Package 'SK4FGA'

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Type Package

Title Scott-Knott for Forensic Glass Analysis

Version 0.1.1

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Description In forensics, it is common and effective practice to analyse glass fragments from the scene and suspects
to gain evidence of placing a suspect at the crime scene.
This kind of analysis involves comparing the physical and chemical attributes of glass fragments that exist on both the
person and at the crime scene, and assessing the significance in a likeness that they share.
The package implements the Scott-
Knott Modification 2 algorithm (SKM2) (Christopher M. Triggs and
James M. Curran and John S. Buckleton and Kevan A.J. Walsh (1997) <doi:10.1016/S0379-0738(96)02037-3>
``The grouping problem in forensic glass analysis: a divisive approach", Forensic Science International, 85(1), 1--14)
for small sample glass fragment analysis using the refractive index (ri) of a set of glass samples.
It also includes an experimental multivariate analog to the Scott-
Knott algorithm for similar analysis on glass samples
with multiple chemical concentration variables and multiple samples of the same item; testing against the Hotellings T^2
distribution (J.M. Curran and C.M. Triggs and J.R. Almirall and J.S. Buckleton and K.A.J. Walsh (1997)
<doi:10.1016/S1355-0306(97)72197-X> ``The interpretation of elemental composition measurements from forensic glass evidence", Science & Justice, 37(4), 241--244).

License GPL (>= 2)

BugReports https://github.com/tobyhayward13/SCI118UOA_ForensicGlassAnalysis/issues

URL https://github.com/tobyhayward13/SCI118UOA_ForensicGlassAnalysis

Encoding UTF-8

LazyData true

Depends R (>= 2.10)

RoxygenNote 7.2.3

LinkingTo Rcpp

Imports Rcpp

NeedsCompilation yes

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James Curran [aut, ctb] (Supervised and contributed to the development of the package.),
Lewis Kendall-Jones [ctb] (Wrote and supported the development of the C++ code.)

Repository CRAN

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Contents

`calculate_lambda_threshold` *Calculate the significance threshold for Lambda.*

Description

For a given significance value, this function uses critical values determined from simulated data formed on 1 million arrays, and returns the quantile estimated at that significance level. For values of k > 20, it assumes a chi squared distribution with k/(pi - 2) degrees of freedom.

Usage

```
calculate_lambda_threshold(k, alpha)
```

Arguments

k	Number of indices.
alpha	Level of significance.

Value

A 100(1-alpha)% quantile estimate from the distribution of Lambda.

---

find_B0 *Calculate B0*

Description

Calculates the B0 value for a given numeric vector of values; assuming they're appropriate values corresponding to glass fragment refractive indices.

Usage

```
find_B0(arr)
```

Arguments

arr	vector of refractive indices.

Value

A numeric corresponding to the maximum between-sum-of-squares estimate from the sample.

---

find_T0 *Calculate T0 for a given list of glass fragments and features.*

Description

Calculates the "T0" value (the split corresponding to the maximum value of T^2) for a given list of data sets corresponding to glass fragment features assuming they're appropriate values corresponding to glass fragment features.

Usage

```
find_T0(data, i = 1, j = length(data))
```

Arguments

data	list of glass fragment chemical (or otherwise) features.
i	Starting element (default = 1)
j	Ending element (default = length(array))

Value

A numeric corresponding to the maximum between-sum-of-squares estimate from the sample.

`find_T2` *Calculate Hotelling's T^2 Statistic for two independent multivariate samples.*

Description

Calculate Hotelling's T^2 Statistic for two independent multivariate samples.

Usage

```
find_T2(d1, d2)
```

Arguments

`d1`	matrix or data.frame type object containing the multivariate data for the first sample.
`d2`	matrix or data.frame type object containing the multivariate data for the second sample.

Value

T^2 value for the two objects.

`generate_indices` *Generate a test array of Glass-Fragment Refractive Indices.*

Description

Returns a vector of randomly generated refractive indices from a expected normal distribution of glass fragments.

Usage

```
generate_indices(n = 10, .sd_multi = 1)
```

Arguments

`n`	Number of refractive indices to generate.
`.sd_multi`	Scale factor of the standard deviation. Greater values imply more variance in the random sample.

Value

A vector of randomly generated RIs.

Examples

```
test_ris = generate_indices(8)
partition(test_ris)

test_ris_varied = generate_indices(.sd_multi = 5)
partition(test_ris_varied)
```

`glass` *glass*

Description

Glass composition data for seven elements from 200 glass items.

Usage

```
data(glass)
```

Format

a 'data.frame' with 2400 rows and 9 columns.

item factor200 levels - which item the measurements came from

fragment factor4 levels - which of the four fragments from each item the observations were made upon

logNaO numericlog of sodium concentration to oxygen concentration

logMgO numericlog of magnesium concentration to oxygen concentration

logAlO numericlog of aluminium concentration to oxygen concentration

logSiO numericlog of silicon concentration to oxygen concentration

logKO numericlog of potassium concentration to oxygen concentration

logCaO numericlog of calcium concentration to oxygen concentration

logFeO numericlog of iron concentration to oxygen concentration

Details

These data are from Grzegorz (Greg) Zadora at the [Institute of Forensic Research](http://ies.krakow.pl/) in Krakow, Poland. They are the log of the ratios of each element to oxygen, so logNaO is the log(10) of the Sodium to Oxygen ratio, and logAlO is the log of the Aluminium to Oxygen ratio. The instrumental method was SEM-EDX.

The ‘item‘ indicates the object the glass came from. The levels for each item are unique to that item. The ‘fragment‘ can be considered a sub-item. When collecting these observations Greg took a glass object, say a jam jar, he would then break it, and extract four fragments. Each fragment would be measured three times upon different parts of that fragment. The fragment labels are repeated, so, for example, fragment "f1" from item "s2" has nothing whatsoever to do with fragment "f1" from item "s101".

For two level models use ‘item‘ as the lower level - three level models can use the additional information from the individual fragments.

Source

Grzegorz Zadora [Institute of Forensic Research](http://ies.krakow.pl/), Krakow, Poland.

References

Aitken, C.G.G. Zadora, G. & Lucy, D. (2007) A Two-Level Model for Evidence Evaluation. *Journal of Forensic Sciences*: **52**(2); 412-419.

`glass2` *glass2*

Description

Glass Fragment Elemental Composition Data on 15 variables.

Usage

```
data(glass2)
```

Format

a ‘data.frame‘ with 16 rows and 16 columns.

item factor761 levels - which item the measurements came from

Li7 numericlog of lithium concentration

Mg25 numericlog of magnesium concentration

Al27 numericlog of aluminium concentration

K39 numericlog of potassium concentration

Ti49 numericlog of titanium concentration

Mn55 numericlog of manganese concentration

Fe57 numericlog of iron concentration

Rb85 numericlog of rubidium concentration

Sr88 numericlog of strontium concentration

Zr90 numericlog of zirconium concentration

Ba137 numericlog of barium concentration

La139 numericlog of lanthanum concentration

Ce140 numericlog of cerium concentration

Nd146 numericlog of neodymium concentration

Pb208 numericlog of lead concentration

Details

Log transformed example casework data

Source

Almirall, Jose; Akmeemana, Anuradha, 2022, "casework.tab", Shiny Glass Application, https://doi.org/10.34703/gzx1-9v95/OB8BS9/CP6WXP, FIU Research Data Portal, V2, UNF:6:jQxEQCGZVvlWtc6owbtp+A== [fileUNF]

References

Anuradha Akmeemana, R. C., Jose Almirall, The Calculation of Calibrated Likelihood Ratios (LRs) for Glass Using a Multivariate Kernel Density Model: Introducing a User-Friendly Graphical User Interface (GUI). In American Academy of Forensic Science, Anaheim, CA, 2020.

`has.children` *has.children*

Description

For internal use only. Determines if a node in the Partition tree has a child.

Usage

```
has.children(part)
```

Arguments

`part`	Node in partition Tree.

Value

Logical determining if the node has any children.

order_euclid — *Order a list of data frames containing numerical columns by their euclidean distance to the mean.*

Description

Meant for internal use only.

Usage

```
order_euclid(alist)
```

Arguments

alist	A list of data frames.

Value

A list of data frames.

partition — *Create Partitions of an RI array.*

Description

Partitions the array of assumed glass fragment refractive indices into statistically significant groups.

Usage

```
partition(array, alpha = 0.05, .debug = FALSE)
```

Arguments

array	Vector of refractive indices.
alpha	Significance parameter "[0,1]". Higher values are more likely to partition the array further.
.debug	Runs debugging.

Value

sk_partition_tree

Examples

```
set.seed(123)
ris = generate_indices(8, 4)
part = partition(ris)
plot(part)
part$groups
```

`partition.multi` *Create Partitions of a multivariate array of objects.*

Description

Partitions the array of assumed glass fragment chemical compositions and features into statistically significant groups.

Usage

```
partition.multi(data, alpha = 0.05, .debug = FALSE)
```

Arguments

`data`	A list of data.frames or matrices corresponding to individual observations of glass fragment features.
`alpha`	Significance parameter "[0,1]". Higher values are more likely to partition the array further.
`.debug`	Runs debugging.

Value

A list of groupings and the tree formed.

Examples

```
test.data = prepare_data(glass, 1)[1:3]
part = partition.multi(test.data)
plot(part)

set.seed(123)
test.data.random = prepare_data(glass, 1)
test.data.random = test.data.random[sample(1:length(test.data.random), 5)]
part = partition.multi(test.data.random)
part$groups
```

plot.sk_partition_tree

Plot S3method for objects of type "sk_partition_tree".

Description

S3method for plotting the resulting tree formed by the partitioning algorithms in the SK4FGA package.

Usage

```
## S3 method for class 'sk_partition_tree'
plot(x, ...)
```

Arguments

x	Output from the function "partition()"
...	Extra details for the plot. Unused.

Value

Plot of the decision tree that is formed by the sk_partition_tree object returned by partition and partition.multi.

Examples

```
data = generate_indices()
part = partition(data)
plot.sk_partition_tree(part)

data(glass)
data.multi = prepare_data(glass, 1)[1:3]
part = partition.multi(data.multi)
plot(part)
```

prepare_data *prepare_data*

Description

Prepare a data file that is in standard form for partition.multi.

Usage

```
prepare_data(data, label = NA)
```

Arguments

data	Inputted data.frame.
label	Column corresponding to the label to be grouped by.

Value

A list of split data.

---

ptsquared *Calculate the Probability for a given T^2 statistic.*

Description

Calculate the Probability for a given T^2 statistic.

Usage

```
ptsquared(t, n1, n2, p)
```

Arguments

t	T^2 statistic.
n1	Number of observations in first sample.
n2	Number of observations in second sample.
p	Number of parameters.

Value

A probability corresponding to a given T^2 statistic and for given arguments.

---

ungroup.partition *ungroup.partition*

Description

Ungroups the tree object in the output from partition()

Usage

```
ungroup.partition(tree)
```

Arguments

tree	tree object returned from partition()

Value

A list object containing the indices of the

vehicle.glass *vehicle.glass*

Description

FIU Vehicle Glass Database V2.0

Usage

```
data(vehicle.glass)
```

Format

a 'data.frame' with 6858 rows and 16 columns.

item factor761 levels - which item the measurements came from

Li7 numericlog of lithium concentration

Mg25 numericlog of magnesium concentration

Al27 numericlog of aluminium concentration

K39 numericlog of potassium concentration

Ti49 numericlog of titanium concentration

Mn55 numericlog of manganese concentration

Fe57 numericlog of iron concentration

Rb85 numericlog of rubidium concentration

Sr88 numericlog of strontium concentration

Zr90 numericlog of zirconium concentration

Ba137 numericlog of barium concentration

La139 numericlog of lanthanum concentration

Ce140 numericlog of cerium concentration

Nd146 numericlog of neodymium concentration

Pb208 numericlog of lead concentration

Details

This freely available research-based database consists of 762 samples of various vehicle glass (windshield, passenger side, driver side, etc.). The samples span various makes and models, and range in year from 2004-2019. All samples were collected from the M&M salvage yard in Ruckersville, VA.

Source

Almirall, Jose; Akmeemana, Anuradha, 2022, "FIU Vehicle Glass Database V2.0.tab", Shiny Glass Application, https://doi.org/10.34703/gzx1-9v95/OB8BS9/XGH0IO, FIU Research Data Portal, V2, UNF:6:YDbwWISU04S+UCtb7aRoBQ== [fileUNF]

References

Anuradha Akmeemana, R. C., Jose Almirall, The Calculation of Calibrated Likelihood Ratios (LRs) for Glass Using a Multivariate Kernel Density Model: Introducing a User-Friendly Graphical User Interface (GUI). In American Academy of Forensic Science, Anaheim, CA, 2020.

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