Package ‘clustMD’

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**Title**  Model Based Clustering for Mixed Data

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**Author**  Damien McParland [aut, cre], Isobel Claire Gormley [aut]

**Maintainer**  Damien McParland <damien.mcparland@ucd.ie>

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**Description**

Model-based clustering of mixed data (i.e. data that consist of continuous, binary, ordinal or nominal variables) using a parsimonious mixture of latent Gaussian variable models.

**Author(s)**

Damien McParland

Damien McParland <damien.mcparland@ucd.ie> Isobel Claire Gormley <claire.gormley@ucd.ie>

**References**


**See Also**

clustMD

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**Byar**

*Byar prostate cancer data set.*

**Description**

A data set consisting of variables of mixed type measured on a group of prostate cancer patients. Patients have either stage 3 or stage 4 prostate cancer.

**Usage**

Byar

**Format**

A data frame with 475 observations on the following 15 variables.

- **Age** a numeric vector indicating the age of the patient.
- **Weight** a numeric vector indicating the weight of the patient.
- **Performance.rating** an ordinal variable indicating how active the patient is: 0 - normal activity, 1 - in bed less than 50% of daytime, 2 - in bed more than 50% of daytime, 3 - confined to bed.
- **Cardiovascular.disease.history** a binary variable indicating if the patient has a history of cardiovascular disease: 0 - no, 1 - yes.
Systolic.blood.pressure a numeric vector indicating the systolic blood pressure of the patient in units of ten.

Diastolic.blood.pressure a numeric vector indicating the diastolic blood pressure of the patient in units of ten.

Electrocardiogram.code a nominal variable indicating the electrocardiogram code: 0 - normal, 1 - benign, 2 - rythmic disturbances and electrolyte changes, 3 - heart blocks or conduction defects, 4 - heart strain, 5 - old myocardial infarct, 6 - recent myocardial infarct.

Serum.haemoglobin a numeric vector indicating the serum haemoglobin levels of the patient measured in g/100ml.

Size.of.primary.tumour a numeric vector indicating the estimated size of the patient’s primary tumour in centimeters squared.

Index.of.tumour.stage.and.histologic.grade a numeric vector indicating the combined index of tumour stage and histologic grade of the patient.

Serum.prostatic.acid.phosphatase a numeric vector indicating the serum prostatic acid phosphatase levels of the patient in King-Armstrong units.

Bone.metastases a binary vector indicating the presence of bone metastasis: 0 - no, 1 - yes.

Stage the stage of the patient’s prostate cancer.

Observation a patient ID number.

SurvStat the post trial survival status of the patient: 0 - alive, 1 - dead from prostatic cancer, 2 - dead from heart or vascular disease, 3 - dead from cerebrovascular accident, 3 - dead from pulmonary embolus, 5 - dead from other cancer, 6 - dead from respiratory disease, 7 - dead from other specific non-cancer cause, 8 - dead from other unspecified non-cancer cause, 9 - dead from unknown cause.

Source


---

**clustMD**

*Model Based Clustering for Mixed Data*

**Description**

A function that fits the clustMD model to a data set consisting of any combination of continuous, binary, ordinal and nominal variables.

**Usage**

```r
clustMD(X, G, CnsIndx, OrdIndx, Nnorms, MaxIter, model, store.params = FALSE, scale = FALSE, startCL = "hc_mclust", autoStop = FALSE, ma.band = 50, stop.tol = NA)
```
Arguments

- **X**: a data matrix where the variables are ordered so that the continuous variables come first, the binary (coded 1 and 2) and ordinal variables (coded 1, 2, ...) come second and the nominal variables (coded 1, 2, ...) are in last position.

- **G**: the number of mixture components to be fitted.

- **CnsIndx**: the number of continuous variables in the data set.

- **OrdIndx**: the sum of the number of continuous, binary and ordinal variables in the data set.

- **Nnorms**: the number of Monte Carlo samples to be used for the intractable E-step in the presence of nominal data. Irrelevant if there are no nominal variables.

- **MaxIter**: the maximum number of iterations for which the (MC)EM algorithm should run.

- **model**: a string indicating which clustMD model is to be fitted. This may be one of: EII, VII, EEI, VEI, EVI, VVI or B0.

- **store.params**: a logical argument indicating if the parameter estimates at each iteration should be saved and returned by the clustMD function.

- **scale**: a logical argument indicating if the continuous variables should be standardised.

- **startCL**: a string indicating which clustering method should be used to initialise the (MC)EM algorithm. This may be one of "kmeans" (K means clustering), "hclust" (hierarchical clustering), "mclust" (finite mixture of Gaussian distributions), "hc_mclust" (model-based hierarchical clustering) or "random" (random cluster allocation).

- **autoStop**: a logical argument indicating whether the (MC)EM algorithm should use a stopping criterion to decide if convergence has been reached. Otherwise the algorithm will run for MaxIter iterations. If only continuous variables are present the algorithm will use Aitken’s acceleration criterion with tolerance stop.tol. If categorical variables are present, the stopping criterion is based on a moving average of the approximated log likelihood values. Let \( t \) denote the current iteration. The average of the \( ma.band \) most recent approximated log likelihood values is compared to the average of another \( ma.band \) iterations with a lag of 10 iterations. If this difference is less than the tolerance the algorithm will be said to have converged.

- **ma.band**: the number of iterations to be included in the moving average calculation for the stopping criterion.

- **stop.tol**: the tolerance of the (MC)EM stopping criterion.

Value

An object of class clustMD is returned. The output components are as follows:

- **model**: The covariance model fitted to the data.

- **G**: The number of clusters fitted to the data.

- **Y**: The observed data matrix.

- **cl**: The cluster to which each observation belongs.
tau
A N x G matrix of the probabilities of each observation belonging to each cluster.

means
A D x G matrix of the cluster means. Where D is the dimension of the combined observed and latent continuous space.

A
A G x D matrix containing the diagonal entries of the A matrix corresponding to each cluster.

Lambda
A G x D matrix of volume parameters corresponding to each observed or latent dimension for each cluster.

Sigma
A D x D x G array of the covariance matrices for each cluster.

BIChat
The estimated Bayesian information criterion for the model fitted.

ICLhat
The estimated integrated classification likelihood criterion for the model fitted.

paramlist
If store.params is TRUE then paramlist is a list of the stored parameter values in the order given above with the saved estimated likelihood values in last position.

Varnames
A character vector of names corresponding to the columns of Y

Varnames_sht
A truncated version of Varnames. Used for plotting.

likelihood.store
A vector containing the estimated log likelihood at each iteration.

References

Examples

data(Byar)
  # Transformation skewed variables
  Byar$Size.of.primary.tumour <- sqrt(Byar$Size.of.primary.tumour)
  Byar$Serum.prostatic.acid.phosphatase <- log(Byar$Serum.prostatic.acid.phosphatase)

  # Order variables (Continuous, ordinal, nominal)
  Y <- as.matrix(Byar[, c(1, 2, 5, 6, 8, 9, 10, 11, 3, 4, 12, 7)])

  # Start categorical variables at 1 rather than 0

  # Standardise continuous variables
  Y[, 1:8] <- scale(Y[, 1:8])

  # Merge categories of EKG variable for efficiency
  Yekg <- rep(NA, nrow(Y))
  Yekg[Y[,12]==1] <- 1
  Yekg[(Y[,12]==2) & (Y[,12]==3) & (Y[,12]==4)] <- 2
  Yekg[(Y[,12]==5) & (Y[,12]==6) & (Y[,12]==7)] <- 3
  Y[, 12] <- Yekg

  ## Not run:
  res <- clustMD(X = Y, G = 3, CnsIndx = 8, OrdIndx = 11, Nnorms = 20000,
                  MaxIter = 500, model = "EV1", store.params = FALSE, scale = TRUE,
Description

A function that fits the clustMD model to a data set consisting of any combination of continuous, binary, ordinal and nominal variables. This function is a wrapper for clustMD that takes arguments as a list.

Usage

clustMDlist(arglist)

Arguments

arglist a list of input arguments for clustMD. See clustMD.

Value

A clustMD object. See clustMD.

References


See Also

clustMD

Examples

data(Byar)

# Transformation skewed variables
Byar$Size.of.primary.tumour <- sqrt(Byar$Size.of.primary.tumour)
Byar$Serum.prostatic.acid.phosphatase <-
log(Byar$Serum.prostatic.acid.phosphatase)

# Order variables (Continuous, ordinal, nominal)
Y <- as.matrix(Byar[, c(1, 2, 5, 6, 8, 9, 10, 11, 3, 4, 12, 7)])

# Start categorical variables at 1 rather than 0
\# Standardise continuous variables
Y[, 1:8] <- scale(Y[, 1:8])

\# Merge categories of EKG variable for efficiency
Yekg <- rep(NA, nrow(Y))
Yekg[Y[, 12]==1] <- 1
Yekg[(Y[, 12]==2)|(Y[, 12]==3)] <- 2
Yekg[(Y[, 12]==5)|(Y[, 12]==6)] <- 3
Y[, 12] <- Yekg

argList <- list(x=Y, G=3, CnsIndx=8, OrdIndx=11, Nnorms=20000,
MaxIter=500, model="EVI", store.params=FALSE, scale=TRUE,
startCL="kmeans", autoStop=FALSE, ma.band=50, stop.tol=NA)

## Not run:
res <- clustMDlist(argList)

## End(Not run)

---

### clustMDparallel

**Run multiple clustMD models in parallel**

#### Description

This function allows the user to run multiple clustMD models in parallel. The inputs are similar to `clustMD()` except `G` is now a vector containing the numbers of components the user would like to fit and `models` is a vector of strings indicating the covariance models the user would like to fit for each element of `G`. The user can specify the number of cores to be used or let the function detect the number available.

#### Usage

\[
\text{clustMDparallel}(x, \text{CnsIndx}, \text{OrdIndx}, G, \text{models}, \text{Nnorms}, \text{MaxIter}, \text{store.params}, \\
\text{scale}, \text{startCL} = \text{"hc_mclust"}, \text{Ncores = NULL, autoStop = FALSE}, \\
\text{ma.band = 50, stop.tol = NA})
\]

#### Arguments

- **X**: a data matrix where the variables are ordered so that the continuous variables come first, the binary (coded 1 and 2) and ordinal variables (coded 1, 2, ...) come second and the nominal variables (coded 1, 2, ...) are in last position.
- **CnsIndx**: the number of continuous variables in the data set.
- **OrdIndx**: the sum of the number of continuous, binary and ordinal variables in the data set.
- **G**: a vector containing the numbers of mixture components to be fitted.
- **models**: a vector of strings indicating which clustMD models are to be fitted. This may be one of: EII, VII, EEI, VEI, EVI, VVI or BD.
Nnorms  
the number of Monte Carlo samples to be used for the intractable E-step in the presence of nominal data.

MaxIter  
the maximum number of iterations for which the (MC)EM algorithm should run.

store.params  
a logical variable indicating if the parameter estimates at each iteration should be saved and returned by the clustMD function.

scale  
a logical variable indicating if the continuous variables should be standardised.

startCL  
a string indicating which clustering method should be used to initialise the (MC)EM algorithm. This may be one of "kmeans" (K means clustering), "hclust" (hierarchical clustering), "mclust" (finite mixture of Gaussian distributions), "hc_mclust" (model-based hierarchical clustering) or "random" (random cluster allocation).

Ncores  
the number of cores the user would like to use. Must be less than or equal to the number of cores available.

autoStop  
a logical argument indicating whether the (MC)EM algorithm should use a stopping criterion to decide if convergence has been reached. Otherwise the algorithm will run for MaxIter iterations.

If only continuous variables are present the algorithm will use Aitken’s acceleration criterion with tolerance stop.tol.

If categorical variables are present, the stopping criterion is based on a moving average of the approximated log likelihood values. let $StS$ denote the current iteration. The average of the $ma.band$ most recent approximated log likelihood values is compared to the average of another $ma.band$ iterations with a lag of 10 iterations. If this difference is less than the tolerance the algorithm will be said to have converged.

$ma.band$  
the number of iterations to be included in the moving average stopping criterion.

stop.tol  
the tolerance of the (MC)EM stopping criterion.

Value

An object of class clustMDparallel is returned. The output components are as follows:

BICarray  
A matrix indicating the estimated BIC values for each of the models fitted.

results  
A list containing the output for each of the models fitted. Each entry of this list is a clustMD object. If the algorithm failed to fit a particular model, the corresponding entry of results will be NULL.

References


See Also

clustMD
Examples

```r
data(Byar)

# Transformation skewed variables
Byar$Size.of.primary.tumour <- sqrt(Byar$Size.of.primary.tumour)
Byar$Serum.prostatic.acid.phosphatase <- log(Byar$Serum.prostatic.acid.phosphatase)

# Order variables (Continuous, ordinal, nominal)
Y <- as.matrix(Byar[, c(1, 2, 5, 6, 8, 9, 10, 11, 3, 4, 12, 7)])

# Start categorical variables at 1 rather than 0

# Standardise continuous variables
Y[, 1:8] <- scale(Y[, 1:8])

# Merge categories of EKG variable for efficiency
Yekg <- rep(NA, nrow(Y))
Yekg[Y[,12]==1] <- 1
Yekg[(Y[,12]==2) | (Y[,12]==3) | (Y[,12]==4)] <- 2
Yekg[(Y[,12]==5) | (Y[,12]==6)] <- 3
Y[, 12] <- Yekg

## Not run:
res <- clustMDparallel(X = Y, G = 1:3, CnsIndx = 8, OrdIndx = 11, Nnorms = 20000,
MaxIter = 500, models = c("EVI", "EII", "VII"), store.params = FALSE, scale = TRUE,
startCL = "kmeans", autoStop= TRUE, ma.band=30, stop.tol=0.0001)
res$BICarray

## End(Not run)
```

---

**getDescription_clustMDparallel**

*Extracts relevant output from clustMDparallel object*

**Description**

This function takes a clustMDparallel object, a number of clusters and a covariance model as inputs. It then returns the output corresponding to that model. If the particular model is not contained in the clustMDparallel object then the function returns an error.

**Usage**

```r
getOutput_clustMDparallel(resParallel, nClus, covModel)
```
Arguments

- `resParallel` a `clustMDparallel` object.
- `nclus` the number of clusters in the desired output.
- `covModel` the covariance model of the desired output.

Value

A `clustMD` object containing the output for the relevant model.

Description

Plots a parallel coordinates plot and dot plot of the estimated cluster means, a barplot of the variances by cluster for diagonal covariance models or a heatmap of the covariance matrix for non-diagonal covariance structures, and a histogram of the clustering uncertainties for each observation.

Usage

```r
## S3 method for class 'clustMD'
plot(x, ...)
```

Arguments

- `x` a `clustMD` object.
- `...` further arguments passed to or from other methods.

Value

Prints graphical summaries of the fitted model as detailed above.

References


See Also

`clustMD`
**plot.clustMDparallel**

*Summary plots for a clustMDparallel object*

**Description**

Produces a line plot of the estimated BIC values corresponding to each covariance model against the number of clusters fitted. For the optimal model according to this criteria, a parallel coordinates plot of the cluster means is produced along with a barchart or heatmap of the covariance matrices for each cluster and a histogram of the clustering uncertainties.

**Usage**

```r
## S3 method for class 'clustMDparallel'
plot(x, ...)
```

**Arguments**

- `x` a `clustMDparallel` object.
- `...` further arguments passed to or from other methods.

**Value**

Produces a number of plots as detailed above.

---

**print.clustMD**

*Print basic details of clustMD object.*

**Description**

Prints a short summary of a `clustMD` object to screen. Details the number of clusters fitted as well as the covariance model and the estimated BIC.

**Usage**

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

**Arguments**

- `x` a `clustMD` object.
- `...` further arguments passed to or from other methods.

**Value**

Prints summary details, as described above, to screen.
See Also

clustMD

print.clustMDparallel  *Print basic details of clustMDparallel object*

Description

Prints basic details of clustMDparallel object. Outputs the different numbers of clusters and the different covariance structures fitted to the data. It also states which model was optimal according to the estimated BIC criterion.

Usage

### S3 method for class 'clustMDparallel'

```r
print(x, ...)
```

Arguments

- `x`  a clustMDparallel object.
- `...`  further arguments passed to or from other methods.

Value

Prints details described above to screen.

See Also

clustMD

summary.clustMD  *Summarise clustMD object*

Description

Prints a summary of a clustMD object to screen. Details the number of clusters fitted as well as the covariance model and the estimated BIC. Also prints a table detailing the number of observations in each cluster and a matrix of the cluster means.

Usage

### S3 method for class 'clustMD'

```r
summary(object, ...)
```
Arguments

object  a clustMD object.
... further arguments passed to or from other methods.

Value

Prints summary of clustMD object to screen, as detailed above.

See Also

clustMD

summary.clustMDparallel

Prints a summary of a clustMDparallel object to screen.

Description

Prints the different numbers of clusters and covariance models fitted and indicates the optimal model according to the estimated BIC criterion. The estimated BIC for the optimal model is printed to screen along with a table of the cluster membership and the matrix of cluster means for this optimal model.

Usage

# S3 method for class 'clustMDparallel'
summary(object, ...)

Arguments

object  a clustMDparallel object.
... further arguments passed to or from other methods.

Value

Prints a summary of the clustMDparallel object to screen, as detailed above.

See Also

clustMD
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