Package 'missForestPredict'

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 Description Missing data imputation based on the 'missForest' algorithm (Stekhoven, Daniel J (2012) <doi:10.1093 bioinformatics="" btr597="">) with adaptations for prediction settings. The function missForest() is used to impute a (training) dataset with missing values and to learn imputation models that can be later used for imputing new observations. The function missForestPredict() is used to impute one or multiple new observations (test set) using the models learned on the training data. For more details see Albu, E., Gao, S., Wynants, L., & Van Calster, B. (2024). missForestPredictMissing data imputation for prediction settings <doi:10.48550 arxiv.2407.03379="">.</doi:10.48550></doi:10.1093> Encoding UTF-8
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Author Elena Albu [aut, cre] (ORCID: <https://orcid.org/0000-0003-2602-0918>, funding: KU Leuven)

Maintainer Elena Albu <elenaa.albu@gmail.com>

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calculate_convergence Calculates convergence based on NMSE

Description

Calculates convergence based on NMSE. Details on the convergence criterion calculation are provided in the package vignettes.

Usage

```
calculate_convergence(err, weights)
```

Arguments

err	dataframe containing OOB or apparent errors for each iteration.
weights	vector of weights in the same format as for the missForest function.

Value

A list with elements

converged	boolean indicating if the algorithm has converged (TRUE) or not (FALSE)
measure_old	the total error of the previous iteration
measure_new	the total error of the last iteration

check_predictor_matrix

Performs checks on a custom predictor matrix

Description

Performs a number of checks on a custom predictor matrix and returns error if the matrix is not in a valid format.

Usage

```
check_predictor_matrix(predictor_matrix, data, verbose = TRUE)
```

Arguments

predictor_matrix	
	custom predictor matrix
data	dataframe to be imputed
verbose	if TRUE, returns human readable message for the checks performed.

Value

No return value, only verifies the validity the provided predictor matrix

```
create_predictor_matrix
```

Creates the default predictor matrix with 0 diagonal and 1 elements in the rest.

Description

Creates a square predictor matrix with number of rows and columns equal to the number of columns of the data. Each row name represents the name of the column to be imputed. Each column name represents a predictor for the imputation model. The values in a row will contain 1 for the variables that should be included as predictors in the imputation model and 0 if the variable should not be included as predictor. The diagonal of the predictor matrix is 0, indicating that variable X will not be a predictor for the imputation model of variable X. All other values are 1, meaning that all other variables will be included in the imputation model. This is the default predictor matrix used.

Usage

```
create_predictor_matrix(data)
```

Arguments

data dataframe to be imputed

predictor matrix that can be used as a start for setting a custom predictor matrix

evaluate_imputation_error

Evaluate the imputation error when true values are known.

Description

Evaluate the imputation error when true values are known. Useful when missing values are simulated and true values are known (the errors are calculated as distances from the true values). For continuous variables, MSE (mean square error) and NMSE (normalized mean square error) are returned. For categorical variables, MER (misclassification error rate) is returned.

Usage

```
evaluate_imputation_error(ximp, xmis, xtrue, all = FALSE)
```

Arguments

ximp	imputed dataframe.
xmis	original dataframe with missing values.
xtrue	true dataframe with no missing values.
all	calculate error on all observations (TRUE) or only on missing observations (FALSE). Default is FALSE.

Details

For details check the advanced vignette on convergence criteria and error monitoring.

Value

Dataframe with variables in rows and performance measures in columns.

missForest

Description

Imputes a dataframe and (if save_models = TRUE) returns imputation models to be used on new observations.

Usage

```
missForest(
  xmis,
 maxiter = 10,
  fixed_maxiter = FALSE,
  var_weights = NULL,
  decreasing = FALSE,
  initialization = "mean/mode",
  x_init = NULL,
  class.weights = NULL,
  return_integer_as_integer = FALSE,
  save_models = TRUE,
  predictor_matrix = NULL,
 proportion_usable_cases = c(1, 0),
  verbose = TRUE,
  convergence_error = "00B",
  . . .
)
```

Arguments

xmis	dataframe containing missing values of class dataframe ("tibble" class tbl_df is also supported). Matrix format is not supported. See details for column format.
maxiter	maximum number of iterations. By default the algorithm will stop when converge is reached or after running for maxiter, whichever occurs first.
fixed_maxiter	if set to TRUE, the algorithm will run for the exact number of iterations specified in maxiter, regardless of the convergence criteria. Default is FALSE.
var_weights	named vector of weights for each variable in the convergence criteria. The names should correspond to variable names. By default the weights are set to the proportion of missing values on each variable.
decreasing	(boolean) if TRUE the order in which the variables are imputed is by decreasing amount of missing values. (the variable with highest amount of missing values will be imputed first). If FALSE the variable with lowest amount of missing values will be imputed first.
initialization	initialization method before running RF models; supported: mean/mode, me- dian/mode and custom. Default is mean/mode.

- x_init if initialization = custom; a complete dataframe to be used as initialization (see vignette for example).
- class.weights a named list containing class.weights parameter to be passed to ranger for categorical variables. The names of the list needs to respect the names of the categorical variables in the dataframe. (See ranger function documentation in ranger package for details).

return_integer_as_integer

Internally, integer columns are treated as double (double precision floating point numbers). If TRUE, the imputations will be rounded to closest integer and returned as integer (This might be desirable for count variables). If FALSE, integer columns will be returned as double (This might be desirable, for example, for patient age imputation). Default is FALSE. The same behaviour will be applied to new observations when using missForestPredict.

- save_models if TRUE, imputation models are saved and a new observation (or a test set) can be imputed using the models learned; saving models on a dataset with a high number of variables will occupy RAM memory on the machine. Default is TRUE.
- predictor_matrix

predictor matrix indicating which variables to use in the imputation of each variable. See documentation for function create_predictor_matrix for details on the matrix format.

proportion_usable_cases

a vector with two components: the first one is a minimum threshold for p_obs and the second one is a maximum threshold for p_miss. Variables for which p_obs is greater than or equal to 1 (by default) will be filtered from the predictor matrix. Variables for which p_miss is lower than or equal to 0 (by default) will be filtered from the predictor matrix. For more details on p_obs and p_miss see the documentation for the prop_usable_cases function. If parameter predictor_matrix is specified, the proportion_usable_cases will be applied to this provided matrix.

verbose (boolean) if TRUE then missForest returns OOB error estimates (MSE and NMSE) and runtime.

convergence_error

Which error should be used for the convergence criterion. Supported values: OOB and apparent. If a different value is provided, it defaults to OOB. See vignette for full details on convergence.

... other arguments passed to ranger function (some arguments that are specific to each variable type are not supported). See vignette for num.trees example.

Details

An adaptation of the original missForest algorithm (Stekhoven et al. 2012) is used. Variables are initialized with a mean/mode, median/mode or custom imputation. Then, they are imputed iteratively "on the fly" for a maximum number of iterations or until the convergence criteria are met. The imputation sequence is either increasing or decreasing. At each iteration, a random forest model is build for each variable using as outcome on the observed (non-missing) values of the variable and as predictors the values of the other variables from previous iteration for the first

missForest

variable in the sequence or current iteration for next variables in the sequence (on-the-fly). The ranger package (Wright et al. 2017) is used for building the random forest models.

The convergence criterion is based on the out-of-boostrap (OOB) error or the apparent error and uses NMSE (normalized mean squared error) for both continuous and categorical variables.

Imputation models for all variables and all iterations are saved (if save_models is TRUE) and can be later applied to new observations.

Both dataframe and tibble (tbl_df class) are supported as input. The imputed dataframe will be retured with the same class. Numeric and integer columns are supported and treated internally as continuous variables. Factor and character columns are supported and treated internally as categorical variables. Other types (like boolean or dates) are not supported. NA values are considered missing values.

Value

Object of class missForest with elements

ximp	dataframe with imputed values	
init	x_init if custom initalization is used; otherwise list of mean/mode or median/mode for each variable	
initialization	value of initialization parameter	
impute_sequence		
	vector variable names in the order in which imputation has been run	
maxiter	maxiter parameter as passed to the function	
models	list of random forest models for each iteration	
return_integer_as_integer		
	Parameter return_integer_as_integer as passed to the function	
integer_columns	3	
	list of columns of integer type in the data	
00B_err	dataframe with out-of-bag errors for each iteration and each variable	

References

- Stekhoven, D. J., & Bühlmann, P. (2012). MissForest-non-parametric missing value imputation for mixed-type data. Bioinformatics, 28(1), 112-118. doi:10.1093/bioinformatics/btr597
- Wright, M. N. & Ziegler, A. (2017). ranger: A fast implementation of random forests for high dimensional data in C++ and R. J Stat Softw 77:1-17. doi:10.18637/jss.v077.i01.

Examples

```
data(iris)
iris_mis <- produce_NA(iris, proportion = 0.1)
imputation_object <- missForest(iris_mis, num.threads = 2)
iris_imp <- imputation_object$ximp</pre>
```

missForestPredict

Description

Imputes a new dataframe based on the missForest models. The same number of iterations as in missForest are used.

Usage

```
missForestPredict(missForestObj, newdata, x_init = NULL)
```

Arguments

missForestObj	missForest object as returned by the missForest function.
newdata	new data to impute. The column names should be the same as in the imputation model.
x_init	initialization dataframe in case custom initialization mode has been used. It needs to be complete dataframe (with no missing values). See vignette for a full example.

Details

A new observation is initialized in the same manner as passed through the initialization parameter to the missForest function. Then, variables are imputed in the same sequence and for the same number of iterations using the random models saved for each iteration. This ensures that a new observation is imputed in the same manner as the training set (imputed by the function missForest). Re-imputing the training set with the missForestPredict will yield the same result as the original imputation returned by the missForest function.

Value

an imputed dataframe

Examples

```
data(iris)
# split train / test and create missing values
id_test <- sample(1:nrow(iris), floor(nrow(iris)/3))
iris_train <- iris[-id_test,]
iris_test <- iris[id_test,]</pre>
```

```
iris_train_miss <- produce_NA(iris_train, proportion = 0.1)
iris_test_miss <- produce_NA(iris_test, proportion = 0.1)</pre>
```

```
# impute train and learn imputation models
iris_train_imp_obj <- missForest(iris_train_miss, save_models = TRUE, num.threads = 2)</pre>
```

```
# impute test
iris_test_imp_new <- missForestPredict(iris_train_imp_obj, newdata = iris_test_miss)
head(iris_test_imp_new)
```

produce_NA

Produces a dataframe with missing values

Description

Produces a dataframe with missing values. For each variable, a random sample of observations of size proportion * nrow(x) will be set to NA.

Usage

produce_NA(x, proportion = 0.1)

Arguments

х	a dataframe
proportion	proportion of missing values to be produced; a vector of size ncol(x) or a single value to be applied to all variables in the dataframe.

Value

dataframe with missing values.

<pre>prop_usable_cases</pre>	Calculates variable-wise proportion of usable cases (missing and ob-
	served)

Description

Calculates variable-wise proportion of usable cases (missing and observed) as in Molenberghs et al. (2014).

Usage

```
prop_usable_cases(data)
```

Arguments

data dataframe to be imputed

Details

missForest builds models for each variable using the observed values of that variable as outcome of a random forest model. It then imputes the missing part of the variable using the learned models.

If all values of a predictor are missing among the observed value of the outcome, the value of p_obs will be 1 and the model built will rely heavily on the initialized values. If all values of a predictor are observed among the observed values of the outcome, p_obs will be 0 and the model will rely on observed values. Low values of p_obs are preferred.

Similarly, if all values of a predictor are missing among the missing values of the outcome, p_miss will have a value of 0 and the imputations (predictions) will heavily rely on the initialized values. If all values of a predictor are observed among the missing value of the outcome, p_miss will have a value of 1 and the imputations (predictions) will rely on real values. High values of p_miss are preferred.

Each row represents a variable to be imputed and each column a predictor.

Value

a list with two elements: p_obs and p_miss

p_obs	the proportion of missing Y_k among observed Y_j ; j in rows, k in columns
p_miss	the proportion of observed Y_k among missing Y_j ; j in rows, k in columns

References

• Molenberghs, G., Fitzmaurice, G., Kenward, M. G., Tsiatis, A., & Verbeke, G. (Eds.). (2014). Handbook of missing data methodology. CRC Press. Chapter "Multiple Imputation"

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