LMU

LUDWIG-
MAXIMILIANS-
UNIVERSITÄT
MÜNCHEN

INSTITUT FÜR STATISTIK

Alexander Hapfelmeier

Random Forest variable importance with missing data

Technical Report Number 121, 2012
Department of Statistics
University of Munich

http://www.stat.uni-muenchen.de

Random Forest variable importance with missing data

Alexander Hapfelmeier
Institut für Medizinische Statistik und Epidemiologie,
Technische Universität München,
Ismaninger Str. 22, 81675 Munich, Germany,
Alexander.Hapfelmeier@tum.de

Kurt Ulm
Institut für Medizinische Statistik und Epidemiologie,
Technische Universität München,
Ismaninger Str. 22, 81675 Munich, Germany

Torsten Hothorn
Institut für Statistik, Ludwig-Maximilians-Universität,
Ludwigstraße 33, 80539 Munich, Germany

February 15, 2012

Abstract

Random Forests are commonly applied for data prediction and interpretation. The latter purpose is supported by variable importance measures that rate the relevance of predictors. Yet existing measures can not be computed when data contains missing values. Possible solutions are given by imputation methods, complete case analysis and a newly suggested importance measure. However, it is unknown to what extend these approaches are able to provide a reliable estimate of a variables relevance. An extensive simulation study was performed to investigate this property for a variety of missing data generating processes. Findings and recommendations: Complete case analysis should not be applied as it inappropriately penalized variables that were completely observed. The new importance measure is much more capable to reflect decreased information exclusively for variables with missing values and should therefore be used to evaluate actual data situations. By contrast, multiple imputation allows for an estimation of importances one would potentially observe in complete data situations.

Keywords: Random Forests, variable importance measures, missing data, multiple imputation, surrogates, complete case analysis

1 Introduction

Random Forests (cf. Breiman, 2001) are popular approaches for regression analysis. On account of their easy applicability and interpretability they are commonly used in many research fields such as social, econometric and clinical science. Further strong advantages over common approaches like regression analysis are their ability to implicitly deal with high dimensional data, missing values, complex interactions and collinearity (cf. Cutler et al., 2007; Lunetta et al., 2004, for corresponding discussions). Likewise, Random Forests provide variable importance measures which can be used to identify variables that are of relevance for prediction. In a subsequent step these measures are often used for variable selection (cf. Tang et al., 2009; Yang and Gu, 2009; Rodenburg et al., 2008; Sandri and Zuccolotto, 2006; Díaz-Uriarte and Alvarez de Andrés, 2006; Altmann et al., 2010; Archer and Kimes, 2008).

So far, it has not been investigated how to proceed for the computation of such measures when there is missing data. Complete case analysis and imputation (e.g. mean, hot-deck, conditional mean and predictive distribution substitution) are two potential solutions to this issue. However, it has been shown that these ad hoc methods may lead to biased inference when the data is not missing completely at random (cf. Schafer and Graham, 2002; Horton and Kleinman, 2007). Multiple imputation by chained equations (MICE; cf. van Buuren et al., 2006; White et al., 2011) is meant to solve this problem and its superiority has been shown in many publications (e.g. Janssen et al., 2009, 2010). A third solution has been proposed earlier (cf. Hapfelmeier et al., 2012) by a new variable importance measure. It is closely related to existing approaches – and therefore retains appreciated properties – yet handles missing values in an intuitive way.

The predictive accuracy of Random Forests has been explored for the analysis of missing data by Rieger et al. (2010); Hapfelmeier et al. (2011): comparisons of models fit with and without imputation of missing values showed only negligible differences. By contrast, the following study focuses on the assessment of a variables relevance by means of importance measures. As a result the ability to produce reliable estimates well differs between complete case analysis, multiple imputation (executed by MICE) and the new importance measure. An extensive simulation study that involves various missing data generating processes is conducted for both, regression and classification problems. Findings about predictive accuracy are retraced in an additional analysis of a simulated test dataset.

2 Missing Data

In early works Rubin (1976, 1987) specifies the issue of correct statistical inference with missing values by the definition of missing data generating processes:

- Missing completely at random (MCAR):
  $P(R|\mathbf{X}_{\text{comp}}) = P(R)$
- Missing at random (MAR):
  $P(R|\mathbf{X}_{\text{comp}}) = P(R|\mathbf{X}_{\text{obs}})$
- Missing not at random (MNAR):
  $P(R|\mathbf{X}_{\text{comp}}) = P(R|\mathbf{X}_{\text{obs}}, \mathbf{X}_{\text{mis}})$

Whether a value is missing is indicated by a binary variable R and depends on its probability distribution $P(R)$. The complete variable set $\mathbf{X}_{\text{comp}}$ consists of the observed values $\mathbf{X}_{\text{obs}}$ and the missing ones $\mathbf{X}_{\text{mis}}$: $\mathbf{X}_{\text{comp}} = \{\mathbf{X}_{\text{obs}}, \mathbf{X}_{\text{mis}}\}$. Therefore in a MCAR scheme the probability for a missing value is independent of the observed and unobserved data. By contrast for MAR this probability is dependent on the observed information. In MNAR the probability depends on unobserved variables or the missing values themselves.

Little and Rubin (2002) showed that usual sample estimates – for example in linear regression – stay unaffected by the MCAR scheme. By contrast, in classification and regression trees even MCAR may induce a systematic bias, that may be carried forward to Random Forests based on biased split selections (cf. Strobl et al., 2007). Also, it is well-known that complete case analysis is prone to biased inference when the data is not MCAR. Therefore, in the following simulation study, one MCAR, four MAR and one MNAR scheme to generate missing values are investigated.

3 Methods

3.1 Random Forests

The most famous representative of recursive partitioning is the CART algorithm (cf. Breiman et al., 1984). It constructs trees by sequential binary splits that produce subsets of the data which are as homogeneous as possible in terms of the outcome. Breiman (1996) also showed that the performance of single trees benefits from "bagging" (bootstrap aggregation). In bagging, several trees are fit to bootstrapped or subsampled data. As a further advancement, Random Forests (Breiman, 2001; Breiman and Cutler, 2008) have been introduced for which splits are performed in random selections of variables. This makes a more diverse set of variables contribute to the joint prediction. The latter is found by averaged values or majority votes of each single tree in a Random Forest. The so called 'out of bag' (OOB) samples – i.e. observations not used to fit the respective trees – can be used for an unbiased estimate of a Random Forests error, viz. the OOB-error.

When there are missing values surrogate splits need to be employed. They mimic the initial split of the data as they try to archive the same partitioning of complete observations. When several surrogate splits are computed they can be ranked according to their ability to resemble the initial split. An observation that contains more than a single missing value is processed along this ranking until a decision is found.

The CART and the C4.5 algorithms – and consequently all Random Forest algorithms based on the same construction principles – have been shown to be prone to biased variable selection (cf. Breiman et al., 1984; Strobl et al., 2007; White and Liu, 1994; Kim and Loh, 2001; Dobra and Gehrke, 2001; Hothorn et al., 2006). Therefore, Random Forests used in this work base on the recursive partitioning approach of Hothorn et al. (2006). It follows the same rationale as Breiman's original approach and guarantees unbiased variable selection and variable importance measures when combined with subsampling (as opposed to bootstrap sampling; cf. Strobl et al., 2007).

3.2 A new variable importance measure for missing data

The most popular and most advanced variable importance measure for Random Forests is the permutation accuracy importance. It is assessed by a comparison of a trees prediction accuracy before and after the random permutation of a predictor variable. If the latter is of relevance the accuracy is supposed to drop as the original association to the response and further predictors is destroyed by permutation; the importance measure takes large values in such a case. The major issue is that there is no straightforward way to compute this measure when there are missing values. In particular, it is not clear how conclusions about the importance of variables can be drawn from the permutation approach when surrogate splits are involved in the computation of the accuracy.

A new approach was proposed earlier (cf. Hapfelmeier et al., 2012) to overcome this pitfall. In order to retain appreciated properties it is closely related to existing methodology, yet differs in one substantial aspect: Instead of permuting the values of a variable X (that may be missing), observations are randomly send to the daughter nodes if a parent node k is split in X. The probability to be sent left is determined by the relative frequency $\hat{p}_k$ of observations that initially went this way. The algorithm to compute the new importance measure is given by:

1. Compute the OOB accuracy of a tree.
2. Randomly assign each observation with $\hat{p}_k$ to the left (or right) child node if the parent node k is split in X.
3. Recompute the OOB accuracy of the tree.
4. Compute the difference between the original and recomputed OOB accuracy.
5. Repeat step 1 to 4 for each tree and use the average difference over all trees as the overall importance score.

This procedure simulates – like for the random permutation in the original permutation importance – the null hypothesis that the allocation of observations does not depend on the particular predictor variable. It solves any problems associated with the occurrence of missing values and the application of surrogate splits as decisions are detached from the raw values of a variable.

3.3 Multivariate Imputation by Chained Equations

Single imputation can lead to severe underestimation of variance (cf. Harel and Zhou, 2007). A simple and popular solution to this problem is the application of multiple imputation (MI; cf. Rubin, 1987, 1996). In a first step a proper MI approach is supposed to draw M estimates $\theta^{(1)}, ..., \theta^{(\mathrm{M})}$ from $\mathrm{P}(\theta|\mathbf{X}_{\mathrm{obs}})$ for the multidimensional parameter θ which determines the data distribution. These are subsequently used in the conditional distributions $\mathrm{P}(\mathbf{X}_{\mathrm{mis}}|\mathbf{X}_{\mathrm{obs}}; \widehat{\theta}^{(\mathrm{t})})$, $\mathrm{t} = 1, ..., \mathrm{M}$ to draw multiple imputations for missing values. This way several imputed datasets are created. Finally, any measure of interest can be assessed by the average of estimates for each of the imputed datasets. Little and Rubin (2002) point out that the approach makes standard complete-data methods applicable to incomplete data (e.g. the original permutation importance measure).

The case of more than one variable with missing values demands for a special imputation procedure. A practical approach which makes it possible to bypass the specification of a joint distribution is MICE (sometimes also called fully conditional specification (FCS); cf. van Buuren et al., 2006; van Buuren, 2007; van Buuren and Groothuis-Oudshoorn, 2010; White et al., 2011). It cycles through incomplete variables to iteratively update imputed values and parameter estimates until convergence. The procedure is repeated several times to produce multiple imputed data sets. An apparent advantage is that imputation of the data can be achieved by a flexible specification of predictive models for each variable.

MICE is especially suitable in MAR settings though Janssen et al. (2010) state that it should also be preferred to ad hoc methods like complete case analysis even in MNAR situations. Likewise He et al. (2009) and White et al. (2011) point out that MICE is also capable to deal with MNAR schemes as the imputation model becomes more general and includes more variables to make MAR plausible.

4 Simulation study

An extensive simulation study was designed to investigate the ability of complete case analysis, multiple imputation by MICE and the new importance measure to produce reliable estimates of a variables relevance. In addition, the predictive accuracy of Random Forests that base on each of these approaches was explored for a simulated test dataset. There are several factors of potential influence that needed to be explored; therefore the amount of missing values, correlation schemes, variable strength and different processes to generate missing values were of particular interest. A detailed explanation of the setup is given in the following.

- *Influence of predictor variables*

  The simulated data contained both, a classification and a regression problem. Therefore, a categorical (binary) and a continuous response were created in dependence of six variables with coefficients β:
  $$\beta = (1, 1, 0, 0, 1, 0)^\top.$$
  Repeated values for β make it possible to compare importances of variables which are, by construction, equally influential but show different correlations and different fractions of missing values. In addition, the non-influential variables with $\beta = 0$ help to investigate possible undesired effects and serve as a baseline.

- *Data generating models*

  A continuous response was modeled by means of a linear model:
  $$y = \mathbf{x}^\top\beta + \epsilon \text{ with } \epsilon \sim N(0, .5).$$
  The binary response was drawn from a Bernoulli distribution $B(1, \pi)$ with π which was assessed by means of a logistic model
  $$\pi = P(Y = 1|\mathbf{X} = \mathbf{x}) = \frac{e^{\mathbf{x}^\top\beta}}{1 + e^{\mathbf{x}^\top\beta}}.$$

The variable set $\mathbf{X}$ itself contained 100 observations drawn from a multivariate normal distribution with mean vector $\vec{\mu} = 0$ and covariance matrix Σ:

- *Correlation*

$$\Sigma = \begin{pmatrix} 1 & 0.3 & 0.3 & 0.3 & 0 & 0 \\ 0.3 & 1 & 0.3 & 0.3 & 0 & 0 \\ 0.3 & 0.3 & 1 & 0.3 & 0 & 0 \\ 0.3 & 0.3 & 0.3 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

  As the variances of each variable are chosen to be 1, the covariance equals the correlation in this special case. The structure of Σ reveals that there is a block of four correlated variables and two uncorrelated ones.

- *Missing values*
  Several MCAR, MAR and MNAR processes to create missing values were implemented. For each scheme, a given fraction $m \in \{0.0, 0.1, 0.2, 0.3\}$ of values is set missing for the variables X_2, X_4 and X_5. The number of observations that contain at least one missing value is given by $1 - (1 - \%_{\text{missing}})^{\text{n}_{\text{variables}}}$. Thus, a dataset that contains three variables with 30% missing values includes $1 - (1 - 0.3)^3 = 65.7\%$ incomplete observations on average. This seems to be a rather huge amount though it is not unlikely for real life data. Therefore, m comprises a wide range of possible scenarios.

  In the MAR setting, the probability for missing values in a variable depended on the values of another variable. In the MNAR scheme this probability was determined by a variables own values. Accordingly, each variable that contained missing values had to be linked to at least one other variable or itself. Table 1 lists the corresponding relations.

Table 1: List of variables that contain missing values determine the probability of missing values.

contains missing values (MCAR, MAR & MNAR)	determines missing values (MAR)	(MNAR)
X_2	X_1	X_2
X_4	X_2	X_4
X_5	X_6	X_5

  The schemes to produce missing values are:

  - MCAR: Values are randomly replaced by missing values.
  - MAR(rank): The probability of a value to be replaced by a missing value rises with the rank the same observation has in the determining variable.
  - MAR(median): The probability of a value to be replaced by a missing value is nine times higher for observations whose value in the determining variable is located above the corresponding median.
  - MAR(upper): Those observations with the highest values of the determining variable are replaced by missing values.
  - MAR(margins): Those observations with the highest and lowest values of the determining variable are replaced by missing values.
  - MNAR(upper): The highest values of a variable are set missing.

An independent test dataset served the purpose to evaluate the predictive accuracy of a Random Forest. It was created the same way as the training data though it contained 5000 observations and was completely observed. The accuracy was assessed by the mean squared error (MSE) which equals the misclassification error rate (MER) in classification problems.

In summary, there were 2 response types investigated for 6 processes to generate and 3 procedures to handle 4 different fractions of missing values. This sums up to as much as 144 simulation settings. The simulation was repeated 1000 times. Corresponding `R`-Code is available online at `http://www2.imse.med.tu-muenchen.de/r-code/hapfelmeier/RF_VI_missingData.r` .

5 Results

The following investigations are based on the classification analysis. Results for the regression problem are presented as supplementary material in section A (cf. Figure 5) as they showed similar properties.

A general finding which holds for each analysis accentuates the well-known fact that unconditional permutation importance measures rate the relevance of correlated variables higher than that of uncorrelated ones (cf. Strobl et al., 2008). This becomes evident by the example of variables 1, 2 and 5. Although they are of equal strength the latter is assigned a lower relevance as it is uncorrelated to any other predictor; in some research fields this effect is appreciated to uncover relations and interactions among variables (cf. Nicodemus et al., 2010; Altmann et al., 2010). Also, there were no artificial effects observed for the non-influential variables in any analysis setting.

Findings for the new variable importance measure which is able to implicitly deal with missing values are displayed by Figure 1. According to expectations, the importance of variables 2, 4 and 5 decreased as they contained a rising amount of missing values. It is interesting to note that meanwhile the importance of variable 1 rose, although it does not seem to be directly affected. However, Hapfelmeier et al. (2012)

showed that this gain of relevance is justified: variables that are correlated and therefore provide similar information replace each other in a Random Forest when some of the information gets lost due to missing values. Accordingly, variable 1 takes over for variable 2 which reflects in an increased selection frequency of variable 1 in the tree building process. In conclusion, this approach is allowed to be affected by the occurrence of missing values as it mirrors the situation at hand, i.e. the relevance a variable takes in a Random Forest under consideration of the information it actually provides. The new importance measure appeared to be well suited for any of the missing data generating processes as results did not differ substantially.

Results for the complete case analysis – given by Figure 2 – showed undesired effects. A rising amount of missing values lead to a decreased importance of the complete variable 1. This is due to the simple fact that some observations are completely discarded from analysis; importance measures typically diminish when Random Forests are fit to less data. However, its importance is not supposed to drop below that of variable 2 which is of equal strength yet contains the missing values. Unfortunately, this latter effect can be observed for every missing data generating process, except for MNAR(upper). It is most pronounced for MAR(upper) and MAR(margins). There is no rational justification for this property as variable 1 sustains its information while other variables loose it. A proper evaluation of a variables relevance is supposed to reflect this fact. Considering this vulnerability of complete case analysis to different missing data generating processes it should not be used for the assessment of importance measures when there is missing data.

An examination of Figure 3 reveals that multiple imputation – with only as few as five imputed data sets – is a convenient way to maintain and recover the importance of variables that would have been observed if there was no missing data at all. This equally held for variables that contained missing values and those which were completely observed; none of their importances was arbitrarily decreased or increased. Even the importance of variable 5 which is only related to the outcome and therefore is associated with a rather weak imputation model remained unaffected by the amount of missing values. The example of variable 4 shows that the imputation of non-influential variables did not induce artificial importances. All missing data generating processes showed these advantageous properties, except for the MNAR(upper) setting.

The prediction error produced by each approach for the independent test sample is displayed in Figure 4. For multiple imputation the prediction accuracy only slightly decreases with a rising amount of missing values. This effect is more pronounced for Random Forests that use surrogate splits; though there are only minor differences to multiple imputation (cf. Rieger et al., 2010; Hapfelmeier et al., 2011, for according findings). Complete case analysis appears to be much worse and leads to very high errors with a rising fraction of missing values. Missing data generating processes are comparable within each approach. However, there is one exception for the MNAR setting that always causes the worst results. A corresponding evaluation of the regression problem is given as supplementary material in section A (cf. Figure 6).

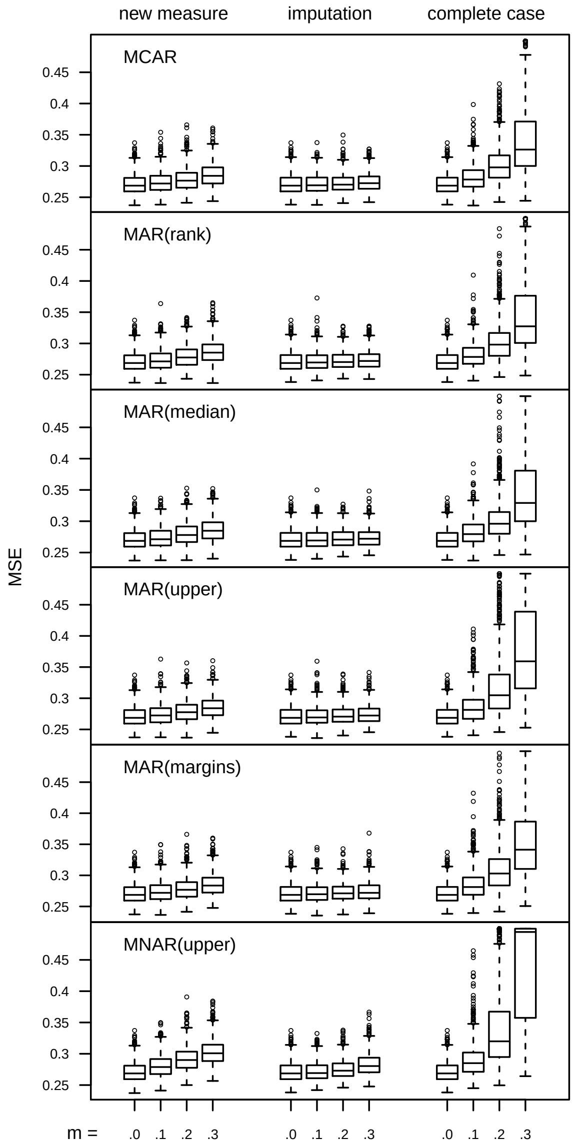


Figure 4: MSE observed for the classification problem (m = % of missing values in X_2, X_4 and X_5).

6 Conclusion

The ability of a new importance measure, complete case analysis and a multiple imputation approach to produce reasonable estimates for a variables importance in Random Forests has been investigated for the case of data that contains missing values. Therefore, an extensive simulation study that employed sev-

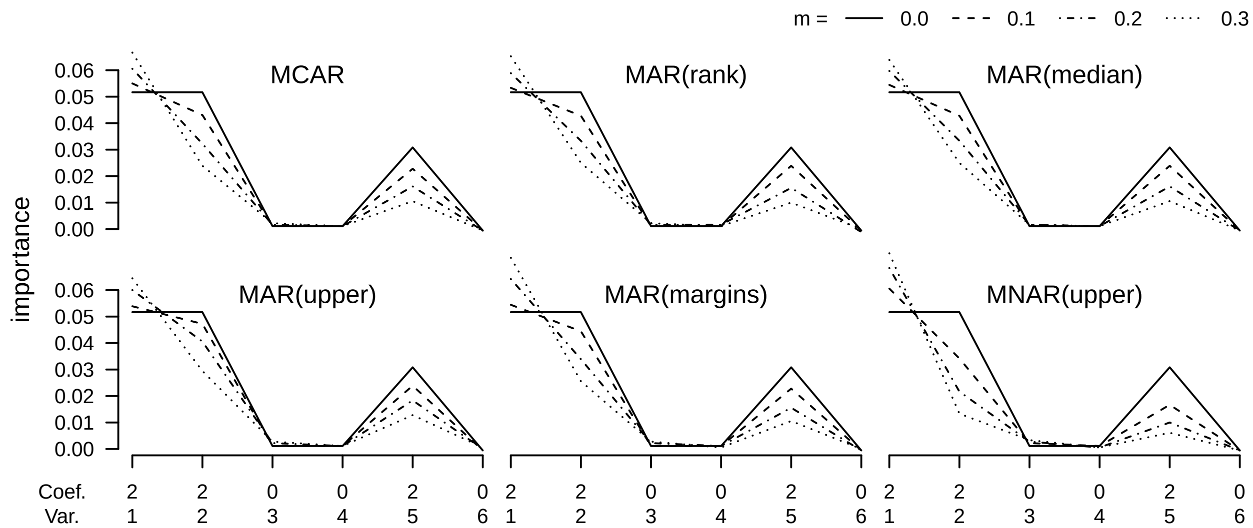


Figure 1: Median variable importance observed for the new importance measure in the classification problem ($m = \%$ of missing values in X_2, X_4 and X_5).

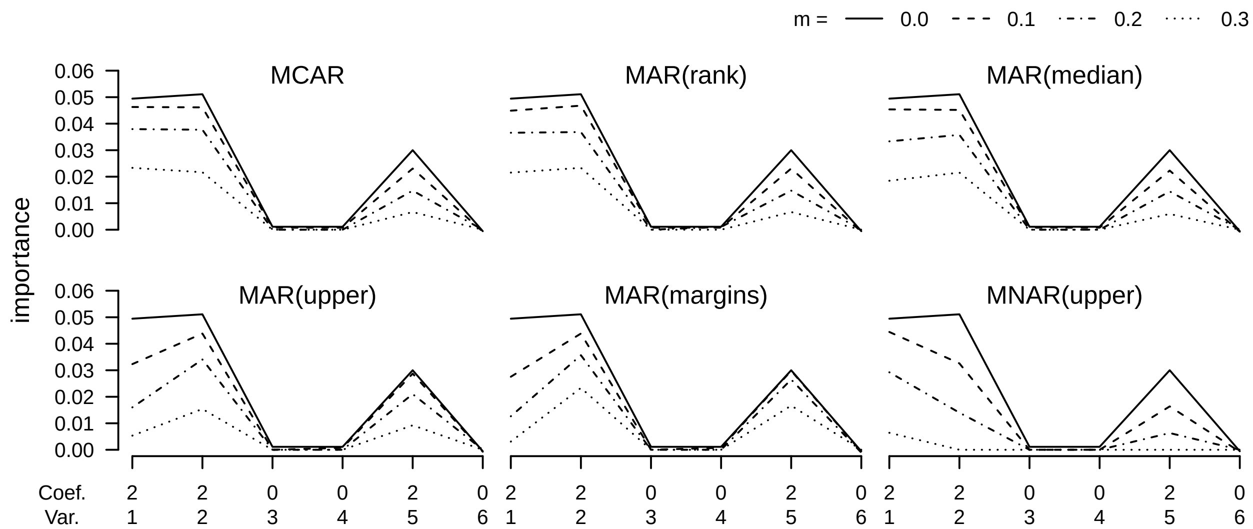


Figure 2: Median variable importance observed for the complete case analysis in the classification problem ($m = \%$ of missing values in X_2, X_4 and X_5).

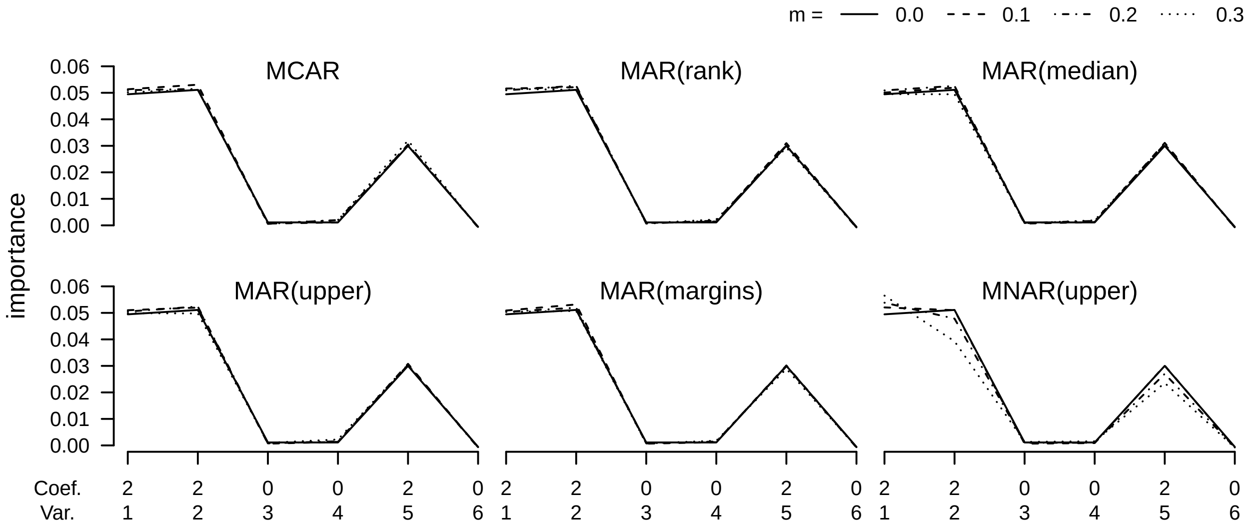


Figure 3: Median variable importance observed for the imputed data in the classification problem (m = % of missing values in X_2, X_4 and X_5).

eral MCAR, MAR and MNAR processes to generate missing values has been conducted. There are some clear recommendations for application: Inappropriate results have been found for the complete case analysis in the MAR settings; it penalized the importance of variables that were completely observed in an arbitrary way. As a consequence the sequence of importances was not able to reflect the true relevance of variables any more. This approach is not recommended for application to real life data. By contrast the new importance measure was able to express the loss of information exclusively for variables that contained missing values. Therefore, it should be used to describe the relevance of a variable under consideration of its actual information. In some cases one might prefer to investigate the relevance a variable would have taken if there had been no missing values. Multiple imputation appeared to serve this purpose very well except for the MNAR setting. An additional evaluation of prediction accuracy revealed that Random Forests that base on multiple imputed data were mostly unaffected by the occurrence of missing values. Results were only slightly worse when surrogate splits were used. Complete case analysis lead to models with the lowest prediction strength.

References

Altmann, A., L. Tolosi, O. Sander, and T. Lengauer (2010). Permutation importance: a corrected feature importance measure. *Bioinformatics 26*(10), 1340–1347.

Archer, K. and R. Kimes (2008). Empirical characterization of random forest variable importance measures. *Computational Statistics & Data Analysis 52*(4), 2249–2260.

Breiman, L. (1996). Bagging predictors. *Machine Learning 24*(2), 123–140.

Breiman, L. (2001). Random forests. *Machine Learning 45*(1), 5–32.

Breiman, L. and A. Cutler (2008). *Random forests.* `http://www.stat.berkeley.edu/users/breiman/RandomForests/cc_home.htm`. (accessed 07.02.2012).

Breiman, L., J. Friedman, C. J. Stone, and R. A. Olshen (1984). *Classification and Regression Trees* (1 ed.). Chapman & Hall/CRC.

Cutler, D. R., T. C. Edwards, K. H. Beard, A. Cutler, K. T. Hess, J. Gibson, and J. J. Lawler (2007). Random forests for classification in ecology. *Ecology 88*(11), 2783–2792.

Díaz-Uriarte, R. and S. Alvarez de Andrés (2006). Gene selection and classification of microarray data using random forest. *BMC Bioinformatics 7*(1), 3.

Dobra, A. and J. Gehrke (2001). Bias correction in classification tree construction. In C. E. Brodley and A. P. Danyluk (Eds.), *Proceedings of the Eighteenth International Conference on Machine Learning (ICML 2001), Williams College, Williamstown, MA, USA*, pp. 90–97. Morgan Kaufmann.

Hapfelmeier, A., T. Hothorn, and K. Ulm (2011). Recursive partitioning on incomplete data using surrogate decisions and multiple imputation. *Computational Statistics & Data Analysis* (0), –.

Hapfelmeier, A., K. Ulm, and T. Hothorn (2012). A new variable importance measure for random forests with missing data. *Statistics and Computing*. under review.

Harel, O. and X.-H. Zhou (2007). Multiple imputation: review of theory, implementation and software. *Statistics in Medicine 26*(16), 3057–3077.

He, Y., A. M. Zaslavsky, M. B. Landrum, D. P. Harrington, and P. Catalano (2009). Multiple imputation in a large-scale complex survey: a practical guide. *Statistical Methods in Medical Research*.

Horton, N. J. and K. P. Kleinman (2007). Much ado about nothing: A comparison of missing data methods and software to fit incomplete data regression models. *The American Statistician 61*(1), 79–90.

Hothorn, T., K. Hornik, C. Strobl, and A. Zeileis (2008). *party: A laboratory for recursive part(y)itioning.* R package version 0.9-9993.

Hothorn, T., K. Hornik, and A. Zeileis (2006). Unbiased recursive partitioning. *Journal of Computational and Graphical Statistics 15*(3), 651–674.

Janssen, K. J., A. R. Donders, F. E. Harrell, Y. Vergouwe, Q. Chen, D. E. Grobbee, and K. G. Moons (2010). Missing covariate data in medical research: to impute is better than to ignore. *Journal of clinical epidemiology 63*(7), 721–727.

Janssen, K. J., Y. Vergouwe, A. R. Donders, F. E. Harrell, Q. Chen, D. E. Grobbee, and K. G. Moons (2009). Dealing with missing predictor values when applying clinical prediction models. *Clinical chemistry 55*(5), 994–1001.

Kim, H. and W. Loh (2001). Classification trees with unbiased multiway splits. *Journal of the American Statistical Association 96*, 589–604.

Little, R. J. A. and D. B. Rubin (2002). *Statistical Analysis with Missing Data, Second Edition* (2 ed.). Wiley-Interscience.

Lunetta, K., B. L. Hayward, J. Segal, and P. Van Eerdewegh (2004). Screening large-scale association study data: exploiting interactions using random forests. *BMC Genetics 5*(1).

Nicodemus, K., J. Malley, C. Strobl, and A. Ziegler (2010). The behaviour of random forest permutation-based variable importance measures under predictor correlation. *BMC Bioinformatics 11*(1), 110.

R Development Core Team (2011). *R: A Language and Environment for Statistical Computing.* Vienna, Austria: R Foundation for Statistical Computing. ISBN 3-900051-07-0.

Rieger, A., T. Hothorn, and C. Strobl (2010). Random forests with missing values in the covariates.

Rodenburg, W., A. G. Heidema, J. M. A. Boer, I. M. J. Bovee-Oudenhoven, E. J. M. Feskens, E. C. M. Mariman, and J. Keijer (2008). A framework to identify physiological responses in microarray-based gene expression studies: selection and interpretation of biologically relevant genes. *Physiological Genomics 33*(1), 78–90.

Rubin, D. B. (1976). Inference and missing data. *Biometrika 63*(3), 581–592.

Rubin, D. B. (1987). *Multiple Imputation for Nonresponse in Surveys.* J. Wiley & Sons, New York.

Rubin, D. B. (1996). Multiple imputation after 18+ years. *Journal of the American Statistical Association 91*(434), 473–489.

Sandri, M. and P. Zuccolotto (2006). Variable selection using random forests. In S. Zani, A. Cerioli, M. Riani, and M. Vichi (Eds.), *Data Analysis, Classification and the Forward Search*, Studies in Classification, Data Analysis, and Knowledge Organization, pp. 263–270. Springer Berlin Heidelberg. 10.1007/3-540-35978-8_30.

Schafer, J. L. and J. W. Graham (2002). Missing data: our view of the state of the art. *Psychol Methods 7*(2), 147–177.

Strobl, C., A.-L. Boulesteix, and T. Augustin (2007). Unbiased split selection for classification trees based on the gini index. *Computational Statistics & Data Analysis 52*(1), 483–501.

Strobl, C., A.-L. Boulesteix, T. Kneib, T. Augustin, and A. Zeileis (2008). Conditional variable importance for random forests. *BMC Bioinformatics 9*(1), 307+.

Strobl, C., A.-L. Boulesteix, A. Zeileis, and T. Hothorn (2007). Bias in random forest variable importance measures: Illustrations, sources and a solution. *BMC Bioinformatics 8*(1), 25+.

Tang, R., J. Sinnwell, J. Li, D. Rider, M. de Andrade, and J. Biernacka (2009). Identification of genes and haplotypes that predict rheumatoid arthritis using random forests. *BMC Proceedings 3*(Suppl 7), S68.

van Buuren, S. (2007). Multiple imputation of discrete and continuous data by fully conditional specification. *Statistical Methods in Medical Research 16*(3), 219–242.

van Buuren, S., J. P. L. Brand, C. G. M. Groothuis-Oudshoorn, and D. B. Rubin (2006). Fully conditional specification in multivariate imputation. *Journal of Statistical Computation and Simulation 76*(12), 1049–1064.

van Buuren, S. and K. Groothuis-Oudshoorn (2010). Mice: Multivariate imputation by chained equations in r. *Journal of Statistical Software in press*, 01–68.

White, A. and W. Liu (1994). Bias in information based measures in decision tree induction. *Machine Learning 15*(3), 321–329.

White, I. R., P. Royston, and A. M. Wood (2011). Multiple imputation using chained equations: Issues and guidance for practice. *Statistics in Medicine 30*(4), 377–399.

Yang, W. and C. C. Gu (2009). Selection of important variables by statistical learning in genome-wide association analysis. *BMC Proceedings 3*(Suppl 7), S70.

A Supplementary Material

Figure 5 displays median importance measures observed for the regression problem.
Figure 6 displays the evaluation of prediction error for the regression problem.

B Computational Details

The R system for statistical computing (R Development Core Team, 2011, version 2.14.1) was used to implement the simulation study. The package `party` (Hothorn et al., 2008, version 1.0) provides unbiased Random Forests based on conditional inference by the function `cforest()`. Its settings were chosen to fit $ntree = 50$ trees. Each node was determined from $mtry = 3$ randomly selected variables and backed by $maxsurrogate = 3$ surrogate splits. There were no restrictions on the significance of a split ($mincriterion = 0$) and trees were grown until terminal nodes contained less than $minsplit = 20$ observations while child nodes had to contain at least $minbucket = 7$ observations. MICE is given by the function `mice()` of the package `mice` (van Buuren and Groothuis-Oudshoorn, 2010, version 2.11). It was used to produce five imputed datasets. A normal linear model was applied to impute continuous variables, a logistic regression for binary variables and a polytomous regression for variables with more than two categories; defaultMethod = c("norm", "logreg", "polyreg"). Each variable contributed to the imputation models. The fraction of imputed data is approximately $1 - (1 - m)^3$, $m \in \{0.0, 0.1, 0.2, 0.3\}$. The computation of permutation importance measures was performed by the function `varimp()` for the complete case analysis and multiple imputation. The new importance measure was implemented following the principles described in section 3.2.

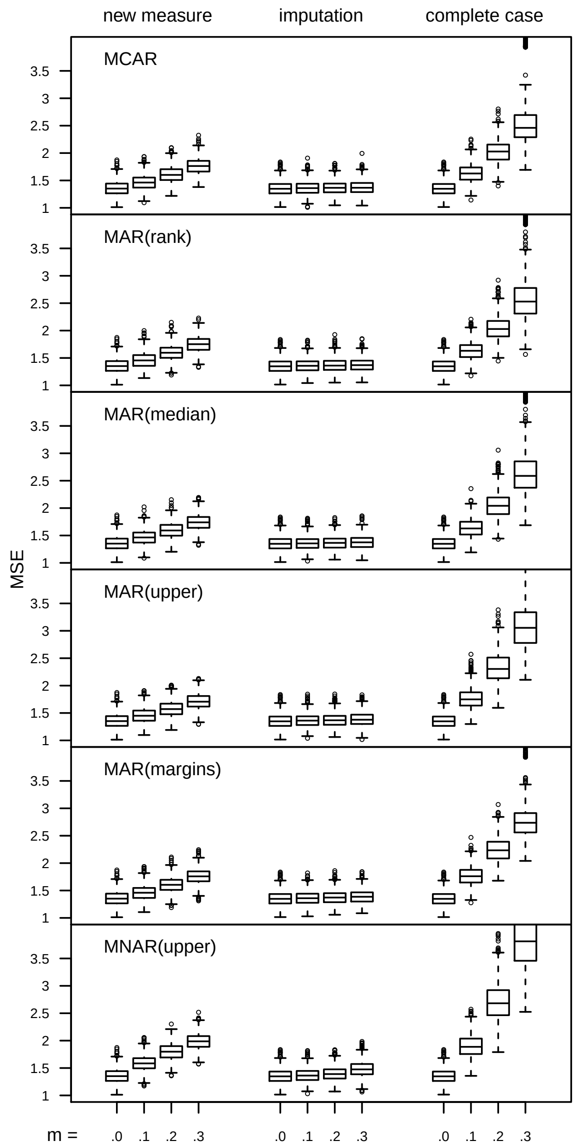
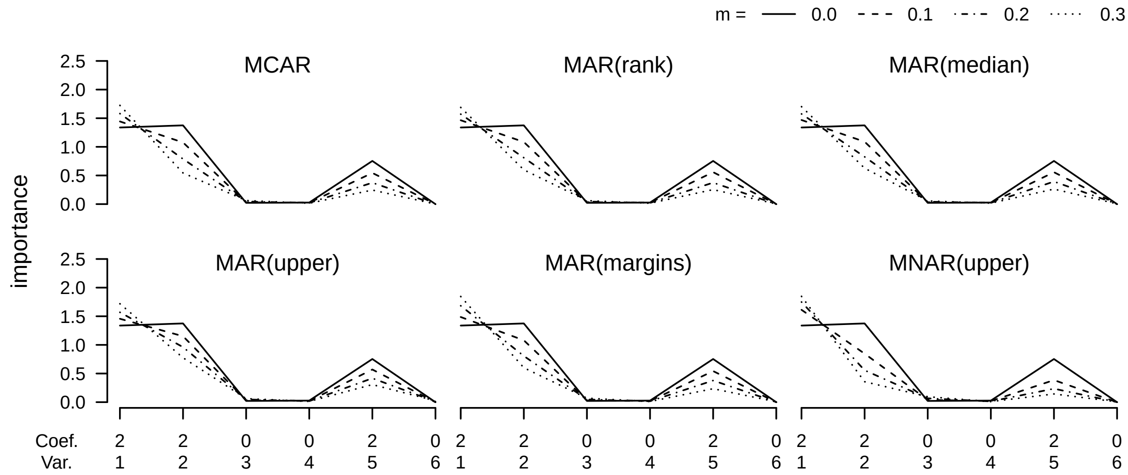
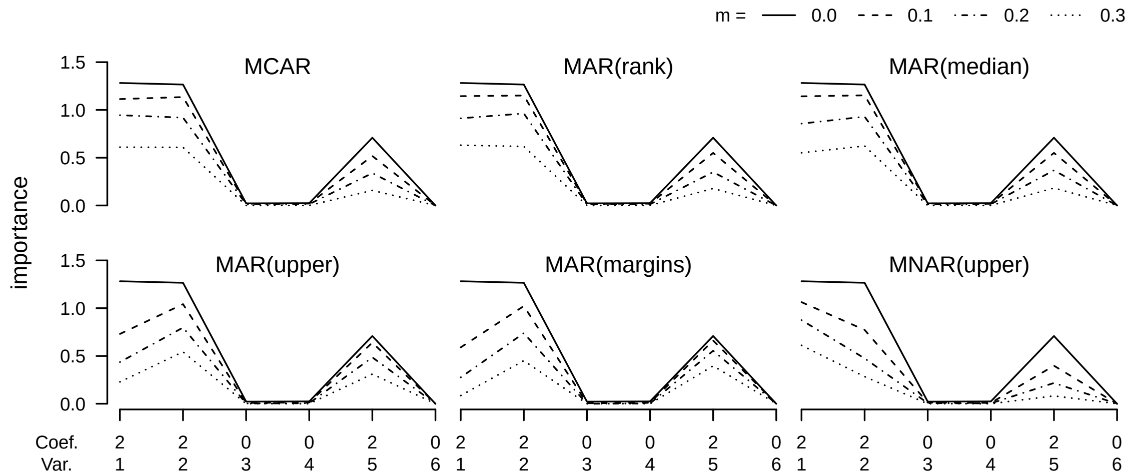


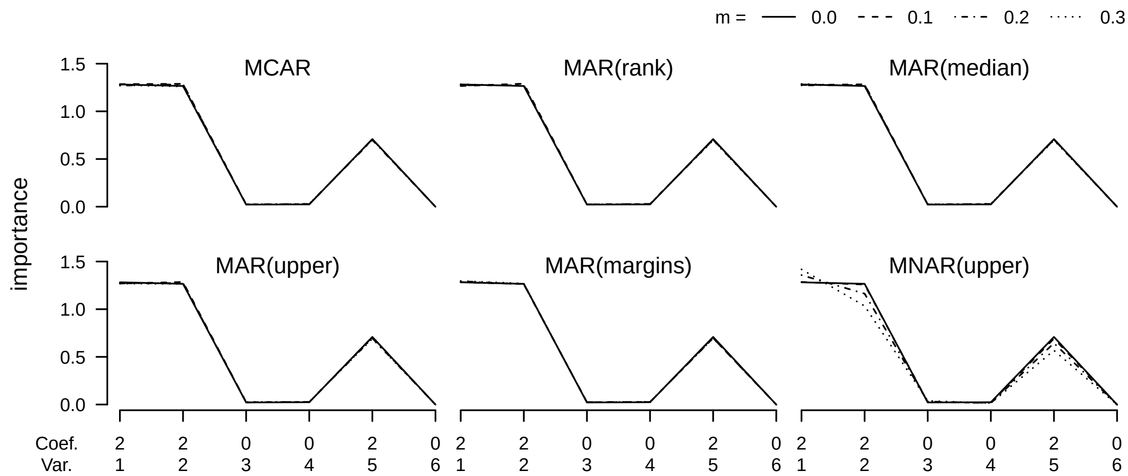
Figure 6: MSE observed for the regression problem (m = % of missing values in X_2, X_4 and X_5).



(a) new importance measure



(b) complete case analysis



(c) multiple imputation

Figure 5: Median variable importance observed for the regression problem ($m = \%$ of missing values in X_2, X_4 and X_5).