Package ‘varrank’

January 29, 2020

Type Package

Title Heuristics Tools Based on Mutual Information for Variable Ranking

Version 0.3

Author Gilles Kratzer [aut, cre] (<https://orcid.org/0000-0002-5929-8935>), Reinhard Furrer [ctb] (<https://orcid.org/0000-0002-6319-2332>)

Maintainer Gilles Kratzer <gilles.kratzer@math.uzh.ch>

Description A computational toolbox of heuristics approaches for performing variable ranking and feature selection based on mutual information well adapted for multivariate system epidemiology datasets. The core function is a general implementation of the minimum redundancy maximum relevance model. R. Battiti (1994) <doi:10.1109/72.298224>. Continuous variables are discretized using a large choice of rule. Variables ranking can be learned with a sequential forward/backward search algorithm. The two main problems that can be addressed by this package is the selection of the most representative variable within a group of variables of interest (i.e. dimension reduction) and variable ranking with respect to a set of features of interest.

Encoding UTF-8

License GPL-3

LazyData true

Suggests Boruta, FSelector, caret, e1071, mlbench, psych, varSelRF, gplots, entropy, testthat, knitr

URL https://www.math.uzh.ch/pages/varrank/

Imports stats, FNN, grDevices

Depends R (>= 3.5.0)

VignetteBuilder knitr

RoxygenNote 6.1.0

NeedsCompilation no

Repository CRAN

Date/Publication 2020-01-29 19:50:02 UTC
Discretization of a Possibly Continuous Data Frame of Random Variables

Description
This function discretizes data frame of possibly continuous random variables through rules for discretization. The discretization algorithms are unsupervised and univariate. See details for the complete list (the desired number of bins could also be provided).

Usage
```r
discretization(data.df = NULL, discretization.method = "cencov", frequency = FALSE)
```

Arguments
- `data.df`: a data frame containing the data to discretize, binary variables must be declared as factors, other as numeric vector. The data frame must be named.
- `discretization.method`: a character vector giving the discretization method to use; see details. If a number is provided, the variable will be discretized by equal binning.
- `frequency`: logical variable to select the output. If set to TRUE a list with the table of count for each bin and the discretized data frame is returned. If set to FALSE only the discretized data frame is returned.

Details
discretization() supports multiple rules for discretization. Below is the list of supported rules.

- `IQR()` stands for interquartile range.
- `fd` stands for the Freedman–Diaconis rule. The number of bins is given by

\[
\text{range}(x) \times n^{1/3} \over 2 \times IQR(x)
\]

The Freedman–Diaconis rule is known to be less sensitive than the Scott’s rule to outlier.
doane stands for doane’s rule. The number of bins is given by

\[ 1 + \log_2 n + \log_2 1 + \frac{|g|}{\sigma_g} \]

is a modification of Sturges’ formula which attempts to improve its performance with non-normal data.

cencov stands for Cencov’s rule. The number of bins is given by:

\[ n^{1/3} \]

rice stands for Rice’ rule. The number of bins is given by:

\[ 2n^{1/3} \]

terrell-scott stands for Terrell-Scott’s rule. The number of bins is given by:

\[ (2n)^{1/3} \]

This is known that Cencov, Rice and Terrell-Scott rules over estimates k compared to other rules due to his simplicity.

sturges stands for Sturges’s rule. The number of bins is given by:

\[ 1 + \log_2(n) \]

scott stands for Scott’s rule. The number of bins is given by:

\[ \frac{\text{range}(x)}{\sigma(x)n}n^{-1/3} \]

kmeans apply the classical k-means clustering to one-dimensional continuous data.

Value
the discretized dataframe or a list containing the table of counts for each bin the discretized dataframe

Author(s)
Gilles Kratzer

References

entropy.data

Computes an Empirical Estimation of the Entropy from a Table of Counts

Description

This function empirically estimates the Shannon entropy from a table of counts using the observed frequencies.

Usage

entropy.data(freqs.table)

Arguments

freqs.table a table of counts.

Details

The general concept of entropy is defined for probability distributions. The `entropy.data` function estimates empirical entropy from data. The probability is estimated from data using frequency tables. Then the estimates are plug-in in the definition of the entropy to return the so-called empirical entropy. A common known problem of empirical entropy is that the estimations are biased due to the sampling noise. This is also known that the bias will decrease as the sample size increases.

Value

Shannon’s entropy estimate on natural logarithm scale.

Author(s)

Gilles Kratzer

Examples

library("varrank")

rv <- rnorm(n = 100, mean = 0, sd = 2)

entropy.data(freqs.table = discretization(data.df = rv,
discretization.method = "fd",
frequency = TRUE)[[1]])
mi.data

Empirical Estimate of the Mutual Information from a Table of Counts

Description

This function estimates the mutual information from observed data.

Usage

mi.data(X, Y, discretization.method=NULL, k=NULL)

Arguments

X  a data frame containing only numeric or continuous variables.
Y  a data frame containing only numeric or continuous variables.
discretization.method  a character vector giving the discretization method to use. See discretization.
k  in case of purely continuous dataset, the mutual information can be computed using the k-nearest neighbours.

Details

The mutual information estimation is computed from the observed frequencies through a plugin estimator based on entropy or using the estimator described in A. Kraskov, H. Stogbauer and P.Grassberger (2004) when the data frame is exclusively made of continuous variables.

The plugin estimator is \( I(X, Y) = H(X) + H(Y) - H(X, Y) \), where \( H() \) is the entropy computed with entropy.data.

Value

Mutual information estimate.

Author(s)

Gilles Kratzer

References


Examples

Y <- rnorm(n = 100, mean = 0, sd = 2)
X <- rnorm(n = 100, mean = 5, sd = 2)

mi.data(X = Y, Y = X, discretization.method = "sturges")
Description

US data, for 1997-2002, from police-reported car crashes in which there is a harmful event (people or property), and from which at least one vehicle was towed. Data are restricted to front-seat occupants, include only a subset of the variables recorded, and are restricted in other ways also.

Usage

nassCDS

Format

A data frame with 26217 observations on the following 15 variables.

- **dvcat**: ordered factor with levels (estimated impact speeds) 1-9km/h, 10-24, 25-39, 40-54, 55+
- **weight**: Observation weights, albeit of uncertain accuracy, designed to account for varying sampling probabilities.
- **dead**: factor with levels alive dead
- **airbag**: a factor with levels none airbag
- **seatbelt**: a factor with levels none belted
- **frontal**: a numeric vector; 0 = non-frontal, 1=frontal impact
- **sex**: a factor with levels f m
- **ageOFocc**: age of occupant in years
- **yearacc**: year of accident
- **yearVeh**: Year of model of vehicle; a numeric vector
- **abcat**: Did one or more (driver or passenger) airbag(s) deploy? This factor has levels deploy nodeploy unavail
- **occRole**: a factor with levels driver pass
- **deploy**: a numeric vector: 0 if an airbag was unavailable or did not deploy; 1 if one or more bags deployed.
- **injSeverity**: a numeric vector; 0:none, 1:possible injury, 2:no incapacity, 3:incapacity, 4:killed; 5:unknown, 6:prior death
- **caseid**: character, created by pasting together the populations sampling unit, the case number, and the vehicle number. Within each year, use this to uniquely identify the vehicle.

Details

Data collection used a multi-stage probabilistic sampling scheme. The observation weight, called national inflation factor (national) in the data from NASS, is the inverse of an estimate of the selection probability. These data include a subset of the variables from the NASS dataset. Variables that are coded here as factors are coded as numeric values in that dataset.
plot.varrank

Source

See also http://www.maths.anu.edu.au/~johnm/datasets/airbags

References


For analyses based on the alternative FARS (Fatal Accident Recording System) data, and associated commentary, see:

Cummings, P; McKnight, B, 2010. Accounting for vehicle, crash, and occupant characteristics in traffic crash studies. Injury Prevention 16: 363-366. [The relatively definitive analyses in this paper use a matched cohort design,

Olson, CM; Cummings, P, Rivara, FP, 2006. Association of first- and second-generation air bags with front occupant death in car crashes: a matched cohort study. Am J Epidemiol 164:161-169. [The relatively definitive analyses in this paper use a matched cohort design, using data taken from the FARS (Fatal Accident Recording System) database.]

The web page http://www-fars.nhtsa.dot.gov/Main/index.aspx has a menu-based interface into the FARS (Fatality Analysis Recording System) data. The FARS database aims to include every accident in which there was at least one fatality.

Examples

data(nassCDS)
xtabs(weight ~ dead + airbag, data=nassCDS)
xtabs(weight ~ dead + airbag + seatbelt + dvcat, data=nassCDS)
tab <- xtabs(weight ~ dead + abcat, data=nassCDS, subset=dvcat=="25-39"&frontal==0)[, c(3,1,2)]
round(tab[2, ]/apply(tab,2,sum)*100,2)

plot.varrank

Visualization of varrank output

Description

plot method for varrank objects with multiple options.
Usage

## S3 method for class 'varrank'
plot(x,

## block separation
colsep = TRUE,
rowsep = TRUE,
sepcol = "white",
sepwidth = c(0.005, 0.005),

## cell labeling
cellnote = TRUE,
notecex = 1.5,
notecol = "black",
digitcell = 3,

## Row/Column Labelling
margins = c(6, 6, 4, 2),
labscrex = 1.2,

## color key + density info
colkey = NULL,
densadj = 0.25,
textlines = 2,

## plot labels
main = NULL,
maincex = 1,
...)

Arguments

x an object of class varrank.

colsep (optional) a logical parameter to indicate if columns should be separated from others by narrow space of color. The default is TRUE.

rowsep (optional) a logical parameter to indicate if rows should be separated from others by narrow space of color. The default is TRUE.

sepcol (optional) the color to use to separate rows or columns. The default is "white".

sepwidth (optional) Vector of length 2 giving the width (colsep) or height (rowsep) the separator box drawn by colsep and rowsep as a function of the width (colsep) or height (rowsep) of a cell. The defaults is c(0.005, 0.005).

cellnote (optional) a logical parameter to indicate if the scores should be displayed in cells.

notecex (optional) numeric scaling factor for scores. The default is 1.5.

notecol (optional) character string specifying the color for cellnote text. Defaults to "black".
digitcell (optional) integer that indicate how many digits of the scores should be displayed. The default is 3.

labels.cex the magnification factor to be used for x and y labels relative to the current setting of cex. The default is 1.2.

margins numerical vector of the form c(bottom, left, top, right) which gives the number of lines of margin to be specified on the four sides of the plot. The default is c(6, 6, 4, 2).

colkey specification for the color scheme to be used. The default is a rainbow color scheme.

densadj numeric scaling value for tuning the kernel width when a density plot is drawn on the color key. (See the adjust parameter for the density function for details.) Defaults is 0.25.

textlines number of lines to display relevance/redundance in the key. Default is 2.

main an overall title for the plot. Default is none.

main.cex main magnification to be used for the plot. Default is 1.

... additional arguments passed to image.

Details

This plot method for varrank objects provides an extensible framework for the visualization varrank output analysis. The user is allowed to specify block separations, display of scores and the color scheme to be used. The other parameters give a full control on the output. The final rendering depends on the algorithm used. For a 'forward' search the key density is on the upper right corner and for a 'backward' search the key density is in the bottom left corner. The default color scheme is continuous heat color from blue to red. A popular alternative for creating color palettes is RColorBrewer, https://cran.r-project.org/package=RColorBrewer.

This plot method is very similar to the heatmap.2 function from gplots, https://cran.r-project.org/package=gplots.

Author(s)

Gilles Kratzer

Examples

if (requireNamespace("mlbench", quietly = TRUE)) {
  library(mlbench)
  data(PimaIndiansDiabetes)
  #forward search for all variables
  out <- varrank(data.df = PimaIndiansDiabetes,
                 method = "estevez",
                 variable.important = "diabetes",
                 discretization.method = "sturges",
                 algorithm = "forward", scheme="mid")
  #default output
Methods for Varrank Objects

Description

Methods for computing on varrank objects.

Usage

## S3 method for class 'varrank'
print(x, digits = 5, ...)

Arguments

- **x**: an object of class varrank.
- **digits**: an integer specifying the number of digits to display in the output.
- **...**: additional arguments passed to print.

Details

digits gives the number of digits that will be displayed in the output. If more information are needed. There exists a summary S3 function that display more details.

Author(s)

Gilles Kratzer

Examples

```r
if (requireNamespace("mlbench", quietly = TRUE)) {
  library(mlbench)
  data(PimaIndiansDiabetes)

  ##forward search for all variables
  varrank.output <- varrank(data.df = PimaIndiansDiabetes,
                             method = "peng",
                             variable.important = "diabetes",
                             discretization.method = "sturges",
                             algorithm = "forward", scheme = "mid")

  ##Print varrank output
  varrank.output
}
```
Description

Methods for detailed display of varrank objects.

Usage

```r
## S3 method for class 'varrank'
summary(object, digits=3, ...)
```

Arguments

- **object**: an object of class varrank.
- **digits**: an integer specifying the number of digits to display in the output.
- **...**: additional arguments passed to summary.

Details

digits gives the number of digits that will be displayed in the output. This method differs of `print.varrank` by the amount of info displayed.

Author(s)

Gilles Kratzer

Examples

```r
if (requireNamespace("mlbench", quietly = TRUE)) {

library(mlbench)
data(PimaIndiansDiabetes)

# forward search for all variables
varrank.output <- varrank(data.df = PimaIndiansDiabetes,
                          method = "peng",
                          variable.important = "diabetes",
                          discretization.method = "sturges",
                          algorithm = "forward", scheme = "mid")

# Print summary output of varrank object
summary(varrank.output)
}
```
Heuristics Tools Based on Mutual Information for Variable Ranking and Feature Selection

Description

This function heuristically estimates the variables ranks based on mutual information with multiple model and multiple search schemes.

Usage

```r
varrank(data.df = NULL, variable.important = NULL, method = c("battiti", "kwak", "peng", "estevez"), algorithm = c("forward", "backward"), scheme = c("mid", "miq"), discretization.method = NULL, ratio = NULL, n.var = NULL, verbose = TRUE)
```

Arguments

- `data.df`: a named data frame with either numeric or factor variables.
- `variable.important`: a list of variables that is the target variables.
- `method`: the method to be used. See ‘Details’. Default is "estevez".
- `algorithm`: the algorithm scheme to be used. Default is "forward".
- `scheme`: the scheme search to be used. "mid" and "miq" stands for the Mutual Information Difference and Quotient schemes, respectively. Those are two ways to combine the relevance and redundancy. They are the two most used mRMRe schemes.
- `discretization.method`: a character vector giving the discretization method to use. See `discretization`.
- `ratio`: parameter to be used in "battiti" and "kwak".
- `n.var`: number of variables to be returned.
- `verbose`: logical. Should a progress bar be plotted? As the search scheme.

Details

By default `varrank` performs a variable ranking based on forward search algorithm using mutual information. The scoring is based on one of the four models implemented. The input dataset can be discrete, continuous or mixed variables. The target variables can be a set. The filter approach based on mutual information is the Minimum Redundancy Maximum Relevance (mRMRe) algorithm. A general formulation of the ensemble of mRMRe techniques is, given a set of features F, a subset of important features C, a candidate feature $f_i$ and possibly some already selected features $f_s$ in $S$. The local score function for a mid scheme (Mutual Information Difference) is expressed as:
\[ g_i(A, C, S, f_i) = MI(f_i; C) - \sum_{f_s} A(f_i, f_s, C) MI(f_i; f_s) \]

Depending of the value method, the value of A and B will be set accordingly to:

- battiti defined \( A=B \), where B is a user defined parameter (called ratio). Battiti (1994).
- kwak defined \( A = B \frac{MI(f_s;C)}{h(f_s)} \), where B a user defined parameter (called ratio). Kwak et al. (2002).
- peng defined \( A=1/|S| \). Peng et al. (2005).
- estevez defined \( A = \frac{1}{|S|} \min(H(f_i), H(f_s)) \). Estévez et al. (2009).

The search algorithm implemented are a forward search i.e. start with an empty set \( S \) and fill in. The the returned list is ranked by decreasing order of relevance. A backward search which start with a full set i.e. all variables except \texttt{variable.important} are considered as selected and the returned list is in increasing order of relevance based solely on mutual information estimation. Thus a backward search will only check for relevance and not for redundancy. \texttt{n.var} is optional if it is not provided, all candidate variables will be ranked.

Value

A list with an entry for the variables ranked and another entry for the score for each ranked variables.

Author(s)

Gilles Kratzer

References

Kratzer, G. and Furrer, R. "varrank: an R package for variable ranking based on mutual information with applications to system epidemiology"

Examples

```r
if (requireNamespace("mlbench", quietly = TRUE)) {
  library(mlbench)
  data(PimaIndiansDiabetes)

  ##forward search for all variables
  out1 <- varrank(data.df = PimaIndiansDiabetes,
                   method = "estevez",
                   variable.important = "diabetes",
                   discretization.method = "sturges",
                   algorithm = "forward", scheme = "mid")

  ##forward search for 3 variables
  out2 <- varrank(data.df = PimaIndiansDiabetes,
                   method = "estevez",
                   variable.important = "diabetes",
                   n.var = 3)
}
```
discretization.method = "sturges",
algorithm = "forward",
scheme = "mid",
n.var=3)

##backward search for all variables
out3 <- varrank(data.df = PimaIndiansDiabetes,
method = "peng",
variable.important = "diabetes",
discretization.method = "sturges",
algorithm = "backward",
scheme = "mid",
n.var=NULL)
}
Index

*Topic **datasets**
  nassCDS, 6

discretization, 2, 5, 12

entropy.data, 4, 5

mi.data, 5

nassCDS, 6

plot.varrank, 7

print.varrank, 10, 11

summary, 10

summary.varrank, 11

varrank, 12