Package 'fingerprint'

July 22, 2025

Version 3.5.7

Date 2018-01-06

Title Functions to Operate on Binary Fingerprint Data

Author Rajarshi Guha <rajarshi.guha@gmail.com>

Maintainer Rajarshi Guha <rajarshi.guha@gmail.com>

BugReports https://github.com/rajarshi/cdkr/issues

Description Functions to manipulate binary fingerprints of arbitrary length. A fingerprint is represented by an object of S4 class 'fingerprint' which is internally represented a vector of integers, such that each element represents the position in the fingerprint that is set to 1. The bitwise logical functions in R are overridden so that they can be used directly with 'fingerprint' objects. A number of distance metrics are also available (many contributed by Michael Fadock). Fingerprints can be converted to Euclidean vectors (i.e., points on the unit hypersphere) and can also be folded using OR. Arbitrary fingerprint formats can be handled via line handlers. Currently handlers are provided for CDK, MOE and BCI fingerprint data.

License GPL Depends methods LazyLoad yes Suggests RUnit NeedsCompilation yes Repository CRAN Date/Publication 2018-01-07 22:44:58 UTC

Contents

as.character																								•	2
balance																								•	3
bit.importance .						•																		•	4
bit.spectrum						•																		•	5
c		•	•	•	• •	•	•	•	•						•	•	•			•	•	•	•	•	6

as.character

cdk.lf, moe.lf, bci.lf	6
count-methods	7
distance-methods	8
euc.vector	11
feature-class	12
feature-methods	13
featvec-class	13
fingerprint-class	14
fold	16
fp.factor.matrix	17
fp.read, fp.read.to.matrix	18
fp.sim.matrix	19
fp.to.matrix	20
fplogical	21
length	21
random.fingerprint	22
shannon	23
show	23
	25
	25

Index

```
as.character
```

Generates a String Representation of a Fingerprint

Description

The function returns a string of 1's and 0's or a character vector of features depending on the nature of the fingerprint supplied.

Usage

```
## S4 method for signature 'fingerprint'
as.character(x)
## S4 method for signature 'featvec'
as.character(x)
## S4 method for signature 'feature'
as.character(x)
```

Arguments

```
х
```

An object of class fingerprint, featvec or feature

Value

A string of 1's and 0's or else a character vector of features (with their counts)

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

balance

Examples

```
# make a fingerprint vector
fp <- new("fingerprint", nbit=32, bits=sample(1:32, 20))
# print out the string representation
as.character(fp)
```

balance

Generate a Balanced Code Fingerprint

Description

It has been noted that the bit density in a fingerprint can affect its ability to retrieve similar compounds from a database primarily due to complexity effects. One approach to alleviating these effects is to generate fingerprints that have a bit density of 50 balanced code approach described by Nisius and Bajorath to convert an ordinary binary fingerprint (whose bit density is not 50 50 (resulting in a fingerprint twice the size of the original).

Usage

balance(fplist)

Arguments

fplist A single fingerprint or a list of fingerprints

Value

A single fingerprint objects or list of fingerprint objects that are "balanced", in that they have a bit density of 50 fingerprints.

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

References

Nisius, B.; Bajorath, J.; ChemMedChem, 2010, 5, 859-868.

See Also

bit.spectrum, bit.importance

bit.importance

Description

This method evaluates the Kullback-Leibler (KL) divergence to rank the individual bits in a binary fingerprint in their ability to discriminate between database and active compounds. This method is implemented based on Nisius and Bajorath and includes an m-estimate correction.

Usage

bit.importance(actives, background)

Arguments

actives	A list of fingerprints for the actives
background	A list of fingerprints representing the background collection

Value

A numeric vector of length equal to the size of the fingerprints. Each element of the vector is the KL divergence for the corresponding bit. If a bit position is never set to 1 in any of the compounds from the actives and the background, then the KL divergence for that position is undefined and NA is returned.

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

References

Nisius, B.; Bajorath, J.; ChemMedChem, 2010, 5, 859-868.

See Also

bit.spectrum

bit.spectrum

Description

The idea of comparing datasets using fingerprints was described in Guha \& Schurer (2008). The idea is that one can summarize the dataset by counting the frequency of occurrence of each bit position. The frequency is normalized by the number of fingerprints considered. Thus a collection of N fingerprints can be converted to a single vector of numbers highlighting the most frequent bits with respect to a given dataset. A plot of this vector looks like a traditional spectrum and hence the name.

The bit spectra for two datasets (assuming that the same types of fingerprints have been used) allows one to compare the similarity of the datasets, without having to do a full pairwise similarity calculation. The difference between the structural features of the datasets can be quantified by evaluating the distance between the two bit spectra.

Usage

```
bit.spectrum(fplist)
```

Arguments

fplist	A list structure with each element being an object of class fingerprint. These
	will can be constructed by hand or read from disk via fp. read.
	All fingerprints in the list should be of the same length.

Value

A numeric vector of length equal to the size of the fingerprints.

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

References

Guha, R.; Schurer, S.; J. Comp. Aid. Molec. Des., 2008, 22, 367-384.

See Also

distance, fp.read

Description

Combine multiple feature objects to give a list of feature objects

Usage

S4 method for signature 'feature'
c(x, ..., recursive = FALSE)

Arguments

х	An object of class feature
	One or more feature objects
recursive	Ignored

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

cdk.lf, moe.lf, bci.lf

Functions to parse lines from fingerprint files

Description

These functions take a single line and parses it to produce a vector of integers which represents the position of the 'on' bits in a fingerprint. This allows the user to use read.fp with arbitrary fingerprint files. A new file format can be handled by defining a new line parser function. Currently the first three functions process fingerprint files obtained from the CDK (http://cdk. sourceforge.net), MOE (http://chemcomp.com), BCI (http://www.digitalchemistry.co. uk/) and the FPS format (http://code.google.com/p/chem-fingerprints/wiki/FPS). The last function can be used for any fingerprint that generates hashed features (such as ECFPs or other circular fingerprints). For these cases, it is assumed that features are unsigned integers, so string features are not handled.

Note that when the fps.lf function is specified, items such as the number of bits or the header flag do not need to be specified, as the format requires a header block containing some of these items.

с

count-methods

Usage

```
cdk.lf(line)
moe.lf(line)
bci.lf(line)
ecfp.lf(line)
fps.lf(line)
jchem.binary.lf(line)
```

Arguments

line

The line to parse

Value

A list with three componenents - the name associated with the fingerprint (if available) and a vector of integers representing bits set to 1 (for the case of the first three methods) or a vector of characters representing hashed features (characteristic of circular fingerprints) or more generally, any string feature. The third component is a (possibly empty) list, which contains the remaining components of a line, when the format allows items other than an a title and the fingerprint (such as the FPS format). The content of the third component is dependent on the line function that is being used.

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

count-methods Get or Set Count of Occurence of a Feature	
--	--

Description

Get or set the count of occurence associated with a feature-class object. The default value for the getter (as defined in the prototype) is 1.

Usage

```
## S4 method for signature 'feature'
count(object)
## S4 replacement method for signature 'feature,numeric'
count(x) <- value</pre>
```

Arguments

object	An object of class feature-class
х	An object of class feature-class
value	A numeric (which will be coerced to integer) indicating the count associated with the feature

Value

An integer representing count of occurence of the feature

Methods

```
signature(object = "feature") Return the count associated with the feature object
signature(x = "feature", value = "numeric") Set the count associated with the feature object
```

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

distance-methods Calculates the Similarity or Dissimilarity Between Two Fingerprints

Description

A number of distance metrics can be calculated for binary fingerprints. Some of these are actually similarity metrics and thus represent the reverse of a distance metric.

The following are distance (dissimilarity) metrics

- Hamming
- Mean Hamming
- Soergel
- Pattern Difference
- Variance
- Size
- Shape

The following metrics are similarity metrics and so the distance can be obtained by subtracting the value fom 1.0

- Tanimoto
- Dice
- Modified Tanimoto
- Simple
- Jaccard
- Russel-Rao
- · Rodgers Tanimoto
- Cosine
- Achiai
- Carbo

distance-methods

- Baroniurbanibuser
- Kulczynski2
- Robust

Finally the method also provides a set of composite and asymmetric distance metrics

- Hamann
- Yule
- Pearson
- Dispersion
- McConnaughey
- Stiles
- Simpson
- Petke
- Tversky

The default metric is the Tanimoto coefficient.

Usage

distance(fp1, fp2, method, a, b)

Arguments

fp1	An object of class fingerprint or featvec
fp2	An object of class fingerprint or featvec
а	Parameter for the Tversky index
b	Parameter for the Tversky index
method	The type of distance metric desired. Partial matching is supported and the deault is tanimoto. Alternative values are
	a gualidaan

- euclidean
- hamming
- meanHamming
- soergel
- patternDifference
- variance
- size
- shape
- jaccard
- dice
- mt
- simple
- russelrao

- rodgerstanimoto
- cosine
- achiai
- carbo
- baroniurbanibuser
- kulczynski2
- robust
- hamann
- yule
- pearson
- mcconnaughey
- stiles
- simpson
- petke
- tversky

If the two fingerprints are of class featvec then the following methods may be specified: tanimoto, robust and dice.

Value

Numeric value representing the distance in the specified metric between the supplied fingerprint objects

Methods

- signature(fp1 = "featvec", fp2 = "featvec", method = "character", a = "missing", b = "missing")
 Similarity method for feature vector type fingerprints, supporting tanimoto, robust and dice
 metrics.
- signature(fp1 = "featvec", fp2 = "featvec", method = "missing", a = "missing", b = "missing")
 Evaluate Tanimoto similarity between two feature vector fingerprints
- signature(fp1 = "fingerprint", fp2 = "fingerprint", method = "character", a = "missing", b = "missing")
 Evaluate similarity (or dissimility) between two binary fingerprints. See below for a list of
 possible similarity (or dissimilarity) metrics
- signature(fp1 = "fingerprint", fp2 = "fingerprint", method = "character", a = "numeric", b = "numeric")
 Evaluate Tversky similarity between two binary fingerprints.
- signature(fp1 = "fingerprint", fp2 = "fingerprint", method = "missing", a = "missing", b = "missing")
 Evaluate Tanimoto similarity between two binary fingerprints

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

euc.vector

References

Fligner, M.A.; Verducci, J.S.; Blower, P.E.; A Modification of the Jaccard-Tanimoto Similarity Index for Diverse Selection of Chemical Compounds Using Binary Strings, *Technometrics*, 2002, 44(2), 110-119

Monve, V.; Introduction to Similarity Searching in Chemistry, MATCH - Comm. Math. Comp. Chem., 2004, 51, 7-38

Examples

```
# make a 2 fingerprint vectors
fp1 <- new("fingerprint", nbit=6, bits=c(1,2,5,6))
fp2 <- new("fingerprint", nbit=6, bits=c(1,2,5,6))
# calculate the tanimoto coefficient
distance(fp1,fp2) # should be 1
# Invert the second fingerprint
fp3 <- !fp2
distance(fp1,fp3) # should be 0
```

euc.vector

Euclidean Representation of Binary Fingerprints

Description

Ordinarily, a binary fingerprint can be considered to represent a corner of a nD hypercube. However in many cases using such a representation can lead to a very sparse space. Consequently one approach is to convert the fingerprint so that it represents points on a nD unit hypersphere.

The resultant fingerprint is then a nD coordinate.

Usage

euc.vector(fp)

Arguments

fp An object of class fingerprint.

Value

A numeric of length equal to the bit length of the fingerprint. The result corresponds to a unit vector for a point on the nD hypersphere

Author(s)

Rajarshi Guha <rguha@indiana.edu>

Examples

```
# make a fingerprint vector
fp <- new("fingerprint", nbit=8, bits=c(1,3,4,5,7))
vec <- euc.vector(fp)</pre>
```

feature-class Class "feature"

Description

This class represents features - arbitrary alphanumeric sequences that are used to characterize molecular substructures (though there is no real restriction to molecules). A feature is associated with an integer count, indicating the occurence of that feature in a molecule. The default value is 1.

Objects from the Class

Objects can be created by calls of the form new("feature", ...).

Slots

feature: Object of class "character" ~ The string representation of a feature

count: Object of class "integer" ~ The occurence of the feature. Default is 1

.Data: ???

Methods

count signature(object = "feature"): Return the count associated with the feature

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

See Also

featvec-class

Examples

```
## create a new feature
f <- new("feature", feature='ABCD', count=as.integer(1))
## modify the feature string and the count
feature(f) <- 'UXYZ'
count(f) <- 10</pre>
```

12

feature-methods

Description

Get or set the character string representing a feature of a feature-class object. The default value for the getter (as defined in the prototype) is the empty string.

Usage

```
## S4 method for signature 'feature'
feature(object)
## S4 replacement method for signature 'feature,character'
feature(x) <- value</pre>
```

Arguments

object	An object of class feature-class
x	An object of class feature-class
value	The character string to replace the current feature string with

Value

An character string representing the feature

Methods

signature(object = "feature") Return the feature associated with the feature object

signature(x = "feature", value = "character") Set the feature associated with the feature
 object

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

featvec-class Class "featvec"

Description

This class represents feature vector style fingerprints, where, rather than a bit string, the fingerprint is represented as a sequence of (signed) integers or strings. Each element of the collection is a representation of a structural feature. For cases where the features are integers, this usually corresponds to a hash of the original feature string.

Objects from the Class

Objects can be created by calls of the form new("featvec", ...). In contrast to traditional binary fingerprints, operations on feature vectors are slightly different and essentially correspond to operations on sets. Thus the logical and (&) would correspond to the union of the two feature vectors.

Slots

- features: Object of class "character" ~~ A vector containing the numeric or character features. Numeric features are treated as character strings
- provider: Object of class "character" ~~ Indicates the source of the fingerprint. Can be useful to keep track of what software generated the fingerprint.
- name: Object of class "character" ~~ The name associated with the fingerprint. If not name is available this gets set to an empty string
- misc: A list to hold arbitrary items associated with a fingerprint (such as extra fields from a fingerprint file)

Methods

```
distance signature(fp1 = "featvec", fp2 = "featvec", method = "missing"): ...
```

```
distance signature(fp1 = "featvec", fp2 = "featvec", method = "character"): ...
```

```
as.character signature(fp = "featvec"): ...
```

```
length signature(fp = "featvec"): ...
```

```
show signature(fp = "featvec"): ...
```

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

See Also

fp.read, fp.read.to.matrix fp.sim.matrix, fp.to.matrix, fp.factor.matrix random.fingerprint

fingerprint-class Class "fingerpint"

Description

This class represents binary fingerprints, usually generated by a variety of cheminformatics software, but not restricted to such

fingerprint-class

Objects from the Class

Objects can be created by calls of the form new("fingerprint", ...). Fingerprints can traditionally thought of as a vector of 1's and 0's. However for large fingerprints this is inefficient and instead we simply store the positions of the bits that are on. Certain operations also need to know the length of the original bit string and this length is stored in the object at construction. Even though we store extra information along with the bit positions, conceptually we still consider the objects as simple bit strings. Thus the usual bitwise logical operations (&, l, !, xor) can be applied to objects of this class.

Slots

- bits: Object of class "numeric" ~~ A vector indicating the bit positions that are on.
- nbit: Object of class "numeric" ~~ Indicates the length of the original bit string.
- folded: Object of class "logical" ~~ Indicates whether the fingerprint has been folded.
- provider: Object of class "character" ~~ Indicates the source of the fingerprint. Can be useful to keep track of what software generated the fingerprint.
- name: Object of class "character" ~~ The name associated with the fingerprint. If not name is available this gets set to an empty string
- misc: Object of class "list" ~~ A holder for arbitrary items that may have been stored along with the fingerprint. Only certain formats allow extra items to be stored with the fingerprint, so in many cases this field is just an empty list

Methods

```
distance signature(fp1 = "fingerprint", fp2 = "fingerprint", method = "missing", a = "missing",
b = "missing"): ...
```

```
distance signature(fp1 = "fingerprint", fp2 = "fingerprint", method = "character", a =
    "missing", b = "missing"): ...
```

```
euc.vector signature(fp = "fingerprint"): ...
```

```
fold signature(fp = "fingerprint"): ...
```

random.fingerprint signature(nbit = "numeric", on = "numeric"): ...

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

See Also

fp.read, fp.read.to.matrix fp.sim.matrix, fp.to.matrix, fp.factor.matrix random.fingerprint

Examples

```
## make fingerprints
x <- new("fingerprint", nbit=128, bits=sample(1:128, 100))
y <- x
distance(x,y) # should be 1
x <- new("fingerprint", nbit=128, bits=sample(1:128, 100))</pre>
```

```
distance(x,y)
folded <- fold(x)
## binary operations on fingerprints
x <- new("fingerprint", nbit=8, bits=c(1,2,3,6,8))
y <- new("fingerprint", nbit=8, bits=c(1,2,4,5,7,8))
x & y
x & y
x | y
!x</pre>
```

fold

Fold a fingerprint

Description

In many situations a fingerprint is generated using a large length (such as 1024 bits or more). As a result of this, the fingerprints for a dataset can be very sparse. One approach to increasing bit density of such fingerprints is to fold them. This is performed by dividing the original fingerprint bitstring into two substrings of equal length and then perform an OR on the two substrings.

It should be noted that many fingerprint generating routines will perform this internally.

Usage

fold(fp)

Arguments

fp

The fingerprint to fold. Should be of class fingerprint.

Value

An object of class fingerprint representing the folded fingerprint.

Author(s)

Rajarshi Guha <rguha@indiana.edu>

Examples

```
# make a fingerprint vector
fp <- new("fingerprint", nbit=64, bits=sample(1:64, 30))
fold(fp)
```

16

fp.factor.matrix Converts a List of Fingerprints to a data.frame of Factors

Description

This function will convert a list of fingerprint objects to a data. frame of factors with levels 1 and 0.

Usage

```
fp.factor.matrix(fplist)
```

Arguments

fplist	A list structure with each element being an object of class fingerprint. These
	will can be constructed by hand or read from disk via fp. read

Value

A matrix with dimensions equal to (length(fplist), length(fplist))

Author(s)

Rajarshi Guha <rguha@indiana.edu>

See Also

distance, fp.read

Examples

```
# make fingerprint objects
fp1 <- new("fingerprint", nbit=6, bits=c(1,2,5,6))
fp2 <- new("fingerprint", nbit=6, bits=c(1,4,5,6))
fp3 <- new("fingerprint", nbit=6, bits=c(2,3,4,5,6))</pre>
```

```
fp.factor.matrix( list(fp1,fp2,fp3) )
```

fp.read, fp.read.to.matrix

Functions to Read Fingerprints From Files

Description

fp.read reads in a set of fingerprints from a file. Fingerprint output from the CDK, MOE and BCI can be handled.

Each fingerprint is represented as a fingerprint object. fp.read returns a list structure, each element being a fingerprint or nfeatvec object, depending on the value of the binary argument.

fp.read.to.matrix is a utility function that reads the fingerprints directly to matrix form (columns are the bit positions and the rows are the objects whose fingerprints have been evaluated). Note that this method does not currently work with feature vector fingerprints.

Usage

fp.read(f='fingerprint.txt', size=1024, lf=cdk.lf, header=FALSE, binary=TRUE)
fp.read.to.matrix(f='fingerprint.txt', size=1024, lf=cdk.lf, header=FALSE)

Arguments

f	File containing the fingperprints
size	The bit length of the fingerprints being considered
lf	A line reading function that parses a single line from a fingerprint file. A number of functions are provided that parse the fingerprints from the output of the CDK, MOE and the BCI toolkit. In addition, support is now available for the FPS format from the chemfp project (http://code.google.com/p/ chem-fingerprints).
header	Indicates whether the first line of the fingerprint file is a header line
binary	If TRUE indicates that a binary fingerprint will be read in. Otherwise indicates that a feature vector style fingerprint (such as from a circular fingerprint) is being read in

Value

A list or matrix of fingerprints

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

See Also

cdk.lf, moe.lf, bci.lf, ecfp.lf, fps.lf

fp.sim.matrix

Description

Given a set of fingerprints, a pairwise similarity can be calculated using the various distance metrics defined for binary strings. This function calculates the pairwise similarity matrix for a set of fingerprint or featvec objects supplied in a list structure. Any of the distance metrics provided by distance can be used and the default is the Tanimoto metric.

Note that if the Euclidean distance is specified then the resultant matrix is a distance matrix and not a similarity matrix

Usage

```
fp.sim.matrix(fplist, fplist2=NULL, method='tanimoto')
```

Arguments

fplist	A list structure with each element being an object of class fingerprint or featvec. These can be constructed by hand or read from disk via fp.read
fplist2	A list structure with each element being an object of class fingerprint or featvec. if NULL then traditional pairwise similarity is calculated with each member in fplist, otherwise the resultant N x M matrix is derived from the similarity between each member of fplist and fplist2
method	The type of distance metric to use. The default is tanimoto. Partial matching is supported.

Value

A matrix with dimensions equal to (length(fplist), length(fplist)) if fplist2 is NULL, otherwise (length(fplist), length(fplist2))

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

See Also

distance, fp.read

Examples

```
# make fingerprint objects
fp1 <- new("fingerprint", nbit=6, bits=c(1,2,5,6))
fp2 <- new("fingerprint", nbit=6, bits=c(1,4,5,6))
fp3 <- new("fingerprint", nbit=6, bits=c(2,3,4,5,6))
fp.sim.matrix( list(fp1,fp2,fp3) )</pre>
```

fp.to.matrix

Description

In general, fingerprint data is read from a file or obtained via calls to an external generator and the return value is a list of fingerprints. This function takes the list and returns a matrix having number of rows equal to the number of fingerprints and the number of columns equal to the length of the fingerprint. Each element is 1 or 0 (1's being specified by the positions in each fingerprint vector)

Usage

```
fp.to.matrix(fplist)
```

Arguments

fplist	A list structure with each element being an object of class fingerprint. These
	will can be constructed by hand or read from disk via fp. read

Value

A matrix with dimensions equal to length(fplist), bit length) where bit length is a property of the fingerprint objects in the list.

Author(s)

Rajarshi Guha <rguha@indiana.edu>

See Also

distance, fp.read

Examples

```
# make fingerprint objects
fp1 <- new("fingerprint", nbit=6, bits=c(1,2,5,6))
fp2 <- new("fingerprint", nbit=6, bits=c(1,4,5,6))
fp3 <- new("fingerprint", nbit=6, bits=c(2,3,4,5,6))</pre>
```

```
fp.to.matrix( list(fp1,fp2,fp3) )
```

fplogical

Description

These functions perform logical operatiosn (AND, OR, NOT, XOR) on the supplied binary fingerprints. Thus for two fingerprints A and B we have

& Logical AND| Logical ORxor Logical XOR! Logical NOT (negation)

Arguments

e1	An object of class fingerprint
e2	An object of class fingerprint

Value

A fingerprint object

Author(s)

Rajarshi Guha <rguha@indiana.edu>

length

Fingerprint Bit Length

Description

Returns the length of the fingerprint. That is, this is the length of the entire bit string and not simply the number of bits that are on.

Usage

```
## S4 method for signature 'fingerprint'
length(x)
```

Arguments

x An object of class fingerprint

Value

The length of the bit string

Author(s)

Rajarshi Guha <rguha@indiana.edu>

random.fingerprint Generate Randomized Fingerprints

Description

A utility function that can be used to generate binary fingerprints of a specified length with a specified number of bit positions (selected randomly) set to 1. Currently bit positions are selected uniformly

Usage

```
random.fingerprint(nbit,on)
```

Arguments

nbit	The length of the fingerprint, that is, the total number of bits. Must be a positive integer.
on	How many positions should be set to 1

Value

An object of class fingerprint

Author(s)

Rajarshi Guha <rguha@indiana.edu>

Examples

```
# make a fingerprint vector
fp <- random.fingerprint(32, 16)
as.character(fp)
```

shannon

Description

This method evaluates the Shannon entropy for a set of fingerprints and utilizes the bit.spectrum method to obtain the relative frequencies of individual bits

Usage

shannon(fplist)

Arguments

fplist	A list structure with each element being an object of class fingerprint. These
	will can be constructed by hand or read from disk via fp. read.
	All fingerprints in the list should be of the same length.

Value

The Shannon entropy for the set of fingerprints

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

See Also

bit.spectrum,fp.read

show

String Representation of a Fingerprint or Feature

Description

Simply summarize the fingerprint or feature

Usage

```
## S4 method for signature 'fingerprint'
show(object)
## S4 method for signature 'featvec'
show(object)
## S4 method for signature 'feature'
show(object)
```

Arguments

object An object of class fingerprint, featvec or feature

Author(s)

Rajarshi Guha <rajarshi.guha@gmail.com>

Index

! (fplogical), 21 !, fingerprint-method (fplogical), 21 * classes feature-class, 12 featvec-class, 13 fingerprint-class, 14 * logic as.character, 2 c, 6 cdk.lf, moe.lf, bci.lf, 6 distance-methods, 8 euc.vector, 11 feature-class, 12 featvec-class, 13 fingerprint-class, 14 fold, 16 fp.factor.matrix, 17 fp.read, fp.read.to.matrix, 18 fp.sim.matrix, 19 fp.to.matrix, 20 fplogical, 21 length, 21 random.fingerprint, 22 show, 23 * methods as.character, 2 fplogical, 21 length, 21 * programming balance, 3 bit.importance,4 bit.spectrum, 5 count-methods, 7 feature-methods, 13 shannon, 23 &(fplogical), 21 &, fingerprint, fingerprint-method (fplogical), 21

as.character, 2

as.character,feature-method
 (as.character), 2
as.character,featvec-method
 (as.character), 2
as.character,fingerprint-method
 (as.character), 2

balance, 3
bci.lf, 18
bci.lf(cdk.lf, moe.lf, bci.lf), 6
bit.importance, 3, 4
bit.spectrum, 3, 4, 5, 23

c, <mark>6</mark>

distance, 5, 17, 19, 20 distance (distance-methods), 8 distance, featvec, featvec, character, missing, missing-method (distance-methods), 8 distance, featvec, featvec, character-method (featvec-class), 13 distance, featvec, featvec, missing, missing, missing-method (distance-methods), 8 distance, featvec, featvec, missing-method (featvec-class), 13 distance, fingerprint, fingerprint, character, missing, missing (distance-methods), 8 distance, fingerprint, fingerprint, character, numeric, numeric (distance-methods), 8 distance, fingerprint, fingerprint, missing, missing, mossing, mos (distance-methods), 8 show, 23 distance-methods, 8 show, feature-method (show), 23 show, featvec-method (show), 23 ecfp.lf, 18 show, fingerprint-method (show), 23 ecfp.lf(cdk.lf, moe.lf, bci.lf), 6 entropy (shannon), 23 xor (fplogical), 21 euc.vector, 11 xor,fingerprint,fingerprint-method euc.vector,fingerprint-method (fplogical), 21 (fingerprint-class), 14 feature (feature-methods), 13 feature, feature-method (feature-methods), 13 feature-class, 12 feature-methods, 13 feature<- (feature-methods), 13</pre> feature<-,feature,character-method</pre> (feature-methods), 13 feature<--methods (feature-methods), 13 featvec-class, 13 fingerprint-class, 14 fold, 16 fold,fingerprint-method (fingerprint-class), 14 fp.factor.matrix, 14, 15, 17 fp.read, 5, 14, 15, 17, 19, 20, 23 fp.read(fp.read, fp.read.to.matrix), 18 fp.read, fp.read.to.matrix, 18 fp.read.to.matrix, 14, 15 fp.sim.matrix, 14, 15, 19 fp.to.matrix, 14, 15, 20 fplogical, 21 fps.lf, 18 fps.lf(cdk.lf, moe.lf, bci.lf), 6 jchem.binary.lf(cdk.lf, moe.lf, bci.lf), 6 length, 21 length,featvec-method(featvec-class), 13 length,fingerprint-method(length),21 moe.lf, *18* moe.lf(cdk.lf, moe.lf, bci.lf), 6 random.fingerprint, 14, 15, 22 random.fingerprint,numeric,numeric-method (fingerprint-class), 14

26