Package ‘MGMM’

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Title Missingness Aware Gaussian Mixture Models

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Description
Parameter estimation and classification for Gaussian Mixture Models (GMMs) in the presence of missing data. This package complements existing implementations by allowing for both missing elements in the input vectors and full (as opposed to strictly diagonal) covariance matrices. Estimating is performed using an expectation conditional maximization algorithm that accounts for missingness of both the cluster assignments and the vector components. The output includes the marginal cluster membership probabilities; the mean and covariance of each cluster; the posterior probabilities of cluster membership; and a completed version of the input data, with missing values imputed to their posterior expectations. For additional details, please see McCaw ZR, Julienne H, Aschard H. “MGMM: an R package for fitting Gaussian Mixture Models on Incomplete Data.” <doi:10.1101/2019.12.20.884551>.

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CalHar ............................................. Calinski-Harabaz Index

Description
CalHar calculates the Calinski-Harabaz index.

Usage
CalHar(data, assign, means)

Arguments
data Observations.
assign Assignments.
means List of cluster means.

Value
Scalar metric.
ChooseK

Cluster Number Selection

Description

Function to choose the number of clusters k. Examines cluster numbers between k0 and k1. For each cluster number, generates boot bootstrap data sets, fits the Gaussian Mixture Model (FitGMM), and calculates quality metrics (ClustQual). For each metric, determines the optimal cluster number k_opt, and the k_1SE, the smallest cluster number whose quality is within 1 SE of the optimum.

Usage

ChooseK(
  data,  
  k0 = 2,  
  k1 = NULL,  
  boot = 100,  
  init_means = NULL,  
  fix_means = FALSE,  
  init_covs = NULL,  
  init_props = NULL,  
  maxit = 10,  
  eps = 1e-04,  
  report = TRUE
)

Arguments

data Numeric data matrix.

k0 Minimum number of clusters.

k1 Maximum number of clusters.

boot Bootstrap replicates.

init_means Optional list of initial mean vectors.

fix_means Fix the means to their starting value? Must provide initial values.

init_covs Optional list of initial covariance matrices.

init_props Optional vector of initial cluster proportions.

maxit Maximum number of EM iterations.

eps Minimum acceptable increment in the EM objective.

report Report bootstrap progress?

Value

List containing Choices, the recommended number of clusters according to each quality metric, and Results, the mean and standard error of the quality metrics at each cluster number evaluated.
See Also

See ClustQual for evaluating cluster quality, and FitGMM for estimating the GMM with a specified cluster number.

Examples

```r
set.seed(100)
mean_list <- list(c(2, 2), c(2, -2), c(-2, 2), c(-2, -2))
data <- rGMM(n = 500, d = 2, k = 4, means = mean_list)
choose_k <- ChooseK(data, k0 = 2, k1 = 6, boot = 10)
choose_k$Choices
```

---

**ClustQual**

*Cluster Quality*

**Description**

Evaluates cluster quality. Returns the following metrics:

- BIC: Bayesian Information Criterion, lower value indicates better clustering quality.
- CHI: Calinski-Harabaz Index, higher value indicates better clustering quality.
- DBI: Davies-Bouldin, lower value indicates better clustering quality.
- SIL: Silhouette Width, higher value indicates better clustering quality.

**Usage**

```
ClustQual(fit)
```

**Arguments**

- `fit` Object of class `mix`.

**Value**

List containing the cluster quality metrics.

**See Also**

See ChooseK for using quality metrics to choose the cluster number.
Examples

```r
set.seed(100)

# Data generation
mean_list = list(
  c(2, 2, 2),
  c(-2, 2, 2),
  c(2, -2, 2),
  c(2, 2, -2)
)
data <- rGMM(n = 500, d = 3, k = 4, means = mean_list)
fit <- FitGMM(data, k = 4)

# Clustering quality
cluster_qual <- ClustQual(fit)
```

---

**DavBou**

*Davies-Bouldin Index*

**Description**

Calculates the Davies-Bouldin index.

**Usage**

```r
DavBou(data, assign, means)
```

**Arguments**

- `data` Observations
- `assign` Assignments
- `means` List of cluster means

**Value**

Scalar index.
Description

Given an $n \times d$ matrix of random vectors, estimates the parameters of a Gaussian Mixture Model (GMM). Accommodates arbitrary patterns of missingness at random (MAR) in the input vectors.

Usage

```r
FitGMM(
  data,  # Numeric data matrix.
  k = 1,  # Number of mixture components. Defaults to 1.
  init_means = NULL,  # Optional list of initial mean vectors.
  fix_means = FALSE,  # Fix the means to their starting value? Must provide initial values.
  init_covs = NULL,  # Optional list of initial covariance matrices.
  init_props = NULL,  # Optional vector of initial cluster proportions.
  maxit = 100,  # Maximum number of EM iterations.
  eps = 1e-06,  # Minimum acceptable increment in the EM objective.
  report = TRUE  # Report fitting progress?
)
```

Arguments

- **data**: Numeric data matrix.
- **k**: Number of mixture components. Defaults to 1.
- **init_means**: Optional list of initial mean vectors.
- **fix_means**: Fix the means to their starting value? Must provide initial values.
- **init_covs**: Optional list of initial covariance matrices.
- **init_props**: Optional vector of initial cluster proportions.
- **maxit**: Maximum number of EM iterations.
- **eps**: Minimum acceptable increment in the EM objective.
- **report**: Report fitting progress?

Details

Initial values for the cluster means, covariances, and proportions are specified using $\mathbf{M}_0$, $\mathbf{S}_0$, and $\mathbf{\pi}_0$, respectively. If the data contains complete observations, i.e. observations with no missing elements, then `fit.GMM` will attempt to initialize these parameters internally using K-means. If the data contains no complete observations, then initial values are required for $\mathbf{M}_0$, $\mathbf{S}_0$, and $\mathbf{\pi}_0$.

Value

- For a single component, an object of class `mvn`, containing the estimated mean and covariance, the final objective function, and the imputed data.
- For a multicomponent model $k > 1$, an object of class `mix`, containing the estimated means, covariances, cluster proportions, cluster responsibilities, and observation assignments.
FitMix

Fit Multivariate Mixture Distribution

Description

Given a matrix of random vectors, estimates the parameters for a mixture of multivariate normal distributions. Accommodates arbitrary patterns of missingness, provided the elements are missing at random (MAR).

See Also

See \texttt{rGMM} for data generation, and \texttt{ChooseK} for selecting the number of clusters.

Examples

```r
# Single component without missingness
# Bivariate normal observations
sigma <- matrix(c(1, 0.5, 0.5, 1), nrow = 2)
data <- rGMM(n = 1e3, d = 2, k = 1, means = c(2, 2), covs = sigma)
fit <- FitGMM(data, k = 1)

# Single component with missingness
# Trivariate normal observations
mean_list <- list(c(-2, -2, -2), c(2, 2, 2))
sigma <- matrix(c(1, 0.5, 0.5, 0.5, 1, 0.5, 0.5, 0.5, 1), nrow = 3)
data <- rGMM(n = 1e3, d = 3, k = 2, means = mean_list, covs = sigma)
fit <- FitGMM(data, k = 2)

# Two components without missingness
# Trivariate normal observations
mean_list <- list(c(-2, -2, -2), c(2, 2, 2))
sigma <- matrix(c(1, 0.5, 0.5, 0.5, 1, 0.5, 0.5, 0.5, 1), nrow = 3)
data <- rGMM(n = 1e3, d = 3, k = 2, means = mean_list, covs = sigma)
fit <- FitGMM(data, k = 2)

# Four components with missingness
# Bivariate normal observations
# Note: Fitting is slow.
mean_list <- list(c(2, 2), c(2, -2), c(-2, 2), c(-2, -2))
sigma <- 0.5 * diag(2)
data <- rGMM(n = 1000,
d = 2,
k = 4,
pi = c(0.35, 0.15, 0.15, 0.35),
m = 0.1,
means = mean_list,
covs = sigma)
fit <- FitGMM(data, k = 4)
```
Usage

FitMix(
  data,
  k = 2,
  init_means = NULL,
  fix_means = FALSE,
  init_covs = NULL,
  init_props = NULL,
  maxit = 100,
  eps = 1e-06,
  report = FALSE
)

Arguments

data Numeric data matrix.
k Number of mixture components. Defaults to 2.
init_means Optional list of initial mean vectors.
fix_means Fix means to their starting values? Must initialize.
init_covs Optional list of initial covariance matrices.
init_props Optional vector of initial cluster proportions.
maxit Maximum number of EM iterations.
eps Minimum acceptable increment in the EM objective.
report Report fitting progress?

Value

Object of class mix.

Description

Given a matrix of n x d-dimensional random vectors, possibly containing missing elements, estimates the mean and covariance of the best fitting multivariate normal distribution.

Usage

FitMVN(
  data,
  init_mean = NULL,
  fix_mean = FALSE,
  init_cov = NULL,
logLik.mix

maxit = 100, 
eps = 1e-06, 
report = TRUE
)

Arguments

data Numeric data matrix.
init_mean Optional initial mean vector.
fix_mean Fix the mean to its starting value? Must initialize.
init_cov Optional initial covariance matrix.
maxit Maximum number of EM iterations.
eps Minimum acceptable increment in the EM objective.
report Report fitting progress?

Value

An object of class mvn.

Description

Log likelihood for Fitted GMM

Usage

## S3 method for class 'mix'
logLik(object, ...)

Arguments

object A mix object.
... Unused.
logLik.mvn  
Log likelihood for Fitted MVN Model

Description
Log likelihood for Fitted MVN Model

Usage
## S3 method for class 'mvn'
logLik(object, ...)

Arguments
object  A mvn object.
...     Unused.

mean.mix  
Mean for Fitted GMM

Description
Mean for Fitted GMM

Usage
## S3 method for class 'mix'
mean(x, ...)

Arguments
x  A mix object.
...  Unused.
mean.mvn

Mean for Fitted MVN Model

Description
Mean for Fitted MVN Model

Usage

```r
## S3 method for class 'mvn'
mean(x, ...)
```

Arguments

- `x` A mvn object.
- `...` Unused.

MGMM

MGMM: Missingness Aware Gaussian Mixture Models

Description
Parameter estimation and classification for Gaussian Mixture Models (GMMs) in the presence of missing data. This package complements existing implementations by allowing for both missing elements in the input vectors and full (as opposed to strictly diagonal) covariance matrices. Estimating is performed using an expectation conditional maximization algorithm that accounts for missingness of both the cluster assignments and the vector components. The output includes the marginal cluster membership probabilities; the mean and covariance of each cluster; the posterior probabilities of cluster membership; and a completed version of the input data, with missing values imputed to their posterior expectations. For additional details, please see McCaw ZR, Julienne H, Aschard H. "MGMM: an R package for fitting Gaussian Mixture Models on Incomplete Data." <doi:10.1101/2019.12.20.884551>.

Author(s)
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mix-class  

*Mixture Model Class*

**Description**

Defines a class to hold Gaussian Mixture Models.

**Slots**

- Assignments  Maximum a posteriori assignments.
- Completed  Completed data, with missing values imputed to their posterior expectations.
- Components  Number of components.
- Covariances  List of fitted cluster covariance matrices.
- Density  Density of each component at each example.
- Means  List of fitted cluster means.
- Objective  Final value of the EM objective.
- Proportions  Fitted cluster proportions.
- Responsibilities  Posterior membership probabilities for each example.

**MixUpdateMeans**  

*Mean Update for Mixture of MVNs with Missingness.*

**Description**

Mean Update for Mixture of MVNs with Missingness.

**Usage**

`MixUpdateMeans(split_data, means, covs, gamma)`

**Arguments**

- `split_data`  Data partitioned by missingness.
- `means`  List of component means.
- `covs`  List of component covariances.
- `gamma`  List of component responsibilities.

**Value**

List containing the updated component means.
Multivariate Normal Model Class

Description
Defines a class to hold multivariate normal models.

Slots
- Completed  Completed data, with missing values imputed to their posterior expectations.
- Covariance  Fitted covariance matrix.
- Mean  Fitted mean vector.
- Objective  Final value of the EM objective.

PartitionData  Partition Data by Missingness.

Description
Partition Data by Missingness.

Usage
PartitionData(data)

Arguments
data  Data.frame.

Value
List containing:
- The original row and column names: ‘orig_row_names’, ‘orig_col_names’.
- The original row and column numbers: ‘n_row’ and ‘n_col’.
- The complete cases ‘data_comp’.
- The incomplete cases ‘data_incomp’.
- The empty cases ‘data_empty’.
- Counts of complete ‘n0’, incomplete ‘n1’, and empty ‘n2’ cases.
- Initial order of the observations ‘init_order’.
Description

Print method for objects of class `mix`.

Usage

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

Arguments

- `x` A `mix` object.
- `...` Unused.

Description

Print for Fitted MVN Model

Usage

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

Arguments

- `x` A `mvn` object.
- `...` Unused.
rGMM

Generate Data from Gaussian Mixture Models

Description

 Generates an \( n \times d \) matrix of multivariate normal random vectors with observations (examples) as rows. If \( k = 1 \), all observations belong to the same cluster. If \( k > 1 \) the observations are generated via two-step procedure. First, the cluster membership is drawn from a multinomial distribution, with mixture proportions specified by \( \pi \). Conditional on cluster membership, the observation is drawn from a multivariate normal distribution, with cluster-specific mean and covariance. The cluster means are provided using \( \text{means} \), and the cluster covariance matrices are provided using \( \text{covs} \). If \( \text{miss} > 0 \), missingness is introduced, completely at random, by setting that proportion of elements in the data matrix to NA.

Usage

\[
\text{rGMM}(n, d = 2, k = 1, \pi = \text{NULL}, \text{miss} = 0, \text{means} = \text{NULL}, \text{covs} = \text{NULL})
\]

Arguments

- \( n \): Observations (rows).
- \( d \): Observation dimension (columns).
- \( k \): Number of mixture components. Defaults to 1.
- \( \pi \): Mixture proportions. If omitted, components are assumed equiprobable.
- \( \text{miss} \): Proportion of elements missing, \( \text{miss} \in [0, 1) \).
- \( \text{means} \): Either a prototype mean vector, or a list of mean vectors. Defaults to the zero vector.
- \( \text{covs} \): Either a prototype covariance matrix, or a list of covariance matrices. Defaults to the identity matrix.

Value

Numeric matrix with observations as rows. Row numbers specify the true cluster assignments.

See Also

For estimation, see \text{FitGMM}.

Examples

\[
\text{set.seed(100)}\\
\text{# Single component without missingness.}\\
\text{# Bivariate normal observations.}\\
\text{cov} \leftarrow \text{matrix}(c(1, 0.5, 0.5, 1), \text{nrow} = 2)\\
\text{data} \leftarrow \text{rGMM}(n = 1e3, d = 2, k = 1, \text{means} = c(2, 2), \text{covs} = \text{cov})
\]
# Single component with missingness.
# Trivariate normal observations.
mean_list <- list(c(-2, -2, -2), c(2, 2, 2))
cov <- matrix(c(1, 0.5, 0.5, 0.5, 1, 0.5, 0.5, 0.5, 1), nrow = 3)
data <- rGMM(n = 1e3, d = 3, k = 2, means = mean_list, covs = cov)

# Two components without missingness.
# Trivariate normal observations.
mean_list <- list(c(-2, -2, -2), c(2, 2, 2))
cov <- matrix(c(1, 0.5, 0.5, 0.5, 1, 0.5, 0.5, 0.5, 1), nrow = 3)
data <- rGMM(n = 1e3, d = 3, k = 2, means = mean_list, covs = cov)

# Four components with missingness.
# Bivariate normal observations.
mean_list <- list(c(2, 2), c(2, -2), c(-2, 2), c(-2, -2))
cov <- 0.5 * diag(2)
data <- rGMM(n = 1000, d = 2, k = 4, 
  pi = c(0.35, 0.15, 0.15, 0.35), 
  miss = 0.1, 
  means = mean_list, 
  covs = cov)

---

**show.mix-method**

*Show for Fitted Mixture Models*

**Description**

Show for Fitted Mixture Models

**Usage**

```r
## S4 method for signature 'mix'
show(object)
```

**Arguments**

- `object` A `mix` object.
### show.mvn-method

**Show for Multivariate Normal Models**

#### Description

Show for Multivariate Normal Models

#### Usage

```r
## S4 method for signature 'mvn'
show(object)
```

#### Arguments

- `object`: A `mvn` object.

### vcov.mix

**Covariance for Fitted GMM**

#### Description

Covariance for Fitted GMM

#### Usage

```r
## S3 method for class 'mix'
vcov(object, ...)
```

#### Arguments

- `object`: A `mix` object.
- `...`: Unused.
Covariance for Fitted MVN Model

## S3 method for class 'mvn'
vcov(object, ...)

### Arguments

- **object**: A mvn object.
- **...**: Unused.

### Description

Covariance for Fitted MVN Model
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