Package ‘MixfMRI’

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Title Mixture fMRI Clustering Analysis

Depends R (>= 3.4.0)

Imports MASS, Matrix, RColorBrewer, fftw, MixSim, EMCluster

Enhances pbdMPI (>= 0.3-4), AnalyzeFMRI, oro.nifti

LazyLoad yes

LazyData yes

Description Utilizing model-based clustering (unsupervised) for functional magnetic resonance imaging (fMRI) data. The developed methods (Chen and Maitra (2018, manuscript)) include 2D and 3D clustering analyses (for p-values with voxel locations) and segmentation analyses (for p-values alone) for fMRI data where p-values indicate significant level of activation responding to stimulus of interesting. The analyses are mainly identifying active voxel/signal associated with normal brain behaviors. Analysis pipelines (R scripts) utilizing this package (see examples in 'inst/workflow/') is also implemented with high performance techniques.

License Mozilla Public License 2.0

BugReports https://github.com/snoweye/MixfMRI/issues

URL https://github.com/snoweye/MixfMRI

NeedsCompilation yes

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**MixfMRI-package**

**R topics documented:**

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**Description**

Utilizing model-based clustering (unsupervised) for fMRI data especially in a distributed manner. The methods includes 2D and 3D clustering analyses and segmentation analyses for fMRI signals where p-values are significant levels of active voxels which respond to stimulate of interesting. The analyses are mainly identifying active voxels/signals from normal brain behaviors. Workflows are also implemented utilizing high performance techniques.

**Details**

- **Package**: MixfMRI
- **Type**: Package
- **License**: GPL (>= 2)
- **LazyLoad**: yes

The main function of this package is `fclust()` that implements model-based clustering algorithm for fMRI signal data and provides unsupervised clustering results for the data. Several workflows implemented with high-performance computing techniques are also built in for automatically pro-
Main algorithms implemented in fclust

**Description**
Main algorithms implemented in fclust.

**Usage**
- `ecm.step.gbd(PARAM.org)`
- `apecma.step.gbd(PARAM.org)`
- `em.step.gbd(PARAM.org)`

**Arguments**
- `PARAM.org`: an initialized `PARAM`, usually returned by `set.global()`, `initial.em.gbd()`, and `initial.RndEM.gbd()`.

**Details**
These are main algorithms implemented in `fclust()`.

**Value**
Return an optimized `PARAM`. 

Author(s)
Wei-Chen Chen and Ranjan Maitra.

References
http://maitra.public.iastate.edu/

See Also
`fclust()`, `set.global()`.

Examples
```r
library(MixfMRI, quietly = TRUE)
demo(fclust3d,'MixfMRI',ask=FALSE,echo=FALSE)
demo(fclust2d,'MixfMRI',ask=FALSE,echo=FALSE)
```
Compute Q values

Author(s)
Wei-Chen Chen and Ranjan Maitra.

References
http://maitra.public.iastate.edu/

See Also
set.global(), fclust(), PARAM, PARAM.org.

Examples

```r
library(MixfMRI, quietly = TRUE)
library(EMCluster, quietly = TRUE)
# FC.CT$algorithm <- "em"
# FC.CT$model.X <- "v"
# FC.CT$ignore.X <- TRUE
FC.CT$check.X.unit <- FALSE

### Test toy1.
set.seed(1234)
X.gbd <- toy1$X.gbd
PV.gbd <- toy1$PV.gbd
PARAM <- set.global(X.gbd, PV.gbd, K = 2)
PARAM.new <- initial.em.gbd(PARAM)
PARAM.toy1 <- em.step.gbd(PARAM.new)
id.toy1 <- .MixfMRIEnv$CLASS.gbd
print(PARAM.toy1$ETA)
RRand(toy1$CLASS.gbd, id.toy1)

### Test toy2.
set.seed(1234)
X.gbd <- toy2$X.gbd
PV.gbd <- toy2$PV.gbd
PARAM <- set.global(X.gbd, PV.gbd, K = 3)
PARAM.new <- initial.em.gbd(PARAM)
PARAM.toy2 <- em.step.gbd(PARAM.new)
id.toy2 <- .MixfMRIEnv$CLASS.gbd
print(PARAM.toy2$ETA)
RRand(toy2$CLASS.gbd, id.toy2)
```

Description

Compute q-values Benjamini and Hochberg’s (1995) approach for controlling FDR.
Compute Q values

Usage

qvalue(p, method = c("BH1995", "BY2001"))

Arguments

- `p` a p-value vector.
- `method` using method by either BH1995 or BY2001

Details

This function computes q-values using Benjamini and Hochberg's (1995) approach for controlling FDR. The function `bhNfdr` is originally written by Dr. Dan Nettleton.

The Benjamini and Yekutieli's (2001) approach for controlling FDR using the function `byNfdr` is coded by Wei-Chen Chen.

Value

Return corresponding q-values for the input p-values.

Author(s)

Dan Nettleton.

Modified by Wei-Chen Chen.

References

http://maitra.public.iastate.edu/

See Also

dpval(), dmixpval().

Examples

```r
library(MixfMRI, quietly = TRUE)
set.seed(1234)
da <- gendataset(phantom = shepp1fMRI, overlap = 0.01)
p <- da$pval[!is.na(da$pval)][1:100]
qvalue(p)
```
Compute Statistics for Log Odds Ratio of Posterior Probability

Description

The function computes statistics for log odds ratio of posterior probability.

Usage

logor.stat(x, fobj, post.z, cov.param = NULL, cov.post.z = NULL, cov.logit.z = NULL, all.x = FALSE, drop.ETA1 = FALSE)

Arguments

x an input list of two elements X.gbd and PV.gbd.
fobj a fclust object.
post.z a matrix of dim = N * K for posterior probabilities, which is also the return value of post.prob().
cov.param a covariance matrix of dim = d * d for parameters, which is also a return of cov.param(). d is total number of parameters which is dependent on data and models.
cov.post.z a covariance list of length equal to number of active voxels, which is also a return of cov.post.z().
cov.logit.z a covariance list of length equal to number of active voxels, which is also a return of cov.logit.z().
all.x all cov matrices for all observations are returned if TRUE, while for only active observations (those of class ids are greater than 1) if FALSE.
drop.ETA1 if drop the ETA[1] from the cov matrix due to the min.1st.prop constrain.

Details

For posterior probability, this function compute log odd ratio, cov matrix of log odd ratio, degrees of freedom, and testing statistics.

Value

A list is returned with four elements: log.or, cov.log.or, df, and test.stat.

Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

http://maitra.public.iastate.edu/
Covariance Matrices

See Also

post.prob(), cov.param(), cov.post.z(), cov.logit.z().

Examples

library(MixfMRI, quietly = TRUE)
.f.CT$model.X <- "I"
.f.CT$CONTROL$debug <- 0
K <- 3

### Fit toy1.
set.seed(1234)
X.gbd <- toy1$X.gbd
X.range <- apply(X.gbd, 2, range)
X.gbd <- t((t(X.gbd) - X.range[1,]) / (X.range[2,] - X.range[1,]))
PV.gbd <- toy1$PV.gbd
fcobj <- fclust(X.gbd, PV.gbd, K = K, min.1st.prop = 0.5)

### Test log odds ratio.
x <- list(X.gbd = X.gbd, PV.gbd = PV.gbd)
post.z <- post.prob(x, fcobj)
lor <- logor.stat(x, fcobj, post.z)

### Check if 95% CE covers log odd ratio = 1.
id <- !is.na(lor$df)
id.cover.0 <- which(lor$test.stat[id] < pchisq(0.95, lor$df[id]))

### Get voxels needed for merging.
id.active <- which(fcobj$class != 1)
id.merge <- id.active[id][id.cover.0]

### Check results.
post.z[id.merge,]
cbind(toy1$X.gbd[id.merge,], toy1$PV.gbd[id.merge])

Covariance Matrices

Description

These functions compute posterior probabilities, Fisher information with covariance matrix of parameters, covariance matrix of posterior probabilities, and covariance matrix of logit posterior probabilities.

Usage

post.prob(x, fcobj)
cov.param(x, fcobj, post.z, drop.ETA1 = FALSE)
cov.post.z(x, fcobj, post.z, cov.param = NULL, all.x = FALSE,
covariance matrices

\[
drop.ETA1 = \text{FALSE}
\]

\[
cov.logit.z(x, \text{fcobj}, \text{post.z}, \text{cov.param} = \text{NULL}, \text{cov.post.z} = \text{NULL},
\text{all.x} = \text{FALSE}, \text{drop.ETA1} = \text{FALSE})
\]

**Arguments**

- **x**
  - an input list of two elements \(X, P\).
- **fcobj**
  - a \text{fclust} object.
- **post.z**
  - a matrix of \(\text{dim} = N \times K\) for posterior probabilities, which is also the return value of \text{post.prob}().
- **cov.param**
  - a covariance matrix of \(\text{dim} = d \times d\) for parameters, which is also a return of \text{cov.param}(). \(d\) is total number of parameters which is dependent on data and models.
- **cov.post.z**
  - a covariance list of length equal to number of active voxels, which is also a return of \text{cov.post.z}().
- **all.x**
  - all cov matrices for all observations are returned if TRUE, while for only active observations (those of class ids are greater than 1) if FALSE.
- **drop.ETA1**
  - if drop the \(\text{ETA}[1]\) from the cov matrix due to the min.Ist.prop constrain.

**Details**

These functions are required to compute covariance matrices of parameters and posterior probabilities.

Use \text{post.prob}() to get the posterior probabilities.

Input the returns of \text{post.prob}() to \text{cov.param}() to obtain the cov matrix for parameters (inversed Fisher information obtained from inner product of gradient of log observed data likelihood). A list is returned with \(I\) for Fisher information, and \text{cov} for the covariance matrix which is inverted by \text{ginv}().

Input the returns of \text{post.prob}() and \text{cov.param}() to \text{cov.post.z}() to obtain the cov matrix for posterior probabilities by the multivariate delta method on the cov matrix for parameters.

Input the returns of \text{post.prob}(), \text{cov.param}(), and \text{cov.post.z}() to \text{cov.logit.z}() to obtain cov matrix for logit posterior probabilities by the multivariate delta method on cov matrix of posterior probabilities.

**Value**

A matrix or a list is returned.

The \text{cov.param}() will return a list containing two elements \(I\) for the Fisher information, and \text{cov} for the covariance matrix by generalized inversed of the Fisher information. The dimension of both elements are \(d \times d\) where \(d = K \times 7 - 4\) for 2D data and \(d = K \times 9 - 4\) for 3D data if \text{drop.ETA1} = \text{TRUE}, otherwise they are \(d = K \times 7 - 3\) and \(d = K \times 9 - 4\), respectively.

The \text{cov.post.z}() will return a list containing cov matrices of posterior probabilities for each valid/selected voxel.

The \text{cov.logit.z}() will return a list containing cov matrices of logit posterior probabilities for each valid/selected voxel.
Covariance Matrices

Author(s)
Weichen Chen and Ranjan Maitra.

References
http://maitra.public.iastate.edu/

See Also
EMCluster::lmt(), lmt.I().

Examples
library(MixFMR1, quietly = TRUE)
library(EMCluster, quietly = TRUE)
.F.CT$model.X <- "I"
.F.CT$CONTROL$debug <- 0
K <- 3

## Fit toy1.
set.seed(1234)
X.gbd <- toy1X.gbd
X.range <- apply(X.gbd, 2, range)
X.gbd <- t((t(X.gbd) - X.range[1,]) / (X.range[2,] - X.range[1,]))
PV.gbd <- toy$PV.gbd
fcobj <- fclust(X.gbd, PV.gbd, K = K, min.1st.prop = 0.5)

## Test cov matrix of posterior z and logit posterior z.
x <- list(X.gbd = X.gbd, PV.gbd = PV.gbd)
post.z <- post.prob(x, fcobj)
cov.param <- cov.param(x, fcobj, post.z = post.z)
cov.post.z <- cov.post.z(x, fcobj, post.z = post.z,
cov.param = cov.param$cov)
cov.logit.z <- cov.logit.z(x, fcobj, post.z = post.z,
cov.param = cov.param$cov,
cov.post.z = cov.post.z)

## Compute cov matrix of log odds ratio for all k > 1.
A <- cbind(rep(-1, K - 1), diag(1, K - 1))
logit.p <- log(post.z[fcobj$class != 1,] / (1 - post.z[fcobj$class != 1,]))
log.or <- logit.p %*% t(A)
cov.log.or <- lapply(cov.logit.z, function(x) A %*% x %*% t(A))

## Check if 0 vector covered by 95% confidence ellipsoid.
id <- 1
plot(log.or[id,],
     xlim = log.or[id, 1] + c(-5, 5),
     ylim = log.or[id, 2] + c(-5, 5),
     main = "1st observation", xlab = "x", ylab = "y")
plotBN(log.or[id,], cov.log.or[[id]])
points(0, 0, col = 2)
These functions compute covariance matrix of logit ETA.

Usage

cov.logit.ETA(x, fobj, cov.param = NULL)

Arguments

- **x**: an input list of two elements `X.gbd` and `PV.gbd`.
- **fobj**: a `fclust` object.
- **cov.param**: a covariance matrix of `dim = d * d` for parameters, which is also a return of `cov.param()`. `d` is total number of parameters which is dependent on data and models.

Details

These functions are required to compute covariance matrices of logit ETA.

Input the returns of `cov.param()` to `cov.logit.ETA()` to obtain the cov matrix for logit ETA by the multivariate delta method on the cov matrix for parameters.

Value

A matrix.

Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

http://maitra.public.iastate.edu/

See Also

`EMCluster::lmt()`, `lmt.I()`.
Examples

```r
library(MixfMRI, quietly = TRUE)
.FC.CT$model.X <- "I"
.FC.CT$CONTROL$debug <- 0
K <- 3

### Fit toy1.
set.seed(1234)
X.gbd <- toy1$X.gbd
X.range <- apply(X.gbd, 2, range)
X.gbd <- t(((t(X.gbd) - X.range[1,]) / (X.range[2,] - X.range[1,])))
PV.gbd <- toy1$PV.gbd
fcobj <- fclust(X.gbd, PV.gbd, K = K, min.1st.prop = 0.5)

### Test cov matrix of posterior z.
x <- list(X.gbd = X.gbd, PV.gbd = PV.gbd)
post.z <- post.prob(x, fcobj)
cov.param <- cov.param(x, fcobj, post.z)
cov.logit.ETA <- cov.logit.ETA(x, fcobj, cov.param = cov.param$ cov)

### Compute cov matrix of eta_k - eta_1 for all k > 1.
A <- cbind(rep(-1, K - 1), diag(1, K - 1))
ETA <- fcobj$param$ETA
log.or <- log(ETA / (1 - ETA)) %%*% t(A)
cov.log.or <- A %%*% cov.logit.ETA %%*% t(A)
```

Density function of p-values

These functions based on normal assumption and transformation to derive a (mixture) density function of p-values.

Usage

```r
dpval(x, mu = 0, log = FALSE)
dmixpval(x, eta, mu)
```

Arguments

- **x**: support of p-values which should be between 0 and 1.
- **mu**: hypothetical mean of testing statistics (in normal distribution) for producing p-values.
- **log**: if return log of density.
- **eta**: mixing proportion of K components if a mixture is assumed.
Example Datasets

Details

Note that eta and mu in dmixpval() are of length K for K component mixtures.

Value

Corresponding density values (to the input x) are returned.

Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

http://maitra.public.iastate.edu/

See Also

gendataset(), qvalue().

Examples

library(MixfMRI, quietly = TRUE)
set.seed(1234)
da <- gendataset(phantom = shepp1fMRI, overlap = 0.01)
x <- da$pval[!is.na(da$pval)][1:100]
dpval(x)
dmixpval(x, mu = da$mu, eta = da$eta)

<table>
<thead>
<tr>
<th>Example Datasets</th>
<th>Example datasets in MixfMRI</th>
</tr>
</thead>
</table>

Description

These are datasets used to demo examples and workflows in this package.

Format

Objects may contain several information and data.

Details

pstats is a 3D example.
pval.2d.complex and pval.2d.mag are 2D examples.
shepp0fMRI, shepp1fMRI, shepp2fMRI and sheppAnat are phantoms generated by Dr. Maitra for simulation studies with different overlap levels for p-values.
toy* are 2D toy examples.
False Discovery Rates for Spatial Signals

Author(s)
Wei-Chen Chen and Ranjan Maitra.

References
http://maitra.public.iastate.edu/

Examples
library(MixfMRI, quietly = TRUE)

### Plotting.
demo(shepp,'MixfMRI',ask=FALSE,echo=FALSE)

---

False Discovery Rates for Spatial Signals

False Discovery Rates for Spatial Signals using Benjamini and Heller (2007)

---

Description
Compute q-values Benjamini and Heller’s (2007) approach for controlling FDR for spatial signals.

Usage
fdr.bh.p1(p, w = rep(1, length(p)), q = 0.05)
fdr.bh.p2(p, w = rep(1, length(p)), q = 0.05)

Arguments
- **p**: a p-value vector. No NA is allowed and all values are in [0, 1].
- **w**: a weight vector for p-values.
- **q**: a desired cutoff for adjusting p-values.

Details
These functions implement first two procedures in Benjamini and Heller (2007) for controlling FDR for spatial signals.

Value
Return the number of rejected hypotheses and all corresponding q-values for the input p-values.

Author(s)
Wei-Chen Chen.
Generalized Cluster-Based Analysis (CBA) Method

References

http://maitra.public.iastate.edu/

See Also

qvalue()

Examples

library(MixfMRI, quietly = TRUE)
set.seed(1234)
da <- gendataset(phantom = shepp1FMRI, overlap = 0.01)
p <- da$psval[!is.na(da$psval)][1:100]
fdr.bh.p1(p)
fdr.bh.p2(p)

---

**Generalized Cluster-Based Analysis (CBA) Method**

**Generalized Cluster-Based Analysis (CBA) Method**

**Description**

Find clusters in 2D or 3D based on a generalized CBA method. The CBA method is originally proposed by Heller, et.al. (2006) using the correlation of two time series as the similarity of two spatial locations.

**Usage**

```r
cba.cor(da.ts, da.m = NULL, adj.dist = TRUE, fun.sim = stats::cor)
cba.cor.2d(da.ts, da.m = NULL, adj.dist = TRUE, fun.sim = stats::cor)
cba.cor.3d(da.ts, da.m = NULL, adj.dist = TRUE, fun.sim = stats::cor)
```

**Arguments**

- `da.ts`: a time series array of dimensions x * y * z * t.
- `da.m`: a mask determining inside of brain or not.
- `adj.dist`: if adjust correlations by distance.
- `fun.sim`: a function computing similarity of two locations.

**Details**

These functions implement the 2D and 3D versions of CBA proposed by Heller, et.al. (2006).

da.ts should have dimensions x * y * z * t for 3D data and x * y * time for 2D data. Similarly, da.m would have x * y * z and x * y correspondingly.
da.m has values 0 or 1 indicating outside or inside a brain, respectively.
fun.sim(a, B) is a function return similarity between a location a and N neighboring locations B where a is of dimension t * 1 and B is of dimension t * N. Ideally, fun.sim() should return values of similarity which take values between 0 and 1 where 0 means totally different and 1 means completely identical of two spatial locations. By default, stats::cor is used. See the example section next for user defined functions for fun.sim().

Value

Return the cluster ids for each voxel. NA for outside of brain if da.m is provided.

Author(s)

Wei-Chen Chen.

References


See Also

fdr.bh.p1(), fdr.bh.p2().

Examples

### Simulated data
library(MixFMRI, quietly = TRUE)
dim <- c(4, 5, 4, 10)
set.seed(123)
da.ts <- array(rnorm(prod(dim)), dim = dim)
id.class <- suppressWarnings(cba.cor(da.ts))
table(id.class)

fun.tanh <- function(a, B){
  d <- 1 / apply(B, 2, function(b){ dist(rbind(as.vector(a), b)) })
  tanh(d)
}
id.class.tanh <- suppressWarnings(cba.cor(da.ts, fun.sim = fun.tanh))
table(id.class.tanh)

fun.logit <- function(a, B){
  d <- dist(t(cbind(a, B)))[1:ncol(B)]
  (1 / (1 + exp(-d))) * 2 - 1
}
id.class.logit <- suppressWarnings(cba.cor(da.ts, fun.sim = fun.logit))
table(id.class.logit)

### Real data
library(AnalyzeFMRI, quietly = TRUE)
library(oro.nifti, quietly = TRUE)
fn <- "pb02_volreg_tlrc.nii"
da <- readNIfTI(fn)
da.ts <- da@.Data

fn <- "mask_anat.nii"
da <- readNIfTI(fn)
da.m <- da@.Data

id.class <- suppressWarnings(cba.cor(da.ts, da.m))
dim(id.class) <- dim(da.m)
length(table(id.class))

---

**Initial**  
*Main initialization functions*

**Description**
Main initialization functions.

**Usage**

```r
initial.em.gbd(PARAM)
initial.RndEM.gbd(PARAM)
```

**Arguments**

PARAM a list of uninitialized parameters, as usual, the returned values of `set.global()`, to be initialized according to data (inside PARAM).

**Details**

`initial.em.gbd()` takes in a template of PARAM (uninitialized), and usually is available by calling `set.global()`, then return an initialized PARAM which is ready for EM runs.

Internally, there are six different initializations implemented for the function `initial.em.gbd()` including `prob.extend`, `prob.simple`, `qnorm.extend`, `qnorm.simple`, `extend`, and `simple`. These methods are mainly based on transformation of original space of data (p-values and voxel locations) into more linear space such that the Euclidean distance more makes sense (fairly) to classify data in groups.

`initial.RndEM.gbd()` implement RndEM initialization algorithm based on repeated calling `initial.em.gbd()`. Note that all configurations are included in PARAM set by `set.global()`.

**Value**

These functions return an initialized PARAM for EM runs based on pre-stored configuration within the input uninitialized PARAM.
Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

http://maitra.public.iastate.edu/

See Also

set.global(), fclust(), PARAM.

Examples

library(MixfMRI, quietly = TRUE)
library(EMCluster, quietly = TRUE)
# .FC.CT$algorithm <- "em"
# .FC.CT$model.X <- "V"
# .FC.CT$ignore.X <- TRUE
.FC.CT$check.X.unit <- FALSE

### Test toy1.
set.seed(1234)
X.gbd <- toy1$X.gbd
PV.gbd <- toy1$PV.gbd
PARAM <- set.global(X.gbd, PV.gbd, K = 2)
PARAM.new <- initial.em.gbd(PARAM)
PARAM.toy1 <- em.step.gbd(PARAM.new)
id.toy1 <- .MixfMRIEnv$CLASS.gbd
print(PARAM.toy1$ETA)
RRand(toy1$CLASS.gbd, id.toy1)

### Test toy2.
set.seed(1234)
X.gbd <- toy2$X.gbd
PV.gbd <- toy2$PV.gbd
PARAM <- set.global(X.gbd, PV.gbd, K = 3)
PARAM.new <- initial.em.gbd(PARAM)
PARAM.toy2 <- em.step.gbd(PARAM.new)
id.toy2 <- .MixfMRIEnv$CLASS.gbd
print(PARAM.toy2$ETA)
RRand(toy2$CLASS.gbd, id.toy2)
Description
These functions test two mixture Gaussian fMRI models with identity covariance matrices and
different numbers of clusters. These functions are similar to the EMCluster::lmt(), but is coded
for fMRI models in MixfMRI.

Usage
\[
\text{lmt.I}(\text{fcobj.0, fcobj.a, X.gbd, PV.gbd, tau = 0.5, n.mc.E.delta = 1000, n.mc.E.chi2 = 1000, verbose = FALSE})
\]
\[
\text{lmt.pv}(\text{fcobj.0, fcobj.a, X.gbd, PV.gbd, tau = 0.5, n.mc.E.delta = 1000, n.mc.E.chi2 = 1000, verbose = FALSE})
\]

Arguments
- \text{fcobj.0} a fclust object for the null hypothesis.
- \text{fcobj.a} a fclust object for the alternative hypothesis.
- \text{X.gbd} a data matrix of N voxel locations. \text{dim(X.gbd) = N x 3} for 3D data and \text{N x 2}
  for 2D data.
- \text{PV.gbd} a p-value vector of signals associated with voxels. \text{length(PV.gbd) = N}.
- \text{tau} proportion of null and alternative hypotheses.
- \text{n.mc.E.delta} number of Monte Carlo simulations for expectation of delta (difference of logL).
- \text{n.mc.E.chi2} number of Monte Carlo simulations for expectation of chisquare statistics.
- \text{verbose} if verbose.

Details
This function calls several subroutines to compute information, likelihood ratio statistics, degrees
of freedom, non-centrality of chi-squared distributions ... etc. Based on Monte Carlo methods
to estimate parameters of likelihood mixture tests, this function return a p-value for testing \(H_0: \text{fcobj.0 v.s. Ha: fcobj.a}\).
\text{lmt.pv()} only uses \text{PV.gbd}.

Value
A list of class \text{lmt.I} are returned.

Author(s)
Wei-Chen Chen and Ranjan Maitra.

References
http://maitra.public.iastate.edu/

See Also
EMCluster::lmt().
Examples

library(MixfMRI, quietly = TRUE)
library(EMCluster, quietly = TRUE)
.FC.CT$model$X <- "I"
.FC.CT$check.X.unit <- FALSE
.FC.CT$CONTROL$debug <- 0

### Fit toy1.
set.seed(1234)
X.gbd <- toy1$X.gbd
PV.gbd <- toy1$PV.gbd
ret.2 <- fclust(X.gbd, PV.gbd, K = 2)
ret.3 <- fclust(X.gbd, PV.gbd, K = 3)
ret.4 <- fclust(X.gbd, PV.gbd, K = 4)
ret.5 <- fclust(X.gbd, PV.gbd, K = 5)

### ARI
RRand(toy1$CLASS.gbd, ret.2$class)
RRand(toy1$CLASS.gbd, ret.3$class)
RRand(toy1$CLASS.gbd, ret.4$class)
RRand(toy1$CLASS.gbd, ret.5$class)

### Test toy1.
(lmt.23 <- lmt.I(ret.2, ret.3, X.gbd, PV.gbd))
(lmt.24 <- lmt.I(ret.2, ret.4, X.gbd, PV.gbd))
(lmt.25 <- lmt.I(ret.2, ret.5, X.gbd, PV.gbd))
(lmt.34 <- lmt.I(ret.3, ret.4, X.gbd, PV.gbd))
(lmt.35 <- lmt.I(ret.3, ret.5, X.gbd, PV.gbd))
(lmt.45 <- lmt.I(ret.4, ret.5, X.gbd, PV.gbd))

### Test toy1 using p-values only.
(lmt.pv.23 <- lmt.pv(ret.2, ret.3, X.gbd, PV.gbd))
(lmt.pv.24 <- lmt.pv(ret.2, ret.4, X.gbd, PV.gbd))
(lmt.pv.25 <- lmt.pv(ret.2, ret.5, X.gbd, PV.gbd))
(lmt.pv.34 <- lmt.pv(ret.3, ret.4, X.gbd, PV.gbd))
(lmt.pv.35 <- lmt.pv(ret.3, ret.5, X.gbd, PV.gbd))
(lmt.pv.45 <- lmt.pv(ret.4, ret.5, X.gbd, PV.gbd))

---

LRT

Likelihood ratio tests

Description

Likelihood ratio tests for merging clusters.
Usage

\[ \text{lrt}(\text{PV.gbd}, \text{CLASS.gbd}, K, H_0.\alpha = .FC.CT\text{LRT}\$H_0.\alpha, \\
    H_0.\beta = .FC.CT\text{LRT}\$H_0.\beta) \]

\[ \text{lrt2}(\text{PV.gbd}, \text{CLASS.gbd}, K, H_0.\text{mean} = .FC.CT\text{LRT}\$H_0.\text{mean}, \\
    \text{upper.}\beta = .FC.CT\text{INIT}\$\text{BETA.}\beta.\text{max}, \text{proc} = \text{c}("1", "2", "\text{weight}") \]

\[ \text{lrt.betamean}(\text{PV.gbd}, \text{CLASS.gbd}, K, \text{proc} = \text{c}("1", "2")) \]

\[ \text{lrt.betaab}(\text{PV.gbd}, \text{CLASS.gbd}, K, \text{proc} = \text{c}("1", "2")) \]

Arguments

- **PV.gbd**: a p-value vector of signals associated with voxels. \( \text{length(PV.gbd)} = N \).
- **CLASS.gbd**: a classification vector of signals associated with voxels. \( \text{length(CLASS.gbd)} = N \).
- **K**: number of clusters.
- **H_0.\alpha**: null hypothesis for the alpha parameter of Beta distribution.
- **H_0.\beta**: null hypothesis for the beta parameter of Beta distribution.
- **H_0.\text{mean}**: null hypothesis for the mean of Beta distribution.
- **upper.\beta**: \( \text{BETA.}\beta.\text{max} \), maximum value of beta parameter of Beta distribution.
- **proc**: q-value procedure for adjusting p-values.

Details

These functions perform likelihood ratio tests for merging clusters. Only p-values coordinates (Beta density) are tested, while voxel location coordinates (multivariate Normal density) are not involved in testing.

\text{lrt.betamean} tests if means of any two pairs of mixture (p-value) component were the same. The chi-square distribution with 1 degree of freedom is used.

\text{lrt.betaab} tests if alpha and beta of any two pairs of mixture (p-value) components were the same. The chi-square distribution with 2 degrees of freedom is used.

Value

A matrix contains MLEs of parameters of Beta distribution under the null hypothesis and the union of null and alternative hypotheses. The matrix also contains testing statistics and p-values.

Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

[http://maitra.public.iastate.edu/](http://maitra.public.iastate.edu/)
Main functions

See Also

PARAM.

Examples

library(MixfMRI, quietly = TRUE)
set.seed(1234)

### Test 2d data.
da <- pval.2d.mag
id <- !is.na(da)
PV.gbd <- da[id]
id.loc <- which(id, arr.ind = TRUE)
X.gbd <- t(t(id.loc) / dim(da))
ret <- fclust(X.gbd, PV.gbd, K = 2, min.1st.prop = 0.95)
# print(ret)

### p-values of rest clusters.
ret.lrt <- lrt(PV.gbd, ret$class, K = 2)
print(ret.lrt)

ret.lrt2 <- lrt2(PV.gbd, ret$class, K = 3)
print(ret.lrt2)

Main MixfMRI function

Description

Main MixfMRI functions.

Usage

fclust(X.gbd, PV.gbd, K = 2,
   PARAM.init = NULL,
   min.1st.prop = .FC.CT$INIT$min.1st.prop,
   max.PV = .FC.CT$INIT$max.PV,
   class.method = .FC.CT$INIT$class.method[1],
   RndEM.iter = .FC.CT$CONTROL$RndEM.iter,
   algorithm = .FC.CT$algorithm[1],
   model.X = .FC.CT$model.X[1],
   ignore.X = .FC.CT$ignore.X,
   stop.unstable = TRUE,
   MPI.gbd = .FC.CT$MPI.gbd, common.gbd = .FC.CT$common.gbd)

set.global(X.gbd, PV.gbd, K = 2,
   min.1st.prop = .FC.CT$INIT$min.1st.prop,
Main functions

max.PV = .FC.CT$INIT$max.PV,
class.method = .FC.CT$INIT$class.method[1],
RndEM.iter = .FC.CT$CONTROL$RndEM.iter,
algorithm = .FC.CT$algorithm[1],
model.X = .FC.CT$model.X[1],
ignore.X = .FC.CT$ignore.X,
check.X.unit = .FC.CT$check.X.unit,
MPI.gbd = .FC.CT$MPI.gbd, common.gbd = .FC.CT$common.gbd)

Arguments

X.gbd a data matrix of N voxel locations. dim(X.gbd) = N x 3 for 3D data and N x 2 for 2D data.
PV.gbd a p-value vector of signals associated with voxels. length(PV.gbd) = N.
K number of clusters to be estimated.
PARAM.init initial parameters.
min.1st.prop lower bound of mixing proportion (ETA) of the 1st cluster (uniform).
max.PV upper bound of p-values where initializations pick from.
class.method classification method for initializations.
RndEM.iter number of RndEM iterations.
algorithm either “ecm” (ECM), “apecm” (APECMa) or “em” (EM) algorithm.
model.X either “I” or “V” for covariance matrix.
ignore.X if X.gbd used in model, TRUE for PV.gbd only.
check.X.unit if X.gbd are all in [0, 1].
stop.unstable if fclust stops if unstable results occur.
MPI.gbd if MPI (“EGM” algorithm) is used.
common.gbd if X.gbd and PV.gbd are in common across all ranks when MPI.gbd = TRUE.

Details

The fclust() contains initialization and EM algorithms for clustering fMRI signal data which have two parts: X.gbd for voxel information either 2D or 3D, PV.gbd for p-value of signals associated with voxels. Each signal is assumed as a mixture distribution with K components with mixing proportion ETA, and each component has two independent coordinates with density functions: Beta and multivariate Normal distributions.

Beta density: The 1st component is restricted by min.1st.prop and Beta(1, 1) distribution. The other K - 1 components have Beta(alpha, beta) distribution with alpha < 1 < beta.

Multivariate Normal density: model.X = "I" is for identity cov matrix of multivariate Normal distribution, and "V" for unstructured cov matrix. ignore.X = TRUE is to ignore X.gbd and normal density, i.e. only Beta density is used.

Currently, APECMa and EM algorithms are implemented with EGM algorithm to speed up convergence if MPI is available. RndEM initialization is also implemented for better chance of good initial values for convergence.

The set.global() has purposes: create a template/storage of parameters, save configurations, and called by fclust() to initial the parameters, such as initial.em.gbd() or initial.RndEM.gbd().
Main functions

Value

A list with class fclust by fclust() is returned which can be summarized by print.fclust().

A list PARAM or PARAM.org is returned by set.global():

N.gbd number of observations (within the rank), and should be equal to N.all if MPI.gbd = FALSE.

N.all numbers of observations (of all ranks if MPI.gbd = TRUE).

N total number of observations (sum(N.all)).

p dimension of an observation (3 for 2D signals, 4 for 3D signals), equivalent to total number of coordinates.

p.X dimension of X.gbd (2 for 2D signals, 3 for 3D signals, 0 when ignore.X = TRUE, number of voxel coordinates.

K number of clusters.

ETA mixing proportion, length K.

log.ETA log(ETA).

BETA a list of length K containing parameters (alpha, beta) of Beta density.

MU a matrix of dimension p.X by K.

SIGMA a list of length K, and each is of dimension K x K.

logL log likelihood value.

min.1st.prop carried from input.

max.PV carried from input.

class.method classification method of initializations.

min.N.CLASS p + 1.

model.X carried from input.

Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

http://maitra.public.iastate.edu/

See Also

print.fclust().
Examples

library(MixfMRI, quietly = TRUE)
library(EMCluster, quietly = TRUE)
# .FC.CT$algorithm <- "em"
# .FC.CT$model.X <- "V"
# .FC.CT$ignore.X <- TRUE
.FC.CT$check.X.unit <- FALSE
set.seed(1234)

### Test toy1.
X.gbd <- toy1$X.gbd[, -3]
PV.gbd <- toy1$PV.gbd
PARAM <- fclust(X.gbd, PV.gbd, K = 2)
print(PARAM)
id.toy1 <- .MixfMRIEnv$CLASS.gbd
print(RRand(toy1$CLASS.gbd, id.toy1))

### Test toy2.
X.gbd <- toy2$X.gbd[, -3]
PV.gbd <- toy2$PV.gbd
PARAM <- fclust(X.gbd, PV.gbd, K = 3)
print(PARAM)
id.toy2 <- .MixfMRIEnv$CLASS.gbd
print(RRand(toy2$CLASS.gbd, id.toy2))

---

MixfMRI Control

Sets of controls in MixfMRI

Description

These sets of controls are used to provide default values in this package.

Format

Objects contain several parameters for methods.

Details

The elements of .FC.CT are default values for main controls of MixfMRI including

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<thead>
<tr>
<th>Elements</th>
<th>Default</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>algorithm</td>
<td>&quot;apecma&quot;</td>
<td>implemented algorithm</td>
</tr>
<tr>
<td>optim.method</td>
<td>&quot;BFGS&quot;</td>
<td>optimization method</td>
</tr>
<tr>
<td>model.X</td>
<td>&quot;I&quot;</td>
<td>cov matrix structure</td>
</tr>
<tr>
<td>ignore.X</td>
<td>FALSE</td>
<td>if using voxel information</td>
</tr>
<tr>
<td>check.X.unit</td>
<td>TRUE</td>
<td>if checking X in [0, 1]</td>
</tr>
<tr>
<td>CONTROL</td>
<td>a list</td>
<td>see CONTROL next for details</td>
</tr>
</tbody>
</table>
The elements of **CONTROL** are default values for optimization controls of implemented EM algorithm including:

<table>
<thead>
<tr>
<th>Elements</th>
<th>Default</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>max.iter</td>
<td>1000</td>
<td>maximum number of EM iterations</td>
</tr>
<tr>
<td>abs.err</td>
<td>1e-4</td>
<td>absolute error of convergence</td>
</tr>
<tr>
<td>rel.err</td>
<td>1e-6</td>
<td>relative error of convergence</td>
</tr>
<tr>
<td>debug</td>
<td>1</td>
<td>debugging level</td>
</tr>
<tr>
<td>RndEM.iter</td>
<td>10</td>
<td>RndEM iterations</td>
</tr>
<tr>
<td>exp.min</td>
<td>(\text{log}(.Machine$double.xmin))</td>
<td>minimum exponential power</td>
</tr>
<tr>
<td>exp.max</td>
<td>(\text{log}(.Machine$double.xmax))</td>
<td>maximum exponential power</td>
</tr>
<tr>
<td>sigma.ill</td>
<td>1e-6</td>
<td>ill condition limit</td>
</tr>
<tr>
<td>DS.max</td>
<td>1e+4</td>
<td>maximum (\text{chol()}) cov matrix</td>
</tr>
<tr>
<td>DS.min</td>
<td>1e-6</td>
<td>minimum (\text{chol()}) cov matrix</td>
</tr>
</tbody>
</table>

The elements of **INIT** are default values or limitations for initial parameters implemented for EM algorithm including:

<table>
<thead>
<tr>
<th>Elements</th>
<th>Default</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>min.1st.prop</td>
<td>0.8</td>
<td>minimum proportion of 1st cluster</td>
</tr>
<tr>
<td>max.PV</td>
<td>0.1</td>
<td>maximum p-value for initialization</td>
</tr>
<tr>
<td>BETA.alpha.min</td>
<td>0 + 1e-6</td>
<td>minimum value of alpha parameter of Beta distribution</td>
</tr>
<tr>
<td>BETA.alpha.max</td>
<td>1 - 1e-6</td>
<td>maximum value of alpha parameter of Beta distribution</td>
</tr>
<tr>
<td>BETA.beta.min</td>
<td>1 + 1e-6</td>
<td>minimum value of beta parameter of Beta distribution</td>
</tr>
<tr>
<td>BETA.beta.max</td>
<td>1e+6</td>
<td>maximum value of beta parameter of Beta distribution</td>
</tr>
<tr>
<td>max.try.iter</td>
<td>10</td>
<td>maximum retry iterations if result is unstable</td>
</tr>
<tr>
<td>class.method</td>
<td>&quot;prob.extned&quot;</td>
<td>classification method at initializations</td>
</tr>
</tbody>
</table>

The elements of **LRT** are default values or limitations for likelihood ratio tests including:

<table>
<thead>
<tr>
<th>Elements</th>
<th>Default</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>H0.alpha</td>
<td>1</td>
<td>null hypothesis alpha parameter of Beta distribution</td>
</tr>
<tr>
<td>H0.beta</td>
<td>1</td>
<td>null hypothesis beta parameter of Beta distribution</td>
</tr>
<tr>
<td>H0.mean</td>
<td>0.05</td>
<td>null hypothesis mean of Beta distribution</td>
</tr>
</tbody>
</table>

**Author(s)**

Wei-Chen Chen and Ranjan Maitra.
Plotting

Main plotting function

Description

Main plotting function in MixfMRI.

Usage

```r
plotfclust(da, posterior, main = NULL, xlim = NULL, ylim = NULL)
plotfclustpv(da, posterior, main = NULL, xlim = NULL, ylim = NULL)

plotpv(da, posterior, PARAM, zlim = c(0, 0.01), plot.mean = TRUE,
       xlab = "", ylab = "", main = NULL, xlim = NULL, ylim = NULL,
       col = my.Y10Rd(), ignore.bg = FALSE)
plotpvlegend(zlim = c(0, 0.01), n.level = 20, main = NULL,
             col = my.Y10Rd())
```

Arguments

- `da` a data set to be plotted.
- `posterior` a posterior data set to be plotted.
- `PARAM` a returning parameter object from `fclust()`.
- `main` title of the plot.
- `xlim` limits of x-axis.
- `ylim` limits of y-axis.
- `zlim` limits of z-axis.
- `xlab` labels of x-axis.
- `ylab` labels of y-axis.
- `plot.mean` if plotting mean values of each cluster.
- `col` colors to be drawn.
- `ignore.bg` if ignoring the background.
- `n.level` number of levels to be plotted.

Details

These are example functions to plot results, simulations, and datasets.
Plotting

Value

Return plots.

Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

http://maitra.public.iastate.edu/

See Also

set.global().

Examples

library(MixfMRI, quietly = TRUE)
set.seed(1234)

### Check 2d data.
da <- pval.2d.complex
id <- !is.na(da)
PV.gbd <- da[id]
hist(PV.gbd, nclass = 100, main = "p-value")

### Test 2d data.
id.loc <- which(id, arr.ind = TRUE)
X.gbd <- t(t(id.loc) / dim(da))
ret <- fclust(X.gbd, PV.gbd, K = 3)
print(ret)

### p-values of rest clusters.
ret.lrt <- lrt(PV.gbd, ret$class, K = 3)
print(ret.lrt)
ret.lrt2 <- lrt2(PV.gbd, ret$class, K = 3)
print(ret.lrt2)

### Plotting.
par(mfrow = c(2, 2), mar = c(0, 0, 2, 0))
plotpv(da, ret$posterior, ret$param,
       zlim = c(0.005, 0.008), main = "Mean of Beta Distribution")
plotpv(da, ret$posterior, ret$param,
       plot.mean = FALSE, main = "p-value")
par(mar = c(5.1, 4.1, 4.1, 2.1))
plotpvlvlegend(zlim = c(0.005, 0.008), main = "Mean of Beta Distribution")
plotpvlvlegend(zlim = c(0, 0.01), main = "p-value")
Description
Print fclust related outputs.

Usage

```r
## S3 method for class 'fclust'
print(x, ...)
```

Arguments

- `x` - an object with the class attributes.
- `...` - other arguments to the `print` function.

Details

`x` is the return result from `fclust()`.

Value

A summary of `fclust` object is printed.

Author(s)

Wei-Chen Chen and Ranjan Maitra.

References

http://maitra.public.iastate.edu/

See Also

`set.global()`, `fclust()`.

Examples

```r
library(MixfMRI, quietly = TRUE)
set.seed(1234)

### Check 2d data.
da <- pval.2d.complex
id <- !is.na(da)
PV.gbd <- da[id]
# hist(PV.gbd, nclass = 100, main = "p-value")

### Test 2d data.
```
Generate datasets for MixfMRI simulations

Description
Generate datasets for MixfMRI simulations

Usage
gendataset(phantom, overlap)

Arguments
phantom a phantom dataset.
overlap a desired overlap level.

Details
This is a function to generate simulated fMRI data based on the input phantom and the desired overlap level for the fMRI p-value.

Value
Return a list contains \( \eta \) for mixing proportion, overlap for the desired level, \( \mu \) for center of p-values, class.id for the true classifications where p-values belong to, tval for the testing statistics, and pval for the p-values of interesting in simulations.

Author(s)
Wei-Chen Chen and Ranjan Maitra.

References
http://maitra.public.iastate.edu/

See Also
set.global().
Examples

```r
library(MixfMRI, quietly = TRUE)
set.seed(1234)
da <- gendataset(phantom = shepp1fMRI, overlap = 0.01)$pval
da2 <- gendataset(phantom = shepp2fMRI, overlap = 0.01)$pval

par(mfrow = c(2, 2), mar = rep(0.05, 4))
image(shepp1fMRI[50:210, 50:210], axes = FALSE)
image(shepp2fMRI[50:210, 50:210], axes = FALSE)
image(da[50:210, 50:210], axes = FALSE)
image(da2[50:210, 50:210], axes = FALSE)
```

Description

Generate datasets with smoothing for MixfMRI simulations

Usage

```r
gcv.smooth2d(y, interval)
```

Arguments

- `y`: a set of p-values in 2d phantom
- `interval`: an interval for optimize function.

Details

The function is used to smooth for Dr. Maitra's 2d phantom simulation. The smoothing method is based on Garcia (2010), CSDA.

Value

Return a list containing two elements `im.smooth` and `par.val`.

Author(s)

Ranjan Maitra.

References

[http://maitra.public.iastate.edu/](http://maitra.public.iastate.edu/)
**Summarized Overlap**

---

**Description**

Compute summarized overlap on a given overlap (symmetric) matrix.

**Usage**

```r
summarized.overlap(overlap.mat)
```

**Arguments**

- `overlap.mat` an overlap (symmetric) matrix.

**Details**

`overlap.mat` is a $p \times p$ matrix containing pair wise overlaps of $p$ experiments. `overlap.mat` is assumed a symmetric matrix. This function returns a summarized overlap based on the input `overlap.mat` that characterizes the overall overlap behavior of the $p$ experiments.

**Value**

A single value is returned.

**Author(s)**

Ranjan Maitra.

**References**

[http://maitra.public.iastate.edu/](http://maitra.public.iastate.edu/)

**Examples**

```r
library(MixfMRI, quietly = TRUE)
set.seed(1234)
p <- 10  # 10 experiments.
overlap.mat <- diag(1, p)
overlap.mat[lower.tri(overlap.mat)] <- runif(p * (p - 1) / 2)
overlap.mat[upper.tri(overlap.mat)] <- t(overlap.mat)[upper.tri(overlap.mat)]
summarized.overlap(overlap.mat)
```
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