

Package: GOFclustering (via r-universe)

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Type Package

Title Goodness-of-Fit Testing for Model-Based Clustering

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Description Performs goodness-of-fit tests for model-based clustering based on the methodology developed in [doi:10.48550/arXiv.2511.04206](https://doi.org/10.48550/arXiv.2511.04206). It implements a test statistic derived from empirical likelihood to verify the distribution of clusters in multivariate Gaussian mixtures and other latent class models.

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FitAndGOFCluster	<i>Fit a Mixture Model and Perform Goodness-of-Fit Test</i>
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Description

High-level function that estimates a clustering model (parametric or non-parametric) and automatically performs the goodness-of-fit test on the posterior probabilities as described in El Kolei and Marbac (2025).

Usage

```
FitAndGOFCluster(
  ech,
  method,
  K,
  kappa = 1/9,
  rho = 3/4,
  xi = 3/4,
  alpha = 0.05,
  basis = "Bernstein",
  size = as.integer(10 * (nrow(ech)^(xi))),
  p = as.integer(round(3 * (nrow(ech)^(kappa)))),
  B = as.integer(round(2 * ((nrow(ech)^(1 - rho)))))
)
```

Arguments

ech	A data frame or matrix where each row is an observation.
method	Character. The clustering method to use: "VarSelLCM" for parametric models or "Mixtools" for non-parametric models.
K	Integer. The number of clusters to be tested.
kappa	Numeric. Tuning parameter for the number of moment conditions p. Default is 1/9.
rho	Numeric. Tuning parameter for the number of blocks B. Default is 3/4.
xi	Numeric. Tuning parameter for the sub-sample size size. Default is 3/4.
alpha	Numeric. Significance level for the test (default is 0.05).
basis	Character or vector of characters. The basis used for the moment conditions ("Bernstein", "indicatorEqualproba", or "indicatorEqualsize"). If a vector is provided, the test is performed for each basis.

size	Integer. Size of the sub-sample for block-splitting. Default is computed based on x_i .
p	Integer. Number of moment conditions. Default is computed based on kappa.
B	Integer. Number of blocks for the test. Default is computed based on rho.

Details

This function automates the estimation and validation. It first fits the model, then calls `GOFClusteringSpe` to compute the test statistics. The test bypasses the curse of dimensionality by working on the unit simplex.

Value

A list containing:

- `clustering`: The fitted model object (VSLCMresults or npEM).
- `GOF`: A list containing the test results for the first basis:
 - `stat`: The 5 statistics: `max` (Max block EL), `sum` (Sum block EL), `ks` (Kolmogorov-Smirnov), `cvm` (Cramer-von Mises), and `ad` (Anderson-Darling).
 - `pvalues`: P-values for `sum`, `ks`, `cvm`, and `ad`.
 - `reject`: Logical indicators of rejection for each test at level alpha.
 - `cvpsi`: The covariance matrix Σ . Its dimension reflects the number of components kept after PCA filtering.
 - `basis`: The basis function used.
 - `hyperparam`: The values of `p` and `B` used.
- `GOF2`: Results for additional bases if provided.

References

El Kolei, S. and Marbac, M. (2025). Goodness-of-fit testing of the distribution of posterior classification probabilities for validating model-based clustering. <doi:10.48550/arXiv.2511.04206>.

Examples

```
# Simulation of Gaussian Mixture Data (K=2, d=5)
set.seed(123)
n <- 180
z <- sample(1:2, n, replace = TRUE, prob = c(1/2,1/2))
ech <- matrix(0, nrow = n, ncol = 5)
for(k in 1:2) ech[z==k,] <- matrix(rnorm(sum(z==k) * 5, ((-1)**k)/sqrt(5), 1), ncol=5)

# --- Case 1: Parametric estimation and test ---
res_param <- FitAndGOFCluster(ech = ech, method = "VarSelLCM", K = 2, p=3, B=3)
print(res_param$GOF$pvalues)

# --- Case 2: Non-parametric estimation and test ---
res_nonparam <- FitAndGOFCluster(ech = ech, method = "Mixtools", K = 2)
print(res_nonparam$GOF$pvalues)
```

Description

Core function to perform the goodness-of-fit test for clustering validation. It takes a matrix of posterior probabilities and a function to generate new posterior probabilities under the null hypothesis (estimated model). This version is agnostic to the clustering package used.

Usage

```
GOFClustering(
  probapost,
  rprobapost,
  size = as.integer(10 * (nrow(probapost)^(3/4))),
  p = as.integer(round(3 * (nrow(probapost)^(1/9)))),
  B = as.integer(round(2 * ((nrow(probapost)^(1/4))))),
  alpha = 0.05,
  basis = "Bernstein"
)
```

Arguments

probapost	A matrix ($n \times K$) of estimated posterior classification probabilities, where n is the number of observations and K is the number of clusters.
rprobapost	A function that generates a new matrix of posterior probabilities under the estimated model. It must take a single argument n (sample size).
size	Integer. Size of the sub-sample used for the block-splitting procedure. Default is $10 * n^{(3/4)}$.
p	Integer. Number of moment conditions. Default is $3 * n^{(1/9)}$.
B	Integer. Number of blocks for the testing procedure. Default is $2 * n^{(1/4)}$.
alpha	Numeric. Significance level (default is 0.05).
basis	Character or vector of characters. The basis used for the moment conditions ("Bernstein", "indicatorEqualproba", or "indicatorEqualsize").

Details

This function implements the Empirical Likelihood test on the unit simplex. The user must provide `rprobapost`, which reflects the uncertainty of the fitted model. For a parametric mixture, this function typically simulates new data from the fitted parameters and returns the resulting posterior probabilities.

Value

A list with the following components:

stat A list of the 5 test statistics: max, sum, ks, cvm, and ad.

pvalues A list of p-values for sum, ks, cvm, and ad.

reject Logical indicators of rejection at level alpha.

cvpsi The estimated covariance matrix Σ after PCA filtering.

basis The basis functions used.

hyperparam The number of moments p and blocks B used.

References

El Kolei, S. and Marbac, M. (2025). Goodness-of-fit testing of the distribution of posterior classification probabilities for validating model-based clustering. <doi:10.48550/arXiv.2511.04206>.

Examples

```
library(VarSelLCM)

# Simulation of a Gaussian Mixture Model (K=2, d=5)
set.seed(123)
n <- 180
z <- sample(1:2, n, replace = TRUE, prob = c(1/2, 1/2))
ech <- matrix(0, nrow = n, ncol = 5)
for(k in 1:2) {
  ech[z==k,] <- matrix(rnorm(sum(z==k) * 5, ((-1)**k)/sqrt(5), 1), ncol=5)
}

# 1. Fit the model using VarSelLCM (without variable selection)
results <- VarSelCluster(ech, 2, vbleSelec = FALSE)

# 2. Define the rprobapost function using the fitted model parameters
# This function simulates data under H0 and computes posterior probabilities
my_rprobapost <- function(n_new) {
  # Simulate labels
  z_sim <- sample(1:results@model@g, n_new, replace = TRUE, results@param@pi)
  # Simulate observations
  ech_sim <- as.data.frame(matrix(NA, n_new, results@data@dataContinuous@d))
  for (j in 1:nrow(results@param@paramContinuous@mu)) {
    for (k in unique(z_sim)) {
      indices <- which(z_sim == k)
      ech_sim[indices, j] <- rnorm(length(indices),
                                  results@param@paramContinuous@mu[j, k],
                                  results@param@paramContinuous@sd[j, k])
    }
  }
}

# Compute log-posterior probabilities
logprobamat <- matrix(log(results@param@pi), n_new, results@model@g, byrow = TRUE)
for (j in 1:nrow(results@param@paramContinuous@mu)) {
  for (k in 1:ncol(logprobamat)) {
```

```

    logprobatmat[, k] <- logprobatmat[, k] +
      dnorm(ech_sim[, j], results@param@paramContinuous@mu[j, k],
            results@param@paramContinuous@sd[j, k], log = TRUE)
  }
}
# Softmax normalization to obtain probabilities
probatmat <- exp(logprobatmat - apply(logprobatmat, 1, max))
probatmat <- probatmat / rowSums(probatmat)
return(probatmat)
}

# 3. Run the general GOF test
test_res <- GOFClustering(probabpost = results@partitions@tik,
                          rprobapost = my_rprobapost,
                          p=3,
                          B=3)

# Print results
print(test_res$pvalues)

```

GOFClusteringSpe

Specific Goodness-of-Fit Test for Clustering Objects

Description

Performs the goodness-of-fit test for a clustering result provided by VarSelLCM or mixtools. This function implements the block-splitting Empirical Likelihood test on the posterior probabilities.

Usage

```
GOFClusteringSpe(results, size, p, B, alpha = 0.05, basis = "Bernstein")
```

Arguments

results	An object of class VSLCMresults (from VarSelLCM) or npEM/spEMsymloc (from mixtools).
size	Integer. Size of the sub-sample for the block-splitting procedure.
p	Integer. Number of moment conditions (equations).
B	Integer. Number of blocks for the testing procedure.
alpha	Numeric. Significance level (default is 0.05).
basis	Character or vector of characters. The basis used for the moment conditions ("Bernstein", "indicatorEqualproba", or "indicatorEqualsize").

Details

This function computes the test statistics by splitting the data into B blocks to account for parameter estimation uncertainty. The moment conditions are projected using Principal Component Analysis (PCA) to handle potential multicollinearity, especially when p is large.

Value

A list with the following components:

stat A list of the 5 test statistics: max (Maximum of block EL statistics), sum (Sum of block EL statistics), ks (Kolmogorov-Smirnov), cvm (Cramer-von Mises), and ad (Anderson-Darling).

pvalues A list of p-values associated with the statistics (except for max which uses a specific critical value).

reject A list of logical indicators. TRUE if the null hypothesis (model adequacy) is rejected at level alpha.

cvpsi The estimated covariance matrix Σ of the moment conditions. Its dimension may be smaller than p due to the PCA filtering.

basis The name of the basis functions used.

hyperparam A list containing the number of moment conditions (p) and the number of blocks (B).

References

El Kolei, S. and Marbac, M. (2025). Goodness-of-fit testing of the distribution of posterior classification probabilities for validating model-based clustering. <doi:10.48550/arXiv.2511.04206>.

Examples

```
# Simulation of Gaussian Mixture Data (K=2, d=5)
set.seed(123)
n <- 180
z <- sample(1:2, n, replace = TRUE, prob = c(1/2,1/2))
ech <- matrix(0, nrow = n, ncol = 5)
for(k in 1:2) ech[z==k,] <- matrix(rnorm(sum(z==k) * 5, ((-1)**k)/sqrt(5), 1), ncol=5)

# --- Case 1: Parametric clustering with VarSelLCM ---
library(VarSelLCM)
res_param <- VarSelCluster(ech, 2, vbleSelec = FALSE)
gof_param <- GOFClusteringSpe(res_param, size=500, p=3, B=3)
print(gof_param$pvalues)
print(dim(gof_param$cvpsi)) # Sigma matrix dimension

# --- Case 2: Non-parametric clustering with mixtools ---
library(mixtools)
res_nonparam <- npMSL(ech, mu0 = 2, verb = FALSE)
gof_nonparam <- GOFClusteringSpe(res_nonparam, size=500, p=3, B=3)
print(gof_nonparam$pvalues)
```

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