, or performing a simultaneous imputation process by using an imputation method that accounts for clustering.(Stata: https://www.stata.com/support/faqs/statistics/clustering-and-mi-impute/) TODO: replace ref.

The selection of each strategy depends mainly on the assumptions in the main analysis and also on the restriction of the analyzed data.

Regarding the restrictions imposed by the data, for instance, the use of cluster indicator variables is restricted in datasets where there are not many clusters and many observations per cluster (Graham, 2009). The last restriction is also required when imputations are performed on each cluster separately. When this restriction cannot be achieved, one can use an imputation model that simultaneously imputes all clusters using a hierarchical model (Allison 2002).

Under this hierarchical imputation model, observations within clusters are correlated and this correlation is modeled by a random effect so the hierarchical model can be estimated even when there are few observations per cluster. However, this strategy is best suited for balanced data (Grund, 2017) and when random effects model is appropriated, i.e. the number of clusters is adequate. (Austin,2018).

Here it is important to evaluate the assumptions imposed by the main model, for instance by using the cluster indicator strategy may lead to bias estimates when the model is based on a hierarchical model (Taaljard,2008). Even when an imputation strategy congenial with the main model is preferred, it is important to consider whether it is appropriate for the data as a less complex imputation strategies may also lead to unbiased estimates in certain scenarios(Bailey 2020). For instance, in causal effect analysis, separately imputation may lead to smaller bias when the size of the smaller exposure cluster is large, compared with an imputation model that includes exposure-confounder interactions. (Zhang,2023).

6. Conclusion

7. Funding

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The views expressed in this paper are the personal views of the authors and may not be understood or quoted as being made on behalf of or reflecting the position of the regulatory agency/agencies or organizations with which the authors are employed/affiliated.

8. References

9. Appendix

Table 3: Notation

Formula lme4	**Details**
`y ~ x1 + (1 | g1)`	Fixed `x1` predictor with random intercept varying among `g1`
`y~x1*x2+ (1| g1)`	Interactions of `x1` and `x2` only in fixed effect
`y ~ x1*x2+ (x2| g1)`	Interactions of `x1` and `x2` only in fixed effect with slope of `x2` randomly varying among `g1`
`y ~ x1*x2+ (x1*x2| g1)`	variance-covariance matrix estimated only with the variance terms of intercept, slope of `x1`, slope of `x2` and interaction `x1*x2`
`y ~ x1*x2+ (x1 | g1)+ (x2| g1)`	variance-covariance matrix estimated separately, i.e, one for intercept and `x1` and another for intercept and `x2`
`y ~ x1 + (x1 | g1) or 1 + x1 + (1 + x1 | g1)`	Fixed `x1` with correlated random intercept and random slope of `x`
`y ~ x1 + (x1 || g1) or 1 + x1 + (1 | g1) + (0 + x1 | g1)`	Fixed `x1` with uncorrelated random intercept and random slope of `x1`
`y ~ (1 | g1) + (1 | g2)`	Random intercept varying among `g1` and among `g2` | |y ~ (1

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