

Package ‘clusternomics’

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Type Package

Title Integrative Clustering for Heterogeneous Biomedical Datasets

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Author Evelina Gabasova

Maintainer Evelina Gabasova <egabasova@gmail.com>

Description Integrative context-dependent clustering for heterogeneous biomedical datasets. Identifies local clustering structures in related datasets, and a global clusters that exist across the datasets.

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LazyData TRUE

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Suggests knitr, rmarkdown, testthat, mclust, gplots, ggplot2

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BugReports <https://github.com/evelinag/clusternomics/issues>

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`clusterSizes`*Estimate sizes of clusters from global cluster assignments.*

Description

Estimate sizes of clusters from global cluster assignments.

Usage

```
clusterSizes(assignments)
```

Arguments

`assignments` Matrix of cluster assignments, where each row corresponds to cluster assignments sampled in one MCMC iteration

Value

Sizes of individual clusters in each MCMC iteration.

Examples

```
# Generate simple test dataset
groupCounts <- c(50, 10, 40, 60)
means <- c(-1.5, 1.5)
testData <- generateTestData_2D(groupCounts, means)
datasets <- testData$data

# Fit the model
# 1. specify number of clusters
clusterCounts <- list(global=10, context=c(3,3))
# 2. Run inference
# Number of iterations is just for demonstration purposes, use
# a larger number of iterations in practice!
results <- contextCluster(datasets, clusterCounts,
  maxIter = 10, burnin = 5, lag = 1,
  dataDistributions = 'diagNormal',
  verbose = TRUE)

# Extract only the sampled global assignments
samples <- results$samples
clusters <- plyr::lapply(1:length(samples), function(i) samples[[i]]$Global)
clusterSizes(clusters)
```

| | |
|--------------------|--|
| coclusteringMatrix | <i>Compute the posterior co-clustering matrix from global cluster assignments.</i> |
|--------------------|--|

Description

Compute the posterior co-clustering matrix from global cluster assignments.

Usage

```
coclusteringMatrix(assignments)
```

Arguments

`assignments` Matrix of cluster assignments, where each row corresponds to cluster assignments sampled in one MCMC iteration

Value

Posterior co-clustering matrix, where element $[i, j]$ represents the posterior probability that data points i and j belong to the same cluster.

Examples

```
# Generate simple test dataset
groupCounts <- c(50, 10, 40, 60)
means <- c(-1.5, 1.5)
testData <- generateTestData_2D(groupCounts, means)
datasets <- testData$data

# Fit the model
# 1. specify number of clusters
clusterCounts <- list(global=10, context=c(3,3))
# 2. Run inference
# Number of iterations is just for demonstration purposes, use
# a larger number of iterations in practice!
results <- contextCluster(datasets, clusterCounts,
  maxIter = 10, burnin = 5, lag = 1,
  dataDistributions = 'diagNormal',
  verbose = TRUE)

# Extract only the sampled global assignments
samples <- results$samples
clusters <- plyr::lapply(1:length(samples), function(i) samples[[i]]$Global)
coclusteringMatrix(clusters)
```

contextCluster *Clusternomics: Context-dependent clustering*

Description

This function fits the context-dependent clustering model to the data using Gibbs sampling. It allows the user to specify a different number of clusters on the global level, as well as on the local level.

Usage

```
contextCluster(datasets, clusterCounts, dataDistributions = "diagNormal",
  prior = NULL, maxIter = 1000, burnin = NULL, lag = 3,
  verbose = FALSE)
```

Arguments

| | |
|-------------------|--|
| datasets | List of data matrices where each matrix represents a context-specific dataset. Each data matrix has the size N times M , where N is the number of data points and M is the dimensionality of the data. The full list of matrices has length C . The number of data points N must be the same for all data matrices. |
| clusterCounts | Number of cluster on the global level and in each context. List with the following structure: <code>clusterCounts = list(global=global, context=context)</code> where <code>global</code> is the number of global clusters, and <code>context</code> is the list of numbers of clusters in the individual contexts (datasets) of length C where <code>context[c]</code> is the number of clusters in dataset c . |
| dataDistributions | Distribution of data in each dataset. Can be either a list of length C where <code>dataDistributions[c]</code> is the distribution of dataset c , or a single string when all datasets have the same distribution. Currently implemented distribution is the 'diagNormal' option for multivariate Normal distribution with diagonal covariance matrix. |
| prior | Prior distribution. If NULL then the prior is estimated using the datasets. The 'diagNormal' distribution uses the Normal-Gamma distribution as a prior for each dimension. |
| maxIter | Number of iterations of the Gibbs sampling algorithm. |
| burnin | Number of burn-in iterations that will be discarded. If not specified, the algorithm discards the first half of the <code>maxIter</code> samples. |
| lag | Used for thinning the samples. |
| verbose | Print progress, by default FALSE. |

Value

Returns list containing the sequence of MCMC states and the log likelihoods of the individual states.

| | |
|---------|---|
| samples | List of assignments sampled from the posterior, each state <code>samples[[i]]</code> is a data frame with local and global assignments for each data point. |
| logliks | Log likelihoods during MCMC iterations. |
| DIC | Deviance information criterion to help select the number of clusters. Lower values of DIC correspond to better-fitting models. |

Examples

```
# Example with simulated data (see vignette for details)
# Number of elements in each cluster
groupCounts <- c(50, 10, 40, 60)
# Centers of clusters
means <- c(-1.5,1.5)
testData <- generateTestData_2D(groupCounts, means)
datasets <- testData$data

# Fit the model
# 1. specify number of clusters
clusterCounts <- list(global=10, context=c(3,3))
# 2. Run inference
# Number of iterations is just for demonstration purposes, use
# a larger number of iterations in practice!
results <- contextCluster(datasets, clusterCounts,
  maxIter = 10, burnin = 5, lag = 1,
  dataDistributions = 'diagNormal',
  verbose = TRUE)

# Extract results from the samples
# Final state:
state <- results$samples[[length(results$samples)]]
# 1) assignment to global clusters
globalAssgn <- state$Global
# 2) context-specific assignments- assignment in specific dataset (context)
contextAssgn <- state[,"Context 1"]
# Assess the fit of the model with DIC
results$DIC
```

empiricalBayesPrior *Fit an empirical Bayes prior to the data*

Description

Fit an empirical Bayes prior to the data

Usage

```
empiricalBayesPrior(datasets, distributions = "diagNormal",
  globalConcentration = 0.1, localConcentration = 0.1, type = "fitRate")
```

Arguments

| | |
|---------------------|--|
| datasets | List of data matrices where each matrix represents a context-specific dataset. Each data matrix has the size N times M , where N is the number of data points and M is the dimensionality of the data. The full list of matrices has length C . The number of data points N must be the same for all data matrices. |
| distributions | Distribution of data in each dataset. Can be either a list of length C where <code>dataDistributions[c]</code> is the distribution of dataset c , or a single string when all datasets have the same distribution. Currently implemented distribution is the 'diagNormal' option for multivariate Normal distribution with diagonal covariance matrix. |
| globalConcentration | Prior concentration parameter for the global clusters. Small values of this parameter give larger prior probability to smaller number of clusters. |
| localConcentration | Prior concentration parameter for the local context-specific clusters. Small values of this parameter give larger prior probability to smaller number of clusters. |
| type | Type of prior that is fitted to the data. The algorithm can fit either rate of the prior covariance matrix, or fit the full covariance matrix to the data. |

Value

Returns the prior object that can be used as an input for the `contextCluster` function.

Examples

```
# Example with simulated data (see vignette for details)
nContexts <- 2
# Number of elements in each cluster
groupCounts <- c(50, 10, 40, 60)
# Centers of clusters
means <- c(-1.5, 1.5)
testData <- generateTestData_2D(groupCounts, means)
datasets <- testData$data

# Generate the prior
fullDataDistributions <- rep('diagNormal', nContexts)
prior <- empiricalBayesPrior(datasets, fullDataDistributions, 0.01, 0.1, 'fitRate')

# Fit the model
# 1. specify number of clusters
clusterCounts <- list(global=10, context=c(3,3))
# 2. Run inference
# Number of iterations is just for demonstration purposes, use
# a larger number of iterations in practice!
results <- contextCluster(datasets, clusterCounts,
  maxIter = 10, burnin = 5, lag = 1,
  dataDistributions = 'diagNormal', prior = prior,
  verbose = TRUE)
```

generatePrior *Generate a basic prior distribution for the datasets.*

Description

Creates a basic prior distribution for the clustering model, assuming a unit prior covariance matrix for clusters in each dataset.

Usage

```
generatePrior(datasets, distributions = "diagNormal",
              globalConcentration = 0.1, localConcentration = 0.1)
```

Arguments

datasets List of data matrices where each matrix represents a context-specific dataset. Each data matrix has the size N times M , where N is the number of data points and M is the dimensionality of the data. The full list of matrices has length C . The number of data points N must be the same for all data matrices.

distributions Distribution of data in each dataset. Can be either a list of length C where `dataDistributions[c]` is the distribution of dataset c , or a single string when all datasets have the same distribution. Currently implemented distribution is the 'diagNormal' option for multivariate Normal distribution with diagonal covariance matrix.

globalConcentration Prior concentration parameter for the global clusters. Small values of this parameter give larger prior probability to smaller number of clusters.

localConcentration Prior concentration parameter for the local context-specific clusters. Small values of this parameter give larger prior probability to smaller number of clusters.

Value

Returns the prior object that can be used as an input for the `contextCluster` function.

Examples

```
# Example with simulated data (see vignette for details)
nContexts <- 2
# Number of elements in each cluster
groupCounts <- c(50, 10, 40, 60)
# Centers of clusters
means <- c(-1.5, 1.5)
testData <- generateTestData_2D(groupCounts, means)
datasets <- testData$data

# Generate the prior
fullDataDistributions <- rep('diagNormal', nContexts)
```

```

prior <- generatePrior(datasets, fullDataDistributions, 0.01, 0.1)

# Fit the model
# 1. specify number of clusters
clusterCounts <- list(global=10, context=c(3,3))
# 2. Run inference
# Number of iterations is just for demonstration purposes, use
# a larger number of iterations in practice!
results <- contextCluster(datasets, clusterCounts,
  maxIter = 10, burnin = 5, lag = 1,
  dataDistributions = 'diagNormal', prior = prior,
  verbose = TRUE)

```

`generateTestData_1D` *Generate simulated 1D dataset for testing*

Description

Generate simple 1D dataset with two contexts, where the data are generated from Gaussian distributions. The generated output contains two datasets, where each dataset contains 4 global clusters, originating from two local clusters in each context.

Usage

```
generateTestData_1D(groupCounts, means)
```

Arguments

| | |
|--------------------------|--|
| <code>groupCounts</code> | Number of data samples in each global cluster. It is assumed to be a vector of four elements: $c(c_{11}, c_{21}, c_{12}, c_{22})$ where c_{ij} is the number of samples coming from cluster i in context 1 and cluster j in context 2. |
| <code>means</code> | Means of the simulated clusters. It is assumed to be a vector of two elements: $c(m_1, m_2)$ where m_1 is the mean of the first cluster in both contexts, and m_2 is the mean of the second cluster in both contexts. |

Value

Returns the simulated datasets together with true assignments.

| | |
|---------------------|---|
| <code>data</code> | List of datasets for each context. This can be used as an input for the <code>contextCluster</code> function. |
| <code>groups</code> | True cluster assignments that were used to generate the data. |

Examples

```
groupCounts <- c(50, 10, 40, 60)
means <- c(-1.5, 1.5)
testData <- generateTestData_1D(groupCounts, means)
# Use the dataset as an input for the contextCluster function for testing
datasets <- testData$data
```

generateTestData_2D *Generate simulated 2D dataset for testing*

Description

Generate simple 2D dataset with two contexts, where the data are generated from Gaussian distributions. The generated output contains two datasets, where each dataset contains 4 global clusters, originating from two local clusters in each context.

Usage

```
generateTestData_2D(groupCounts, means, variances = NULL)
```

Arguments

| | |
|-------------|---|
| groupCounts | Number of data samples in each global cluster. It is assumed to be a vector of four elements: $c(c_{11}, c_{21}, c_{12}, c_{22})$ where c_{ij} is the number of samples coming from cluster i in context 1 and cluster j in context 2. |
| means | Means of the simulated clusters. It is assumed to be a vector of two elements: $c(m_1, m_2)$ where m_1 is the mean of the first cluster in both contexts, and m_2 is the mean of the second cluster in both contexts. Because the data are two-dimensional, the mean is assumed to be the same in both dimensions. |
| variances | Optionally, it is possible to specify different variance for each of the clusters. The variance is assumed to be a vector of two elements: $c(v_1, v_2)$ where v_1 is the variance of the first cluster in both contexts, and v_2 is the variance of the second cluster in both contexts. Because the data are two-dimensional, the variance is diagonal and the same in both dimensions. |

Value

Returns the simulated datasets together with true assignments.

| | |
|--------|--|
| data | List of datasets for each context. This can be used as an input for the contextCluster function. |
| groups | True cluster assignments that were used to generate the data. |

Examples

```
groupCounts <- c(50, 10, 40, 60)
means <- c(-1.5, 1.5)
testData <- generateTestData_1D(groupCounts, means)
# Use the dataset as an input for the contextCluster function for testing
datasets <- testData$data
```

| | |
|------------------|---|
| numberOfClusters | <i>Estimate number of clusters from global cluster assignments.</i> |
|------------------|---|

Description

Estimate number of clusters from global cluster assignments.

Usage

```
numberOfClusters(assignments)
```

Arguments

`assignments` Matrix of cluster assignments, where each row corresponds to cluster assignments sampled in one MCMC iteration

Value

Number of unique clusters in each MCMC iteration.

Examples

```
# Generate simple test dataset
groupCounts <- c(50, 10, 40, 60)
means <- c(-1.5, 1.5)
testData <- generateTestData_2D(groupCounts, means)
datasets <- testData$data

# Fit the model
# 1. specify number of clusters
clusterCounts <- list(global=10, context=c(3,3))
# 2. Run inference
# Number of iterations is just for demonstration purposes, use
# a larger number of iterations in practice!
results <- contextCluster(datasets, clusterCounts,
  maxIter = 10, burnin = 5, lag = 1,
  dataDistributions = 'diagNormal',
  verbose = TRUE)

# Extract only the sampled global assignments
samples <- results$samples
```

```
clusters <- plyr::laply(1:length(samples), function(i) samples[[i]]$Global)
numberOfClusters(clusters)
```

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