Package 'PHM'

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addPosteriorMatrix

Compute Posterior Matrix based on PHM merging

Description

Compute Posterior Matrix based on PHM merging

Usage

```
addPosteriorMatrix(phm, data, initK = length(phm))
```

Arguments

Output from	PHM()
Output from	Ρŀ

data $N \times D$ matrix of observations

initK Number of clusters from which to start computing the posterior matrix

Details

TODO: Fill me in

Value

List of the same structure as from PHM() with posterior_matrix and labels fields calculated for the specified elements.

computeDeltaPmcMatrix ΔP _mc Matrix computation

Description

Compute the $\Delta P_{\rm mc}$ matrix for a set of clusters, where the ij^{th} element is $\Delta P_{\rm mc}^{(i,j)}$.

Usage

```
computeDeltaPmcMatrix(paramsList, integralControl = list())
```

Arguments

paramsList List containing lists with each component GMM parameters. See generateDistbnFunc for format of components.

integralControl

List specifying arguments to pass to cubature::cubintegrate(). See details.

Details

#' Each step of the PHM algorithm reduces the overall $P_{\rm mc}$ by the $\Delta P_{\rm mc}$ value of the merged clusters. For each pair of clusters $j,k,\Delta P_{\rm mc}$ is

$$\Delta P_{\rm mc}^{(j,k)} = \int \pi_j(x) \, \pi_k(x) P(x) dx$$

Where the relationship $P_{\rm mc} = \sum_{i < j} 2\Delta P_{\rm mc}^{(i,j)}$ See computePmc for description of integralControl parameters.

Value

 $K \times K$ matrix with each pair of clusters' contribution to P_{mc}

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
partition <- c(rep(1, 100), rep(2, 100), rep(3, 100))
params <- constructPmcParamsPartition(partition, dat, G=1:5)
computeDeltaPmcMatrix(params)</pre>
```

computeMonteCarloDeltaPmcMatrix

Monte Carlo ΔP _mc *Matrix computation*

Description

Compute the $\Delta P_{\rm mc}$ matrix for a set of clusters, where the ij^{th} element is $\Delta P_{\rm mc}^{(i,j)}$.

Usage

```
computeMonteCarloDeltaPmcMatrix(
  paramsList,
  mcSamples = 1e+06,
  batchSize = mcSamples,
  numCores = 1,
  verbose = F
)
```

Arguments

paramsList	List containing lists with each component GMM parameters. See constructPmcParamsMclust for format of components.
mcSamples	Numeric for number of MC samples to use to approximate the integral.
batchSize	Numeric for the observations to assign to each core. Helps with memory concerns. Default mcSamples.
numCores	Number of cores to use in parallel::mclapply call. Default is 1.
verbose	Boolean whether to print output messages

Details

Each step of the PHM algorithm reduces the overall $P_{\rm mc}$ by the $\Delta P_{\rm mc}$ value of the merged clusters. For each pair of clusters j,k we estimate their $\Delta P_{\rm mc}^{(j,k)}$ value.

$$\Delta \hat{P}_{\text{mc}}^{(j,k)} = \frac{1}{M} \sum_{i=1}^{M} \pi_j(x_i) \, \pi_k(x_i)$$

Where the M observations are sampled from the overall data density P(x). Note that $\Delta \hat{P}_{\mathrm{mc}}^{(j,k)} = \Delta \hat{P}_{\mathrm{mc}}^{(k,j)}$

Value

 $K \times K$ matrix with each pair of clusters' $\Delta P_{\rm mc}$ value.

Examples

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
partition <- c(rep(1, 100), rep(2, 100), rep(3, 100))
params <- constructPmcParamsPartition(partition, dat, G=1:5)
computeMonteCarloDeltaPmcMatrix(params, 1e5, verbose=T)</pre>
```

Description

Compute Monte Carlo estimate of $P_{
m mc}$ for a given cluster configuration based on estimated GMM densities

Usage

```
computeMonteCarloPmc(
  paramsList,
  mcSamples = 1e+05,
  batchSize = mcSamples,
  numCores = 1,
  verbose = F
)
```

Arguments

paramsList	List containing lists with each component GMM parameters. See constructPm-cParamsMclust for format of components.
mcSamples	Numeric for number of MC samples to use to approximate the integral.
batchSize	Numeric for the observations to assign to each core. Helps with memory concerns. Default mcSamples.
numCores	Number of cores to use in parallel::mclapply call. Default is 1.
verbose	Boolean whether to print output messages

Details

 $P_{
m mc}$ can be difficult to evaluate as standard cubature methods tend to perform poorly in higher dimensions. We can approximate it for a K-cluster configuration using a Monte Carlo integral of the form

$$\hat{P}_{\text{mc}} = \frac{1}{M} \sum_{i=1}^{M} \sum_{j=1}^{K} 2 (1 - \pi_j(x_i)) \ \pi_j(x_i)$$

Where the M observations are sampled from the overall data density P(x)

Value

Monte Carlo estimate of P_{mc}

Examples

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
partition <- c(rep(1, 100), rep(2, 100), rep(3, 100))
params <- constructPmcParamsPartition(partition, dat, G=1:5)
computeMonteCarloPmc(params, 1e5, verbose=T)</pre>
```

computePairwisePmcMatrix

Pairwise P_mc Matrix computation

Description

TODO: FILL ME IN

Usage

```
computePairwisePmcMatrix(paramsList, mc = T, ...)
```

Arguments

Value

K imes K matrix with Pairwise $P_{
m mc}$ values for each pair of clusters export

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computePmc

Cubature P_mc computation

Description

Compute Pmc for a given Gaussian mixture distribution based on cubature package

Usage

```
computePmc(paramsList, integralControl = list())
```

Arguments

paramsList

List containing lists with each component GMM parameters. See generateDistbnFunc for format of components.

integralControl

List specifying arguments to pass to cubature::cubintegrate(). See details.

Details

For a given cluster configuration, the overall misclassification probability $P_{
m mc}$ can be evaluated as

$$P_{\rm mc} = \sum_{j=1}^{K} \int 2 (1 - \pi_j(x)) \ \pi_j(x) P(x) dx$$

This integral is implemented using the cubature function. the integralControl variable accepts arguments to the cubature::cubintegrate() function The defaults for this function are:

- method: Which integration method is to be used. Default is hcubature
- lowerLimit and upperLimit: The bounds of integration. Default is $\pm\infty$.
- maxEval: Sets the maximum number of integral evaluations. Default is 1e6
- relTol: Sets the convergence tolerance for the integration. Default is 1e-5

Value

Output from the cubature::cubintegrate() function.

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
partition <- c(rep(1, 100), rep(2, 100), rep(3, 100))
params <- constructPmcParamsPartition(partition, dat, G=1:5)
computePmc(params)</pre>
```

constructPmcParamsMclust

Construct P_mc parameter list from Mclust output

Description

Take the output of Mclust() and format it for consumption by compute*Pmc and PHM() functions

Usage

```
constructPmcParamsMclust(mclustObj, singleElement = F)
```

Arguments

```
mclustObj Output of Mclust() function call
singleElement Boolean, whether to combine into a single list element
```

Details

This function takes the parameters object from the output of Mclust() and transforms it to define a GMM for use in the compute*Pmc and PHM functions. The output is a list of lists, where each sublist corresponds of the parameters of a single cluster distribution (default is a single Gaussian component, K = 1).

If singleElement = TRUE, then all components will be combined into a single list.

The parameters in each sublist are

- mean should be a DxK matrix where each column corresponds to a component mean
- var should be a DxDxK array where each slice corresponds to a covariance matrix
- prob should be a K dimensional vector for the proportions within the parent mixture

Value

List of lists where each sublist contains the parameters for the mixture component or a single list if singleEleemnt is TRUE.

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
mcl <- Mclust(dat)
constructPmcParamsMclust(mcl)</pre>
```

constructPmcParamsPartition

Construct P_mc parameter list from a partition

Description

Estimates the mixture model density for a partition of the data using Mclust

Usage

```
constructPmcParamsPartition(partition, data, ...)
```

Arguments

```
partition Vector of labels for observations
data Numeric matrix
```

... Parameters passed to mclust::Mclust()

Details

Performs a naive density estimation, fitting a GMM to each partition separately. Only observations in a cluster are considered to fit the GMM.

See constructPmcParamsMclust() for a description of the output.

Value

List of lists where each sublist contains the proportion, mean, covariance matrix estimates for each cluster.

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
partition <- c(rep(1, 100), rep(2, 100), rep(3, 100))
params <- constructPmcParamsPartition(partition, dat, G=1:5)</pre>
```

constructPmcParamsWeightedPartition

Construct P_mc parameter list from a partition with weights

Description

Estimates the weighted mixture model density for a partition of the data using Mclust.

Usage

```
constructPmcParamsWeightedPartition(
  partition,
  data,
  weights = NULL,
  threshold = 1e-04,
  linkFunc = min,
  verbose = F,
  ...
)
```

Arguments

Details

This procedure attempts to account for clustering uncertainty when estimating the cluster densities. For a given observation x_i and cluster C_j we estimate its cluster-specific weight based on an observation-cluster distance $d(x_i, C_j)$. By default we take the observation-cluster distance to be the smallest Euclidean distance to any member in that cluster, and compute the weight for cluster j as:

$$w_{ij} = \frac{e^{-d(x_i, C_j)}}{\sum_{k=1}^{K} e^{-d(x_i, C_k)}}$$

constructPmcParamsPartition() is a special case of this procedure with weights of 1 if an observation is in a cluster and 0 otherwise. The weights are then passed to a weighted EM procedure to estimate the cluster-specific density via GMM.

See constructPmcParamsMclust() for a description of the output.

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Value

List of lists where each sublist contains the proportion, mean, covariance matrix estimates for each cluster

Examples

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
partition <- c(rep(1, 100), rep(2, 100), rep(3, 100))
params_w <- constructPmcParamsWeightedPartition(partition, dat, G=1:5)</pre>
```

PHM

PHM Algorithm

Description

Implements the PHM algorithm which constructs a clustering hierarchy by successively merging clusters with the largest $\Delta P_{\rm mc}$ values.

Usage

```
PHM(
    mclustObj = NULL,
    paramsList = NULL,
    partition = NULL,
    data = NULL,
    verbose = T,
    computePosterior = T,
    partitionWeightedDensity = T,
    partitionModel = "VVI",
    partitionMaxComponents = 10,
    mc = T,
    ...
)
```

Arguments

mclustObj	Output from mclust::Mclust()
paramsList	A list generated from constructPmcParamsMclust(), constructPmcParamsPartition(), constructPmcParamsPartition() providing the initial cluster parameter estimates
partition	A vector providing obseration partition memberships for the initial state
data	An $N \times D$ matrix of observations
verbose	Boolean whether to suppress debug statements

... Parameters pased to either computeDeltaPmcMatrix() or computeMonteCarloDeltaPmcMatrix() to evaluate the $\Delta P_{\rm mc}$ matrix

Value

A list of lists for each step of the PHM algorithm. Each sublist contains

- clusters: Number of clusters K at this merge
- posterior_matrix: $N \times K$ matrix of posterior cluster probabilities
- labels: Partition of the observations
- pmc_change: Value of $\Delta P_{
 m mc}$ leading to this value of K
- params: Cluster-specific densities
- pmc_components: Number of original clusters involved in this merge
- pmc_accum: Accumulated ΔP_{mc} in this subtree (unused)
- min_merge_pmc: Minimum value of $\Delta P_{
 m mc}$ for all merges in this subtree
- merge_components: Index of components merged in this step
- pmc: Overall $P_{\rm mc}$ remaining in the cluster configuration
- pmc_matrix: $\Delta P_{
 m mc}$ matrix for the remaining clusters

Examples

```
set.seed(1)
dat <- matrix(c(rnorm(200), rnorm(200, 3), rnorm(200, -3)), ncol=2, byrow=T)
partition <- c(rep(1, 100), rep(2, 100), rep(3, 100))
params <- constructPmcParamsPartition(partition, dat, G=1:5)
phm <- PHM(paramsList=params, data=dat, partition=partition)</pre>
```

 $\verb|plotPHMD| endrogram|$

Visualize PHM merging procedure via Dendrogram

Description

Visualize the PHM merging procedure using a dendrogram. Visualization options, such as displaying the merge $\Delta P_{\rm mc}$ value and tracking group membership across merges is included.

plotPHMDendrogram 13

Usage

```
plotPHMDendrogram(
  phm,
  colors = NULL,
  scaleHeights = c("log10", "unscaled", "pmcdist"),
  heightValue = c("merge", "min"),
  threshold = 0,
  suppressLabels = F,
 mergeLabels = c("delta", "pmc", "percent"),
 mergeLabelsSize = 2,
 mergeLabelsBorderSize = 0.15,
 mergeLabelsPadding = 0.15,
 mergeLabelsR = 0.1,
 displayAxis = c("box", "label", "index", "none"),
  displayAxisSize = NULL,
  colorAxis = NULL,
  groupProbs = NULL,
 groupColorMax = "black",
  groupColorMin = "lightgray"
)
```

Output from PHM()

Arguments

phm

colors	Vector of K hex codes to color the leaf node labels
scaleHeights	String specifying how to set the heights in the dendrogram. See Details for more information.
heightValue	Whether to use the $\Delta P_{\rm mc}$ or $\min \Delta P_{\rm mc}$ value to determine branch height for a merge. See Details for more information.
	From the shall for the factor of the state o

threshold Error threshold for the integral past which to represent the merges as dashed

lines

suppressLabels Boolean whether or not to display $P_{
m mc}$ reduction labels on the dendrogram or

not

mergeLabels String indicating what value to display in the labels on the dendrogram

mergeLabelsSize

Text size for the numeric value in the labels on the dendrogram

mergeLabelsPadding

Padding for the merge label text

mergeLabelsR Radius for the rounded edges of the merge label box

displayAxis String indicating what label to place on the leaf nodes of the dendrogram. See

Details for more information.

displayAxisSize

Text size for the leaf node labels

colorAxis Whether or not to color the labels on the leaf nodes

groupProbs Vector of class probability conditional on base group membership

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```
groupColorMax Color of lines corresponding to high group probability groupColorMin Color of lines corresponding to low group probability
```

Details

There are two options for the value for the P_{mc} height for merging subtrees S_1, S_2 ($m = |S_1| + |S_2|$):

```
• "merge": \binom{m}{2}^{-1}\Delta P_{\mathrm{mc}}^{(\mathcal{S}_1,\mathcal{S}_2)}
• "min": \min_{i\in\mathcal{S}_1,\;j\in\mathcal{S}_2}\Delta P_{\mathrm{mc}}^{(i,j)}
```

Once the value for the tree height is obtained, there are three options to scale.

- "unscaled": The height can be left unscaled
- "log10": A \log_{10} scaling can be applied to the height to better reveal different clustering resolutions.
- "pmcdist": A spline-based scaling where we map the value to a linear distance between two Gaussian clusters.

The displayAxis parameter controls what to display on the axes of the heatmap. box displays a standard box, which is most useful for color-coded axes. label displays the cluster label, as specified in the phm parameters. index displays the numeric index of each cluster in the phm parameter list. none suppresses the cluster label entirely, and is mose useful for when there are a large number of clusters.

Value

A ggplot object

plotPHMDistruct

Generate the distruct plot from the posterior matrix

Description

Visualize a distruct plot based on either a partition or the posterior cluster probabilities.

Usage

```
plotPHMDistruct(
   phm,
   K = length(phm),
   colors = NULL,
   labels = NULL,
   axisTextSize = 6,
   partition = F
)
```

plotPHMMatrix 15

Arguments

phm	Output from the PHM() function
K	Number of clusters for which to generate the distruct plot
colors	Optinal vector with colors for the mixture components
labels	Ground truth class labels for the observations (ordered factor vector)
axisTextSize	Size for axis labels
partition	Whether to visualize from the posterior matrix or partition labels

Details

In the case of visualizing for a partition, the posterior probabilities are set to 1 if it is the cluster the observation is assigned to and 0 otherwise.

Value

A ggplot object

plotPHMMatrix Vis	ualize PHM dendrogram structure with a heatmap
-------------------	--

Description

For a pair of clusters i, j, the heatmap position i, j is the value of $\Delta P_{\rm mc}$ where the clusters are first merged. This allows for a more straightforward visualization of the multi-resolution structure of heatmaps when combined with the dendrogram.

Usage

```
plotPHMMatrix(
   phm,
   colors = NULL,
   displayAxis = c("box", "label", "index", "none"),
   displayAxisSize = NULL,
   colorAxis = NULL,
   gridColor = "black",
   fillLimits = NULL,
   fillScale = c("log10", "pmcdist"),
   legendPosition = "none"
)
```

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Arguments

phm Output from PHM()

colors Vector of *K* hex codes to color the leaf node labels

displayAxis String indicating what label to place along the axis (corresponding to clusters).

See Details for more information.

displayAxisSize

Text size for the axis labels

colorAxis Whether or not to color the axis labels gridColor What color to make the heatmap grid

fillLimits Optional vector to manually set limits of the fill scaling. Default is to use the

min and max $\Delta P_{\rm mc}$ values from phm

fillScale Whether to use $\log_{10} \Delta P_{
m mc}$ or the spline scaling for the heatmap color

legendPosition Where to put the legend for the heatmap colors. Default is to suppress.

Details

Consider a pair of initial clusters i, j, and let \mathcal{S} be the smallest subtree containing both i, j (\mathcal{S}_i contains cluster i and \mathcal{S}_j contains cluster j). The pairwise value for i, j, $\rho(i, j)$ is based on $\Delta P_{\mathrm{mc}}^{(\mathcal{S}(i),\mathcal{S}(j))}$, which is the ΔP_{mc} value at which i, j are merged into a single cluster.

As with the dendrogram heights (plotPHMDendrogram()) there are multiple options for scaling $\rho(i,j)$. The first is log10 scaling, where $\rho(i,j) = \log_{10} \Delta P_{\rm mc}$. The second is a spline-based scaling, pmcdist, where we map the $\Delta P_{\rm mc}$ value to a linear distance between two Gaussian clusters.

The displayAxis parameter controls what to display on the axes of the heatmap. box displays a standard box, which is most useful for color-coded axes. label displays the cluster label, as specified in the phm parameters. index displays the numeric index of each cluster in the phm parameter list. none suppresses the cluster label entirely, and is mose useful for when there are a large number of clusters.

Value

A ggplot object

plotPmc2D $ext{Visualize regions contributing to } P_{mc in a 2D plot}$

Description

Visualize the point-specific $P_{\rm mc}$ over a grid of points to visually inspect cluster contributions to $P_{\rm mc}$

plotPmc2D

Usage

```
plotPmc2D(
  paramsList,
  data,
  partition,
  colors = RColorBrewer::brewer.pal(length(paramsList), "Paired"),
  xlim = NULL,
 ylim = NULL,
  suppressPmc = F,
  numPmcPatches = 200,
  logPmcThreshold = -4,
  logPmcMidpoint = 0.6 * logPmcThreshold,
  PmcColor = "#222",
  suppressDensity = F,
  densityLevels = c(0.01, 0.1),
  densityLevelWidth = 0.3,
  suppressObservations = F,
  pointSize = 0.5,
  labelSize = 2,
  textSize = 9,
  legendPosition = "none"
)
```

Arguments

suppressDensity

paramsList	A list generated from constructPmcParamsMclust(), constructPmcParamsPartition(), constructPmcParamsPartition() providing the initial cluster parameter estimates. Parameters should be $2D$	
data	A $N \times 2$ matrix containing observations	
partition	A vector containing class labels	
colors	Vector of K hex codes to color the leaf node labels	
xlim	Vector with min/max values for the x-axis NULL sets this based on the maximum and minimum x-values for observations	
ylim	Vector with min/max values for the y-axis NULL sets this based on the maximum and minimum y-values for observations	
suppressPmc	Flag whether to display the regions contributing to $P_{ m mc}$ in the plot	
numPmcPatches	Number of points along each axis in the P_{mc} grid to evaluate. Higher values gives a smoother visualization	
logPmcThreshold		
	Threshold for $P_{\rm mc}$ values to display. All coordinates with $\log_{10} P_{\rm mc}$ below this value will be ignored.	
logPmcMidpoint	Midpoint in the $P_{ m mc}$ color gradient	
PmcColor	Hex value for the maximum value in the $P_{ m mc}$ color gradient	

Flag whether to overlay the cluster-specific densities

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densityLevels Values of the density at which to display the level curves densityLevelWidth

Line width for the density curves

suppressObservations

Flag whether to display the observations from data

pointSize Size of the data scatterplot points labelSize Text size for the cluster labels textSize Text size for the plots

legendPosition Where to put the legend for the heatmap colors. Default is to suppress

Details

For an arbitrary point x, using the Monte Carlo evaluation of $P_{\rm mc}$ its point-specific $P_{\rm mc}$ can be calculated as

$$\sum_{k=1}^{K} \pi_k(\mathbf{x})(1 - \pi_k(\mathbf{x})) \times f(x = \mathbf{x})$$

Where $f(\mathbf{x})$ is the overall data density evaluated at a point. Note that for a sample of M points, the average of these point-specific P_{mc} values produce the Monte Carlo estimate of P_{mc} described in Turfah and Wen (2025).

The point-specific $P_{\rm mc}$ of each point in a grid is evaluated and visualized. The cluster-specific density level sets and/or the partitioned observations can be overlaid over this to better understand how the $P_{\rm mc}$ value was obtained.

Value

A ggplot object

plotPmcMatrix

Plot ΔP _mc *matrix*

Description

Visualize the matrix of ΔP_{mc} values

Usage

```
plotPmcMatrix(
   phm,
   K = length(phm),
   colors = NULL,
   displayAxis = c("box", "label", "index", "none"),
   displayAxisSize = NULL,
   colorAxis = NULL,
   visScale = c("absolute", "percent"),
   visSize = 2,
```

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```
visThreshold = 0.001,
visDigits = 3
)
```

Arguments

phm Output from PHM()

K Number of clusters for which to visualize the heatmap colors Vector of K hex codes to color the leaf node labels

displayAxis String indicating what label to place along the axis (corresponding to clusters)

displayAxisSize

Text size for the axis labels

colorAxis Whether or not to color the axis labels

visScale Whether to display the raw $\Delta P_{\rm mc}$ values or scale them to be percent of total

 $P_{
m mc}$

visSize Text size for the values inside the heatmap

visThreshold At what value suppress the value and show "< (visThreshold)"

visDigits Number of digits to round the displayed values

Value

A ggplot object

thresholdPHM Find a clustering for a given P_{mc} threshold

Description

Each step of the PHM algorithm reduces $P_{\rm mc}$. This gives the results from the PHM algorithm terminated when $P_{\rm mc}$ falls below some specified threshold.

Usage

```
thresholdPHM(phm, threshold = 0.01)
```

Arguments

phm Output of PHM()

threshold $P_{\rm mc}$ threshold, default is 0.01

Value

Result of the PHM merging procedure terminated when the $P_{
m mc}$ threshold is satisfied export

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