

# Package ‘pmclust’

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**Title** Parallel Model-Based Clustering

**Depends** R (>= 3.0.0), methods, rlecuyer, pbdMPI (>= 0.2-2), MASS

**Enhances** MixSim, pbdSLAP (>= 0.1-7), pbdBASE (>= 0.3-0), pbdDMAT (>= 0.2-4)

**LazyLoad** yes

**LazyData** yes

**Description** The pmclust aims to utilize model-based clustering (unsupervised) for high dimensional and ultra large data, especially in a distributed manner. The package employs Rmpi to perform a expectation-gathering-maximization (EGM) algorithm for finite mixture Gaussian models. The unstructured dispersion matrices are assumed in the Gaussian models. The implementation is default in the single program multiple data (SPMD) programming model. The code can be executed through Rmpi and independent to most MPI applications. See the High Performance Statistical Computing (HPSC) website for more information, documents and examples.

**License** GPL (>= 2)

**URL** <http://r-pbd.org/>

**BugReports** <http://group.r-pbd.org/>

**MailingList** Please send questions and comments regarding pbdR to RBigData@gmail.com

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pmclust-package	<i>Parallel Model-Based Clustering</i>
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## Description

The pmclust aims to utilize model-based clustering (unsupervised) for high dimensional and ultra large data, especially in a distributed manner. The package employs pbdMPI to perform a parallel version of expectation and maximization (EM) algorithm for finite mixture Gaussian models. The unstructured dispersion matrices are assumed in the Gaussian models. The implementation is default in the single program multiple data (SPMD) programming model. The code can be executed through pbdMPI and independent to most MPI applications. See the High Performance Statistical Computing (HPSC) website for more information, documents and examples.

## Details

Package:	pmclust
Type:	Package
License:	GPL
LazyLoad:	yes

The main function is `pmclust` implementing the parallel EM algorithm for mixture multivariate Gaussian models with unstructured dispersions. This function groups a data matrix `X.gbd` or `X.spmd` into K clusters where `X.gbd` or `X.spmd` is potentially huge and taken from the global environment `.GlobalEnv` or `.pmclustEnv`.

Other main functions `em.step`, `aecm.step`, `apecm.step`, and `apecma.step` may provide better performance than the `em.step` in terms of computing time and convergent iterations.

`kmeans.step` provides the fastest clustering among above algorithms, but it is restricted by Euclidean distance and spherical dispersions.

### Author(s)

Wei-Chen Chen <wccsnow@gmail.com> and George Ostrouchov

### References

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

Chen, W.-C. and Maitra, R. (2011) "Model-based clustering of regression time series data via APECM – an AECM algorithm sung to an even faster beat", *Statistical Analysis and Data Mining*, **4**, 567-578.

Chen, W.-C., Ostrouchov, G., Pugmire, D., Prabhat, M., and Wehner, M. (2013) "A Parallel EM Algorithm for Model-Based Clustering with Application to Explore Large Spatio-Temporal Data", *Technometrics*, (revision).

Dempster, A.P., Laird, N.M. and Rubin, D.B. (1977) "Maximum Likelihood from Incomplete Data via the EM Algorithm", *Journal of the Royal Statistical Society Series B*, **39**, 1-38.

Lloyd, S. P. (1982) "Least squares quantization in PCM", *IEEE Transactions on Information Theory*, **28**, 129-137.

Meng, X.-L. and Van Dyk, D. (1997) "The EM Algorithm – an Old Folk-song Sung to a Fast New Tune", *Journal of the Royal Statistical Society Series B*, **59**, 511-567.

### See Also

`em.step`, `aecm.step`, `apecm.step`,  
`apecma.step`, `kmeans.step`.  
`em.step.dmat`, `kmeans.step.dmat`.

### Examples

```
## Not run:
### Under command mode, run the demo with 2 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 2 Rscript -e 'demo(gbd_em,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(gbd_aecm,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(gbd_apecm,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(gbd_apecma,"pmclust",ask=F,echo=F)'
```

```

mpiexec -np 2 Rscript -e 'demo(gbd_kmeans,"pmclust",ask=F,echo=F)'

mpiexec -np 2 Rscript -e 'demo(ex_em,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(ex_aecm,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(ex_apecm,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(ex_apecma,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(ex_kmeans,"pmclust",ask=F,echo=F)'

mpiexec -np 2 Rscript -e 'demo(dmat_em,"pmclust",ask=F,echo=F)'
mpiexec -np 2 Rscript -e 'demo(dmat_kmeans,"pmclust",ask=F,echo=F)'

## End(Not run)

```

---

as functions

*Convert between X.gbd (X.spmd) and X.dmat*


---

## Description

This function will convert a matrix of format from GBD row-major to ddmatrix vice versa.

## Usage

```

as.dmat(X.spmd, bldim = pbdDMAT::.BLDIM, ICTXT = pbdDMAT::.ICTXT,
        comm = .SPMD.CT$comm)

as.gbd(X.dmat, comm = .SPMD.CT$comm)
as.spmd(X.dmat, comm = .SPMD.CT$comm)

```

## Arguments

X.spmd	an input dataset of format GBD/SPMD row-major to be converted.
X.dmat	an input dataset of format ddmatrix to be converted.
bldim	block dimension, see <b>pbdBASE</b> and <b>pbdDMAT</b> for details.
ICTXT	block context, see <b>pbdBASE</b> and <b>pbdDMAT</b> for details.
comm	communicator, see <b>pbdMPI</b> for details.

## Details

This function will provide a quick conversion to the input data X.spmd which is a default dataset to be clustered in **pmclust**. Usually, this matrix is distributed in GBD row-major format. For fully utilizing **pbdBASE** and **pbdDMAT**, it need to be converted to ddmatrix format.

## Value

A ddmatrix is returned.

**Author(s)**

Wei-Chen Chen <wccsnow@gmail.com> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[kmeans.step.dmat.](#)

**Examples**

```
## Not run:  
# Examples can be found in the help pages of  
# kmeans.step.dmat().  
  
## End(Not run)
```

---

assign.N.sample

*Obtain a Set of Random Samples for X.spmd*

---

**Description**

This utility function samples data randomly from [X.spmd](#) to form a relatively small subset of original data. The EM algorithm on the smaller subset is typically performing fast and capturing rough structures of entire dataset.

**Usage**

```
assign.N.sample(total.sample = 5000, N.org.spmd)
```

**Arguments**

`total.sample` a total number of samples which will be selected from the original data [X.spmd](#).  
`N.org.spmd` the original data size, i.e. `nrow(X.spmd)`.

**Details**

This utility function performs simple random sampling without replacement for the original dataset [X.spmd](#). Different random seeds should be set before calling this function.

**Value**

A list variable will be returned and containing:

N	total sample size across all $S$ processors
N.spmd	sample size of given processor
N.allspmds	a collection of sample sizes for all $S$ processors
ID.spmd	index of selected samples ranged from 1 to N.org.spmd

Note that N and N.allspmds are the same across all  $S$  processors, but N.spmd and ID.spmd are most likely all distinct. The lengths of these elements are 1 for N and N.spmd,  $S$  for N.allspmd, and N.spmd for ID.spmd.

### Author(s)

Wei-Chen Chen <wccsnow@gmail.com> and George Ostrouchov.

### References

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

### See Also

[set.global](#)

### Examples

```
## Not run:
# Save code in a file "demo.r" and run in 4 processors by
# > mpiexec -np 4 Rscript demo.r

### Setup environment.
library(pmclust, quiet = TRUE)
comm.set.seed(123)

### Generate an example data.
N.org.spmd <- 5000 + sample(1:1000, 1)
ret.spmd <- assign.N.sample(total.sample = 5000, N.org.spmd)
cat("Rank:", comm.rank(), " Size:", ret.spmd$N.spmd,
    "\n", sep = "")

### Quit.
finalize()

## End(Not run)
```

## Description

The EM-like algorithm for model-based clustering of finite mixture Gaussian models with unstructured dispersions.

\*.dmat's are `ddmatrix` versions.

## Usage

```
em.step(PARAM.org)
aecm.step(PARAM.org)
apecm.step(PARAM.org)
apecma.step(PARAM.org)
kmeans.step(PARAM.org)

em.step.dmat(PARAM.org)
kmeans.step.dmat(PARAM.org)
```

## Arguments

PARAM.org      an original set of parameters generated by `set.global`.

## Details

A global variable called `X.spmd` should exist in the `.pmclustEnv` environment, usually the working environment. The `X.spmd` is the data matrix to be clustered, and this matrix has a dimension `N.spmd` by `p`.

A `PARAM.org` will be a local variable inside all EM-like functions `em.step`, `aecm.step`, `apecm.step`, `apecma.step`, and `kmeans.step`. This variable is a list containing all parameters related to models. This function also updates in the parameters by the EM-like algorithms, and return the convergent results. The details of list elements are initially generated by `set.global`.

## Value

A convergent results will be returned the other list variable containing all new parameters which represent the components of models. See the help page of `PARAM` or `PARAM.org` for details.

## Author(s)

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

## References

- High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>
- Programming with Big Data in R Website: <http://r-pbd.org/>
- Chen, W.-C. and Maitra, R. (2011) “Model-based clustering of regression time series data via APECM – an AECM algorithm sung to an even faster beat”, *Statistical Analysis and Data Mining*, **4**, 567-578.
- Chen, W.-C., Ostrouchov, G., Pugmire, D., Prabhat, M., and Wehner, M. (2013) “A Parallel EM Algorithm for Model-Based Clustering with Application to Explore Large Spatio-Temporal Data”, *Technometrics*, (revision).
- Dempster, A.P., Laird, N.M. and Rubin, D.B. (1977) “Maximum Likelihood from Incomplete Data via the EM Algorithm”, *Journal of the Royal Statistical Society Series B*, **39**, 1-38.
- Lloyd, S. P. (1982) “Least squares quantization in PCM”, *IEEE Transactions on Information Theory*, **28**, 129-137.
- Meng, X.-L. and Van Dyk, D. (1997) “The EM Algorithm.an Old Folk-song Sung to a Fast New Tune”, *Journal of the Royal Statistical Society Series B*, **59**, 511-567.

## See Also

[set.global](#), [mb.print](#), [set.global.dmat](#).

## Examples

```
## Not run:
# Save code in a file "demo.r" and run in 4 processors by
# > mpiexec -np 4 Rscript demo.r

### Setup environment.
library(pmclust, quiet = TRUE)
comm.set.seed(123)

### Generate an example data.
N.allspmds <- rep(5000, comm.size())
N.spmd <- 5000
N.K.spmd <- c(2000, 3000)
N <- 5000 * comm.size()
p <- 2
K <- 2
data.spmd <- generate.basic(N.allspmds, N.spmd, N.K.spmd, N, p, K)
X.spmd <- data.spmd$X.spmd

### Run clustering.
PARAM.org <- set.global(K = K)           # Set global storages.
# PARAM.org <- initial.em(PARAM.org)     # One initial.
PARAM.org <- initial.RndEM(PARAM.org)    # Ten initials by default.
PARAM.new <- apecma.step(PARAM.org)      # Run APECMa.
em.update.class()                        # Get classification.

### Get results.
```



```

N.CLASS <- get.N.CLASS(K)
comm.cat("# of class:", N.CLASS, "\n")

### Quit.
finalize()

## End(Not run)

```

---

generate.basic

*Generate Examples for Testing*


---

## Description

This function will generate a small set of data for testing algorithms.

## Usage

```
generate.basic(N.allspmds, N.spmd, N.K.spmd, N, p, K)
```

## Arguments

N.allspmds	a collection of sample sizes for all $S$ processors, i.e. a vector of length $S$ .
N.spmd	total sample size of given processor.
N.K.spmd	sample size of each clusters given processor, i.e. sum over N.K.spmd is N.spmd, a vector of length $K$ .
N	total sample size across all $S$ processors, i.e. sum over N.spmd is N.
p	dimension of data <code>X.spmd</code> , i.e. <code>ncol(X.spmd)</code> .
K	number of clusters.

## Details

For all  $S$  processors, this function will generate in total  $N$  observations from  $K$  clusters in  $p$  dimensions.

The clusters centers and dispersions are generated automatically inside the code. Currently, it is not allowed for users to change, but it is not difficult to specify them by mimicking this code.

## Value

A set of simulated data and information will be returned in a list variable including:

K	number of clusters, as the input
p	dimension of data <code>X.spmd</code> , as the input
N	total sample size, as the input
N.allspmds	a collection of sample sizes for all $S$ processors, as the input
N.spmd	total sample size of given processor, as the input
N.K.spmd	sample size of each clusters given processor, as the input
<code>X.spmd</code>	generated data set with dimension with dimension $N.spmd * p$
<code>CLASS.spmd</code>	true id of each data, a vector of length $N.spmd$ and has values from 1 to K
<code>N.CLASS.spmd</code>	true sample size of each clusters, a vector of length K

**Author(s)**

Wei-Chen Chen <wccsnow@gmail.com> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[generate.MixSim](#).

**Examples**

```
## Not run:
# Examples can be found in the help pages of em.step(),
# aecm.step(), apecm.step(), and apecma.step().

## End(Not run)
```

---

generate.MixSim

*Generate MixSim Examples for Testing*

---

**Description**

This function utilizes **MixSim** to generate sets of data for testing algorithms.

**Usage**

```
generate.MixSim(N, p, K, MixSim.obj = NULL, MaxOmega = NULL,
                BarOmega = NULL, PiLow = 1.0, sph = FALSE, hom = FALSE)
```

**Arguments**

N	total sample size across all $S$ processors, i.e. sum over $N$ . <code>spmd</code> is $N$ .
p	dimension of data $X$ . <code>spmd</code> , i.e. <code>ncol(X.spmd)</code> .
K	number of clusters.
MixSim.obj	an object returned from <a href="#">MixSim</a> .
MaxOmega	maximum overlap as in <a href="#">MixSim</a> .
BarOmega	averaged overlap as in <a href="#">MixSim</a> .
PiLow	lower bound of mixture proportion as in <a href="#">MixSim</a> .
sph	sph as in <a href="#">MixSim</a> .
hom	hom as in <a href="#">MixSim</a> .

**Details**

If `MixSim.obj` is `NULL`, then `BarOmega` and `MaxOmega` will be used in `MixSim` to obtain a new `MixSim.obj`.

**Value**

A set of simulated data and information will be returned in a list variable including:

<code>K</code>	number of clusters, as the input
<code>p</code>	dimension of data <code>X.spmd</code> , as the input
<code>N</code>	total sample size, as the input
<code>N.allspmds</code>	a collection of sample sizes for all $S$ processors, as the input
<code>N.spmd</code>	total sample size of given processor, as the input
<code>X.spmd</code>	generated data set with dimension with dimension <code>N.spmd * p</code>
<code>CLASS.spmd</code>	true id of each data, a vector of length <code>N.spmd</code> and has values from 1 to <code>K</code>
<code>N.CLASS.spmd</code>	true sample size of each clusters, a vector of length <code>K</code>
<code>MixSim.obj</code>	the true model where data <code>X.spmd</code> generated from

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

**References**

Melnykov, V., Chen, W.-C. and Maitra, R. (2012) "MixSim: Simulating Data to Study Performance of Clustering Algorithms", *Journal of Statistical Software*, (accepted).

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[generate.basic.](#)

**Examples**

```
## Not run:
# Save code in a file "demo.r" and run in 4 processors by
# > mpiexec -np 4 Rscript demo.r

### Setup environment.
library(pmclust, quiet = TRUE)

### Generate an example data.
N <- 5000
p <- 2
K <- 2
data.spmd <- generate.MixSim(N, p, K, BarOmega = 0.01)
X.spmd <- data.spmd$X.spmd
```

```

### Run clustering.
PARAM.org <- set.global(K = K)           # Set global storages.
# PARAM.org <- initial.em(PARAM.org)     # One initial.
PARAM.org <- initial.RndEM(PARAM.org)    # Ten initials by default.
PARAM.new <- apecma.step(PARAM.org)      # Run APECMA.
em.update.class()                        # Get classification.

### Get results.
N.CLASS <- get.N.CLASS(K)
comm.cat("# of class:", N.CLASS, "\n")
comm.cat("# of class (true):", data.spmid$N.CLASS.spmid, "\n")

### Quit.
finalize()

## End(Not run)

```

---

get.N.CLASS

*Obtain Total Elements for Every Clusters*


---

## Description

This function will collect the total elements for every clusters from all processors that the all reduced calls with the sum operation will be performed.

get.N.CLASS.dmat is a ddmatrix version of get.N.CLASS.

The get.CLASS returns class ids.

## Usage

```
get.N.CLASS(K)
```

```
get.N.CLASS.dmat(K)
```

```
get.CLASS(PARAM)
```

## Arguments

K	the total number of clusters.
PARAM	a set of parameters.

## Details

The final results are distributed in all processors including the total elements for each cluster. The global variable `CLASS.spmid` stores the identification for each observation on each processors. This function will first summary `CLASS.spmid` in K categories, then use the all reduce function with the sum operation to add the numbers by clusters. The `COMM.RANK 0` will be used to take care the printing.

**Value**

K numbers will be returned that are the total elements for each cluster. Sum of these K numbers should be equal to N the total number of observations.

**Author(s)**

Wei-Chen Chen <wccsnow@gmail.com> and George Ostrouchov.

**References**

Programming with Big Data in R Website: <http://r-pbd.org/>

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

**See Also**

[em.step](#), [aecm.step](#), [apecm.step](#),  
[apecma.step](#), [kmeans.step](#),  
[kmeans.step.dmat](#).

**Examples**

```
## Not run:  
# Examples can be found in the help pages of em.step(),  
# aecm.step(), apecm.step(), apecma.step(), and kmeans.step().  
  
# Examples for ddmatrix version can be found in the help pages of  
# kmeans.step.dmat().  
  
## End(Not run)
```

---

Independent logL

*Independent Function for Log Likelihood*

---

**Description**

This function is for debugging only and for checking if the observed data log likelihood is consistent for each EM iteration.

`indep.logL.dmat` is a `ddmatrix` version of `indep.logL`.

**Usage**

```
indep.logL(PARAM)
```

```
indep.logL.dmat(PARAM)
```

**Arguments**

PARAM            a set of parameters.

**Details**

This function will provide an observed data log likelihood based on the current parameter `PARAM`. This function will take in information from `global`, but no global variables will be updated by this function.

This function also don't take care the numerical issues, so the return value may be inaccurate sometimes.

**Value**

An observed data log likelihood will be returned. This value can quickly compare with the log likelihood computed inside `em.onestep`. Small difference is allowed, but large difference indicates bugs of code or illness of data.

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[set.global](#), [em.onestep](#).

**Examples**

```
## Not run:  
# This is a core function for em.estep()  
# see the source code for details.  
# Reset .pmclustEnv$CONTROL$debug to turn on this function  
# automatically for each EM iteration.  
  
## End(Not run)
```

---

 Initialization      *Initialization for EM-like Algorithms*


---

**Description**

These functions implement initialization of EM-like algorithms for model-based clustering based on `X.spmd`, and initialization of K-means algorithm by randomly picking samples from data based on `X.spmd`.

\*.dmat's are `ddmatrix` versions.

**Usage**

```
initial.RndEM(PARAM)
initial.em(PARAM, MU = NULL)
initial.center(PARAM, MU = NULL)

initial.RndEM.dmat(PARAM)
initial.em.dmat(PARAM, MU = NULL)
initial.center.dmat(PARAM, MU = NULL)
```

**Arguments**

PARAM            an original set of parameters generated by `set.global`.

MU                a center matrix with  $\text{dim} = p \times K$ .

**Details**

For `initial.RndEM`, the procedure is implemented by randomly picking `.pmclustEnv$CONTROL$RndEM.iter` starting points from data `X.spmd` and run one E-step to obtain the log likelihood. Then pick the starting point with the highest log likelihood as the best choice to pursue the MLEs in further EM iterations.

This function repeatedly run `initial.em` by `.pmclustEnv$CONTROL$RndEM.iter` random starts and pick the best initializations from the random starts.

For `initial.em`, it takes `X.spmd` from the global environment and randomly pick  $K$  of them as the centers of  $K$  groups. If `MU` is specified, then this `MU` will be the centers. The default identity dispersion in `PARAM$SIGMA` will be used. Then, one E-step will be called to obtain the log likelihood and new classification will be updated.

This function is used to implement the `RndEM` procedure for more elaborate initialization scheme in `initial.RndEM`. Potentially, several random starts should be tried before running EM algorithms. This can benefit in two aspects including: shorter convergent iterations and better classification results.

For `initial.center`, if `MU` is given, then the center will be assigned according.

**Value**

The best initial starting points `PARAM` will be returned among all random starting points. The number of random starting points is assigned by `set.global` to a list variable `CONTROL`. See the help page of `initial.em` and `set.global` for details.

**Author(s)**

Wei-Chen Chen <wccsnow@gmail.com> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

Maitra, R. (2009) "Initializing partition-optimization algorithms", *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **6:1**, 114-157.

**See Also**

[set.global](#), [em.step](#), [aecm.step](#),  
[apecm.step](#), [apecma.step](#), [kmeans.step](#).  
[set.global.dmat](#), [kmeans.step.dmat](#).

**Examples**

```
## Not run:  
# Examples can be found in the help page of em.step(),  
# aecm.step(), apecm.step(), apecma.step(), and kmeans.step().  
  
# Examples for ddmatrix version can be found in the help pages of  
# kmeans.step.dmat().  
  
## End(Not run)
```

---

mb.print

*Print Results of Model-Based Clustering*

---

**Description**

This function will print summarized messages for model-based clustering.

**Usage**

```
mb.print(PARAM, CHECK)
```



**Arguments**

PARAM a set of convergent parameters to be printed.  
CHECK a set of checking parameters to be printed.

**Details**

This function will provide a quick summary from the PARAM and CHECK typically the output of clusterings when algorithms stop. The `COMM.RANK 0` will be used to take care the printing.

**Value**

Summarized messages will print/cat on screen by default.

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[em.step](#), [aecm.step](#), [apecm.step](#),  
[apecma.step](#).

**Examples**

```
## Not run:  
# Examples can be found in the help pages of em.step(),  
# aecm.step(), apecm.step(), and apecma.step().  
  
## End(Not run)
```

---

One E-Step

*Compute One E-step and Log Likelihood Based on Current Parameters*

---

**Description**

This function will perform one E-step based on current parameters. This is a core function of [em.onestep](#).

`e.step.dmat` is a `ddmatrix` version of `e.step`.

**Usage**

```
e.step(PARAM, update.logL = TRUE)

e.step.dmat(PARAM, update.logL = TRUE)
```

**Arguments**

PARAM	a set of parameters.
update.logL	TRUE for update observed data log likelihood.

**Details**

This function will base on the current parameter to compute the densities for all observations for all K components, and update the `Z.spmd` matrix. If the `update.logL` is true, then the log likelihood `W.spmd.rowSums` will be also updated before the end of this function.

Sum of `W.spmd.rowSums` of all processors will be the observed data log likelihood for the current iteration.

**Value**

Several global variables will be overwritten after this call including `Z.spmd`, `W.spmd.rowSums`, `W.spmd`, `U.spmd`, and `Z.colSums`.

**Computing Issues**

Since the clusters can be degenerated or highly flat, these cause very large positive or negative exponents in densities. The log likelihood will tend to be inaccurate (not finite). Since the mixture structures can be over fit, this also cause very tiny mixing proportions. The poster probabilities can also unstable (NaN).

These can be solved by rescaling the range of exponents carefully and adjust the scaling factor on the log values. See `CONTROL` for details about constrains on E- and M-steps.

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[set.global](#), [em.onestep](#), [m.step](#).

## Examples

```
## Not run:  
# This is a core function for em.onestep()  
# see the source code for details.  
  
## End(Not run)
```

---

One M-Step

*Compute One M-Step Based on Current Posterior Probabilities*

---

## Description

This function will perform one M-step based on current posterior probabilities. This is a core function of [em.onestep](#).

`m.step.dmat` is a `ddmatrix` version of `m.step`.

## Usage

```
m.step(PARAM)
```

```
m.step.dmat(PARAM)
```

## Arguments

PARAM            a set of parameters.

## Details

This function will base on the current posterior probabilities [Z.spmd](#) to estimate the parameters [PARAM](#) mainly including mixing proportions [ETA](#), centers of clusters [MU](#), and dispersions of clusters [SIGMA](#).

## Value

Returning a new [PARAM](#) which maximizes the complete data log likelihood for the current iteration.

## Author(s)

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

## References

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[set.global](#), [em.onestep](#), [e.step](#).

**Examples**

```
## Not run:  
# This is a core function for em.onestep()  
# see the source code for details.  
  
## End(Not run)
```

---

One Step of EM algorithm

*One EM Step for GBD*

---

**Description**

One EM step only for model-based clustering of finite mixture Gaussian models with unstructured dispersions. This is a core function of [em.step](#).

`em.onestep.dmat` is a `ddmatrix` version of `em.onestep`.

**Usage**

```
em.onestep(PARAM)
```

```
em.onestep.dmat(PARAM)
```

**Arguments**

PARAM            an original set of parameters generated by [set.global](#).

**Details**

A global variable called `X.spmd` should exist in the `.pmclustEnv` environment, usually the working environment. The `X.spmd` is the data matrix to be clustered, and this matrix has a dimension `N.spmd` by `p`.

The `PARAM` will be a local variable for the current iteration inside `em.onestep`, and this variable is a list containing all parameters related to models. This function also updates in the parameters by the EM algorithm, and return a new `PARAM` for the next iteration. The details of list elements are initially generated by [set.global](#).

**Value**

This function is one EM step. The global variables will be updated and a new `PARAM` will be returned. See the help page of `PARAM` or `PARAM.org` for details.

**Author(s)**

Wei-Chen Chen <wccsnow@gmail.com> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[set.global](#), [e.step](#), [m.step](#).

**Examples**

```
## Not run:  
# This is a core function for em.step()  
# see the source code for details.  
  
## End(Not run)
```

---

pmclust and pkmeans      *Parallel Model-Based Clustering and Parallel K-means Algorithm*

---

**Description**

Parallel Model-Based Clustering and Parallel K-means Algorithm

**Usage**

```
pmclust(X = NULL, K = 2, MU = NULL,  
        algorithm = .PMC.CT$algorithm, RndEM.iter = .PMC.CT$RndEM.iter,  
        CONTROL = .PMC.CT$CONTROL, method.own.X = .PMC.CT$method.own.X,  
        rank.own.X = .SPMD.CT$rank.source, comm = .SPMD.CT$comm)  
  
pkmeans(X = NULL, K = 2, MU = NULL,  
        algorithm = c("kmeans", "kmeans.dmat"),  
        CONTROL = .PMC.CT$CONTROL, method.own.X = .PMC.CT$method.own.X,  
        rank.own.X = .SPMD.CT$rank.source, comm = .SPMD.CT$comm)
```

**Arguments**

X	a GBD row-major matrix or a ddmatrix.
K	number of clusters.
MU	pre-specified centers.
algorithm	types of EM algorithms.

RndEM.iter	number of Rand-EM iterations.
CONTROL	a control for algorithms, see <a href="#">CONTROL</a> for details.
method.own.X	how X is distributed.
rank.own.X	who own X if method.own.X = "single".
comm	MPI communicator.

### Details

These are high-level functions for several functions in **pmclust** including: data distribution, setting global environment `.pmclustEnv`, initializations, algorithm selection, etc.

The input X is either in `ddmatrix` or `gbd`. It will be converted in `gbd` row-major format and copied into `.pmclustEnv` for computation. By default, **pmclust** uses a `GBD` row-major format (`gbdr`). While `common` means that X is identical on all processors, and `single` means that X only exist on one processor `rank.own.X`.

### Value

These functions return a list with class `pmclust` or `pkmeans`.

See the help page of [PARAM](#) or [PARAM.org](#) for details.

### Author(s)

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

### References

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

### See Also

[set.global](#), [e.step](#), [m.step](#).  
[set.global.dmat](#), [e.step.dmat](#), [m.step.dmat](#).

### Examples

```
## Not run:
# Save code in a file "demo.r" and run in 4 processors by
# > mpiexec -np 4 Rscript demo.r

### Setup environment.
library(pmclust, quiet = TRUE)

### Load data
X <- as.matrix(iris[, -5])

### Distribute data
jid <- get.jid(nrow(X))
```

```

X.gbd <- X[jid,]

### Standardized
N <- allreduce(nrow(X.gbd))
p <- ncol(X.gbd)
mu <- allreduce(colSums(X.gbd / N))
X.std <- sweep(X.gbd, 2, mu, FUN = "-")
std <- sqrt(allreduce(colSums(X.std^2 / (N - 1))))
X.std <- sweep(X.std, 2, std, FUN = "/")

### Clustering
library(pmclust, quiet = TRUE)
comm.set.seed(123, diff = TRUE)

ret.mb1 <- pmclust(X.std, K = 3)
comm.print(ret.mb1)

ret.kms <- pkmeans(X.std, K = 3)
comm.print(ret.kms)

### Finish
finalize()

## End(Not run)

```

---

print.object

*Functions for Printing or Summarizing Objects According to Classes*


---

## Description

Several classes are declared in **pmclust**, and these are functions to print and summary objects.

## Usage

```

## S3 method for class 'pmclust'
print(x, ...)
## S3 method for class 'pkmeans'
print(x, ...)

```

## Arguments

x                    an object with the class attributes.  
...                   other possible options.

## Details

These are useful functions for summarizing.

**Value**

The results will cat or print on the STDOUT by default.

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[pmclust](#), [pkmeans](#).

**Examples**

```
## Not run:
library(pmclust, quiet = TRUE)

# Functions applied by directly type the names of objects.

## End(Not run)
```

---

Read Me First

*Read Me First Function*

---

**Description**

This function print the annotations of all variables used in this package.

\*.dmat's are ddmatrix versions.

**Usage**

```
readme()
```

```
readme.dmat()
```

**Details**

This package is optimized in the way by pre-specifying several global variables in `.pmclustEnv`. These variables will be overwrote by EM algorithms. Users should use these names to access the results and utilize them with cautions.

`readme.dmat` is a ddmatrix version of `readme`.



**Value**

A readme message will print on screen by default and explain the global variables used in this package, including:

CHECK	convergent checking
CLASS.spmid	true id of each data, a vector of length N.spmid and has values from 1 to K
COMM.RANK	rank of current processor, obtained from comm.rank of pbdMPI
COMM.SIZE	total processors in MPI world, obtained from comm.size of pbdMPI
CONTROL	controls for EM iterations
PARAM	set or parameters
SAVE.param	(debug only) save parameters for every iterations
SAVE.iter	(debug only) save computing time for every iterations
U.spmid	temporary storage for density
W.spmid	temporary storage for $\eta * \text{density}$
W.spmid.rowSums	temporary storage for rowSums of W.spmid
X.spmid	generated data set with dimension with dimension N.spmid * p
Z.colSums	temporary storage for rowSums of Z.spmid
Z.spmid	posterior probabilities
p.times.logtwopi	$p * \log(2 * \pi)$

Each variable may contain several elements if it is a list, some variables are used for temporary storages in order to optimize computing, and some variables are used for constant variables. These variables may be restricted, and only generated by the function `set.global`.

One can access these variables via the global environment `.pmclustEnv` such as `.pmclustEnv$CONTROL`.

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[set.global](#), [set.global.dmat](#).

**Examples**

```
## Not run:
readme()
readme.dmat()

## End(Not run)
```

---

Set Global Variables    *Set Global Variables According to the global matrix X.gbd (X.spmd) or X.dmat*

---

### Description

This function will set several sets of variables globally in the environment `.pmclustEnv` according to the global matrix `X.gbd/X.spmd`.

`set.global.dmat` is a `ddmatrix` version of `set.global.gbd`.

### Usage

```
set.global.gbd(K = 2, X.gbd = NULL, PARAM = NULL,
  algorithm = c("em", "aecm", "apecm", "apecma", "kmeans"),
  RndEM.iter = 10)
set.global.dmat(K = 2, X.dmat = NULL, PARAM = NULL,
  algorithm = c("em.dmat", "kmeans.dmat"),
  RndEM.iter = 10)

set.global(K = 2, X.spmd = NULL, PARAM = NULL,
  algorithm = c("em", "aecm", "apecm", "apecma", "kmeans"),
  RndEM.iter = 10)
```

### Arguments

<code>K</code>	an original set of parameters generated by <code>set.global</code> .
<code>X.gbd</code>	an input GBD matrix.
<code>X.dmat</code>	an input <code>ddmatrix</code> .
<code>X.spmd</code>	an input SPMD matrix.
<code>PARAM</code>	an original set of parameters generated by <code>set.global</code> .
<code>algorithm</code>	an original set of parameters generated by <code>set.global</code> .
<code>RndEM.iter</code>	number of RndEM iterations.

### Details

WARNING: A global variable named `X.gbd/X.spmd` should be set before calling `set.global` where `X.gbd/X.spmd` is a matrix containing data with dimension `N.spmd * p`. i.e. `N.spmd` observations and `p` variables.

WARNING: A global variable named `X.dmat` should be set before calling `set.global.dmat` where `X.dmat` is a `ddmatrix` (in block-cyclic format) containing data with dimension `N * p`.

`X.gbd/X.spmd` and `X.dmat` are supposed to exist in `.GlobalEnv`. If not, they should be as an input object and will be copied into `.pmclustEnv` which is less efficient.

**Value**

A new set of **PARAM** will be returned and several global variables will be set according to the data `X.gbd/X.spm`.

Sets of global variables are store in the default environment `.pmclustEnv`.

Use [readme](#) to see all global variables set by this function.

Use [readme.dmat](#) to see all global variables of `ddmatrix` version set by this function.

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

**References**

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[em.step](#), [aecm.step](#), [apecm.step](#),  
[apecma.step](#).

**Examples**

```
## Not run:  
# Examples can be found in the help pages of em.step(),  
# aecm.step(), apecm.step(), apecma.step(), and kmeans.step().  
  
# Examples for ddmatrix version can be found in the help pages of  
# kmeans.step.dmat().  
  
## End(Not run)
```

---

Set of CONTROL

*A Set of Controls in Model-Based Clustering.*

---

**Description**

This set of controls are used to guide all algorithms implemented in this package.

**Format**

A list variable contains several parameters for computing.

**Details**

`.PMC.CT` stores all default controls for `pmclust` and `pkmeans` including

algorithm	algorithms implemented
algorithm.gbd	algorithms implemented for gbd/spmd
algorithm.dmat	algorithms implemented for ddmatrix
method.own.X	how X is distributed
CONTROL	a CONTROL list as in next

The elements of CONTROL or .pmclustEnv\$CONTROL are

max.iter	maximum number of iterations (1000)
abs.err	absolute error for convergence (1e-4)
rel.err	relative error for convergence (1e-6)
debug	debugging flag (0)
RndEM.iter	number of RndEM iterations (10)
exp.min	minimum exponent ( $\log(.Machine\$double.xmin)$ )
exp.max	maximum exponent ( $\log(.Machine\$double.xmax)$ )
U.min	minimum of diagonal of chol
U.max	maximum of diagonal of chol

These elements govern the computing including number of iterations, convergent criteria, ill conditions, and numerical issues. Some of them are machine dependent.

Currently, the algorithm could be em, aecm, apecm, apecma, and kmeans for GBD and ddmatrix (with \*.dmat). The method.own.X could be gbdr, common, single, and ddmatrix.

### Numerical Issues

For example, exp.min and exp.max will control the range of densities function before taking logarithm. If the density values were no in the range, they would be rescaled. The scaling factor will be also recorded for post adjustment for observed data log likelihood. This will provide more accurate posterior probabilities and observed data log likelihood.

Also, U.min and U.max will control the output of chol when decomposing SIGMA in every E-steps. If the diagonal terms were out of the range, a PARAM\$U.check would be set to FALSE. Only the components with TRUE U.check will estimate and update the dispersions in M-steps for the rest of iterations.

These problems may cause wrong posteriors and log likelihood due to the degenerate and inflated components. Usually, this is a sign of overestimate the number of components K, or the initialization do not provide good estimations for parameters. See [e.step](#) for more information about computing.

### Author(s)

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

### References

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

**See Also**

[set.global.gbd](#), [set.global.dmat](#), and [set.global](#).

**Examples**

```
## Not run:
# Use set.global() to generate one of this.
# X.spmf should be pre-specified before calling set.global().

## End(Not run)
```

---

Set of PARAM

*A Set of Parameters in Model-Based Clustering.*


---

**Description**

This set of parameters are used in initialization, EM iterations, and final convergent results. All share the same structure in a list variable.

**Format**

A list variable contains several parameters for computing.

**Details**

The elements of PARAM or PARAM.org are

N	number of observations
p	dimension of each observation, total number of variables
K	number of clusters
ETA	mixing proportion
log.ETA	log of mixing proportion
MU	centers, $\text{dim} = p \times K$
SIGMA	dispersions, a list containing $K$ elements, each element is a matrix, $\text{dim} = p \times p$
U	Choleski of SIGMA, the same size of SIGMA
U.check	checks of each elements of U, length $K$
logL	log likelihood
min.N.CLASS	minimum number of elements in a cluster (restrictions)

The model parameters are ETA, MU, and SIGMA, while log.ETA, U, U.check, and min.N.CLASS are only used in computing.

**Author(s)**

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

## References

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

## See Also

[set.global.](#)

## Examples

```
## Not run:  
# Use set.global() to generate one of this.  
# X.spm� should be pre-specified before calling set.global().  
  
## End(Not run)
```

---

Update Class of EM or Kmeans Results

*Update CLASS.spm� Based on the Final Iteration*

---

## Description

Update [CLASS.spm�](#) based on the final iteration of EM-like algorithms.

\*.dmat's are `ddmatrix` versions.

## Usage

```
em.update.class()  
kmeans.update.class()  
  
em.update.class.dmat()  
kmeans.update.class.dmat()
```

## Details

This function takes [Z.spm�](#) from the global environment `.pmclustEnv` and update [CLASS.spm�](#), and provides the identification of groups for all data.

## Value

[CLASS.spm�](#) will be updated.

## Author(s)

Wei-Chen Chen <[wccsnow@gmail.com](mailto:wccsnow@gmail.com)> and George Ostrouchov.

## References

High Performance Statistical Computing (HPSC) Website: <http://thirteen-01.stat.iastate.edu/snoweye/hpsc/>

Programming with Big Data in R Website: <http://r-pbd.org/>

## See Also

[em.step](#), [aecm.step](#), [apecm.step](#),  
[apecma.step](#), [kmeans.step](#),  
[kmeans.step.dmat](#).

## Examples

```
## Not run:  
# Examples can be found in the help pages of em.step(),  
# aecm.step(), apecm.step(), apecma.step(), and kmeans.step().  
  
# Examples for ddmatrix version can be found in the help pages of  
# kmeans.step.dmat().  
  
## End(Not run)
```

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