# Package 'IMIFA'

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Type Package

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**Title** Infinite Mixtures of Infinite Factor Analysers and Related Models

Version 2.1.8

Description Provides flexible Bayesian estimation of Infinite Mixtures of Infinite Factor Analysers and related models, for nonparametrically clustering high-dimensional data, introduced by Murphy et al. (2020) <doi:10.1214/19-BA1179>. The IMIFA model conducts Bayesian nonparametric model-based clustering with factor analytic covariance structures without recourse to model selection criteria to choose the number of clusters or cluster-specific latent factors, mostly via efficient Gibbs updates. Model-specific diagnostic tools are also provided, as well as many options for plotting results, conducting posterior inference on parameters of interest, posterior predictive checking, and quantifying uncertainty.

**Depends** R (>= 4.0.0) **License** GPL (>= 2) **Encoding** UTF-8

URL https://cran.r-project.org/package=IMIFA

BugReports https://github.com/Keefe-Murphy/IMIFA

LazyData true

**Imports** matrixStats (>= 0.53.1), mclust (>= 5.4), mvnfast, Rfast (>= 1.9.8), slam, viridisLite

Suggests gmp (>= 0.5-4), knitr, mcclust, rmarkdown, Rmpfr

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NeedsCompilation no

**70** 

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IMIFA-package	IMIFA: Infinite Mixtures of Infinite Factor Analysers and Related Models

### **Description**

A package for Bayesian nonparametric clustering of high-dimensional data sets, providing functions for fitting, diagnostic tools and plotting for Infinite Mixtures of Infinite Factor Analysers and the full suite of related models introduced by Murphy et al. (2020) <doi: 10.1214/19BA1179>. Allows model based clustering with factor analytic covariance structures without recourse to model selection criteria to choose the number of clusters or cluster-specific latent factors. Model-specific diagnostic tools are also provided, as well as many options for plotting results, conducting posterior inference on parameters of interest, posterior predictive checking, and quantifying uncertainty.

#### **Details**

Type: PackagePackage: IMIFAVersion: 2.1.8

• Date: 2021-12-19 (this version), 2017-02-02 (original release)

• Licence: GPL (>=2)

### Usage

The three most important functions in the **IMIFA** package are: mcmc\_IMIFA, for fitting the model, get\_IMIFA\_results, for extracting results from objects of the "IMIFA" class generated by mcmc\_IMIFA, and the dedicated plotting function plot.Results\_IMIFA, for plotting results pertaining to parameters of inferential interest from objects of class "Results\_IMIFA" generated by get\_IMIFA\_results.

Other functions also exist, e.g. for simulating data from a multivariate mixture of factor analysers, many functions for soliciting good priors, and many functions related to plotting.

mcmc\_IMIFA: This function estimates models in the IMIFA family under the Bayesian paradigm. Most importantly, one must specify the method in the form of an acronym (e.g. "MIFA" for Mixtures of Infinite Factor Analysers) and ranges of values for range.G, the number of clusters, and range.Q, the number(s) of (cluster-specific) latent factors as required by said method.

get\_IMIFA\_results: Raw simulation objects generated by mcmc\_IMIFA() are passed to this function in order to extract results of interest and conduct further post-processing if necessary.

plot.Results\_IMIFA: Results obtained from get\_IMIFA\_Results are passed to this function with the type of plot desired specified by plot.meth (e.g. "trace") and the parameter of interest specified by param (e.g. "loadings").

# References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <doi:10.1214/19-BA1179>.

### See Also

```
Further details and examples are given in the associated vignette document: vignette("IMIFA", package = "IMIFA")
```

### Author(s)

```
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Maintainer: Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### See Also

Useful links:

- https://cran.r-project.org/package=IMIFA
- Report bugs at https://github.com/Keefe-Murphy/IMIFA

bnpControl

Control settings for the Bayesian Nonparametric priors for infinite mixture models (or shrinkage priors for overfitted mixtures)

# **Description**

Supplies a list of arguments for use in mcmc\_IMIFA pertaining to the use of the Bayesian Non-parametric Pitman-Yor / Dirichlet process priors with the infinite mixture models "IMFA" and "IMIFA". Certain arguments related to the Dirichlet concentration parameter for the overfitted mixtures "OMFA" and "OMIFA" can be supplied in this manner also.

# Usage

#### **Arguments**

learn.alpha

For the "IMFA" and "IMIFA" methods: A logical indicating whether the Pitman-Yor / Dirichlet process concentration parameter is to be learned (defaults to TRUE), or remain fixed for the duration of the chain. If being learned, a Ga(a, b) prior is assumed for alpha; updates take place via Gibbs sampling when discount is zero and via Metropolis-Hastings when discount > 0. If not being learned, alpha *must* be supplied.

In the special case of discount < 0, alpha must be supplied as a positive integer multiple of abs(discount); in this instance, learn. alpha is forced to TRUE and alpha is updated with the changing number of components as the positive integer.

For the "OMFA" and "OMIFA" methods: A logical indicating whether the Dirichlet concentration parameter is to be learned (defaults to TRUE) or remain fixed for the duration of the chain. If being learned, a Ga(a, b \* G) is assumed for alpha, where G is the number of mixture components range. G, and updates take place via Metropolis-Hastings. If not being learned alpha *must* be supplied.

alpha.hyper

For the "IMFA" and "IMIFA" methods: A vector of length 2 giving hyperparameters for the prior on the Pitman-Yor / Dirichlet process concentration parameter alpha. If isTRUE(learn.alpha), these are shape and rate parameters of a Gamma distribution. Defaults to Ga(2, 4). Choosing a larger rate is particularly important, as it encourages clustering. The prior is shifted to have support on (-discount, Inf) when non-zero discount is supplied and remains fixed (i.e. learn.d=FALSE) or when learn.d=TRUE.

**For the** "OMFA" **and** "OMIFA" **methods:** A vector of length 2 giving hyperparameters a and b for the prior on the Dirichlet concentration parameter alpha. If isTRUE(learn.alpha), these are shape and rate parameters of a Gamma distribution. Defaults to Ga(2, 4). Note that the supplied rate will be multiplied by range.G, to encourage clustering, such that the form of the prior is Ga(a, b \* G).

discount

The discount parameter used when generalising the Dirichlet process to the Pitman-Yor process. Defaults to 0, but typically must lie in the interval [0, 1). If greater than zero, alpha can be supplied greater than -discount. By default, Metropolis-Hastings steps are invoked for updating this parameter via learn.d. The special case of discount < 0 is allowed, in which case learn.d=FALSE is forced and alpha must be supplied as a positive integer multiple of abs(discount). Fixing discount > 0.5 is discouraged (see learn.alpha).

learn.d

Logical indicating whether the discount parameter is to be updated via Metropolis-Hastings (defaults to TRUE, unless discount is supplied as a negative value).

d.hyper

Hyperparameters for the Beta(a,b) prior on the discount parameter. Defaults to Beta(1,1), i.e. Uniform(0,1).

ind.slice

Logical indicating whether the independent slice-efficient sampler is to be employed (defaults, typically, to TRUE). If FALSE the dependent slice-efficient sampler is employed, whereby the slice sequence  $\xi_1,\ldots,\xi_g$  is equal to the decreasingly ordered mixing proportions. When thresh &/or exchange are set to TRUE (see below), this argument is forced to FALSE.

rho

Parameter controlling the rate of geometric decay for the independent slice-efficient sampler, s.t.  $\xi=(1-\rho)\rho^{g-1}$ . Must lie in the interval [0,1). Higher values are associated with better mixing but longer run times. Defaults to 0.75, but 0.5 is an interesting special case which guarantees that the slice sequence  $\xi_1,\ldots,\xi_g$  is equal to the *expectation* of the decreasingly ordered mixing proportions. Only relevant when ind.slice is TRUE.

trunc.G

The maximum number of allowable and storable clusters under the "IMIFA" and "IMFA" models. The number of active clusters to be sampled at each iteration is adaptively truncated, with trunc.G as an upper limit for storage reasons. Defaults to max(min(N-1,50),range.G)) and must satisfy range.G <= trunc.G < N. Note that large values of trunc.G may lead to memory capacity issues.

kappa

The spike-and-slab prior distribution on the discount hyperparameter is assumed to be a mixture with point-mass at zero and a continuous Beta(a,b) distribution. kappa gives the weight of the point mass at zero (the 'spike'). Must lie in the interval [0,1]. Defaults to 0.5. Only relevant when isTRUE(learn.d). A value of 0 ensures non-zero discount values (i.e. Pitman-Yor) at all times, and *vice versa*. Note that kappa will default to exactly 0 if alpha<=0 and learn.alpha=FALSE.

IM.lab.sw

Logical indicating whether the two forced label switching moves are to be implemented (defaults to TRUE) when running one of the infinite mixture models. Note: when exchange=TRUE (see below), this argument is instead forced to FALSE.

thresh

Logical indicating whether the threshold of Fall and Barat (2014) should be incorporated into the slice sampler. See the reference for details. This is an experimental feature (defaults to FALSE) and can work with or without exchange below. Setting thresh=TRUE is **not** recommended unless both learn.alpha and learn.d are FALSE. Setting thresh to TRUE also forces ind.slice to FALSE (see above).

exchange

Logical indicating whether the exchangeable slice sampler of Fall and Barat (2014) should be used instead. See the reference for details. This argument can work with or without thresh=TRUE above, though it is also an experimental argument and thus defaults to FALSE. When TRUE, the arguments ind.slice and IM.lab.sw (see above) are both forced to FALSE.

zeta

For the "IMFA" and "IMIFA" methods: Tuning parameter controlling the acceptance rate of the random-walk proposal for the Metropolis-Hastings steps when learn.alpha=TRUE, where 2 \* zeta gives the full width of the uniform proposal distribution. These steps are only invoked when either discount is non-zero and fixed or learn.d=TRUE, otherwise alpha is learned by Gibbs updates. Must be strictly positive (if invoked). Defaults to 2.

**For the** "OMFA" **and** "OMIFA" **methods:** Tuning parameter controlling the standard deviation of the log-normal proposal for the Metropolis-Hastings steps when learn.alpha=TRUE. Must be strictly positive (if invoked). Defaults to 0.75.

tune.zeta

A list with the following named arguments, used for tuning zeta (which is either the width of the uniform proposal for the "IMFA" or "IMIFA" methods or

the standard deviation of the log-normal proposal for the "OMFA" or "OMIFA" methods) for alpha, via diminishing Robbins-Monro type adaptation, when the alpha parameter is learned via Metropolis-Hastings steps:

heat The initial adaptation intensity/step-size, such that larger values lead to larger updates. Must be strictly greater than zero. Defaults to 1 if not supplied but other elements of tune.zeta are.

lambda Iteration rescaling parameter which controls the speed at which adaptation diminishes, such that lower values cause the contribution of later iterations to diminish more slowly. Must lie in the interval (0.5, 1]. Defaults to 1 if not supplied but other elements of tune.zeta are.

target The target acceptance rate. Must lie in the interval [0, 1]. Defaults to 0.441, which is optimum for univariate targets, if not supplied but other elements of tune.zeta are.

start.zeta The iteration at which diminishing adaptation begins. Defaults to 100.

stop.zeta The iteration at which diminishing adaptation is to stop completely. Defaults to Inf, such that diminishing adaptation is never explicitly made to stop. Must be greater than start.zeta.

At least one tune.zeta argument must be supplied for diminishing adaptation to be invoked. tune.zeta arguments are only relevant when learn.alpha is TRUE (and, for the "IMFA" and "IMIFA" methods, when either of the following is also true: the discount remains fixed at a non-zero value, or when learn.d is TRUE and kappa < 1). Since Gibbs steps are invoked for updating alpha when discount == 0 under the "IMFA" or "IMIFA" methods, adaption occurs according to a running count of the number of iterations with non-zero sampled discount values for those methods.

If diminishing adaptation is invoked, the posterior mean zeta will be stored. Since caution is advised when employing adaptation, note that acceptance rates of between 10-50% are generally considered adequate.

Catches unused arguments.

### **Details**

The crucial concentration parameter alpha is documented within the main mcmc\_IMIFA function, and is relevant to all of the "IMIFA", "IMFA", "OMIFA", and "OMFA" methods.

All arguments here are relevant to the "IMFA" and "IMIFA" methods, but the following are also related to the "OMFA" and "OMIFA" methods, and may behave differently in those instances: learn.alpha, alpha.hyper, zeta, and tune.zeta.

#### Value

A named list in which the names are the names of the arguments related to the BNP prior(s) and the values are the values supplied to the arguments.

#### Note

Certain supplied arguments will be subject to further checks within mcmc\_IMIFA. G\_priorDensity and G\_moments can help with soliciting sensible DP/PYP priors.

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Under the "IMFA" and "IMIFA" methods, a Pitman-Yor process prior is specified by default. A Dirichlet process prior can be easily invoked when the discount is fixed at 0 and learn.d=FALSE. The normalized stable process can also be specified as a prior distribution, as a special case of the Pitman-Yor process, when alpha remains fixed at 0 and learn.alpha=FALSE (provided the discount is fixed at a strictly positive value or learn.d=TRUE). The special case of the Pitman-Yor process with negative discount is also allowed as an experimental feature for which caution is advised, though learn.d and learn.alpha are forced to FALSE and TRUE, respectively, in this instance.

### Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

Kalli, M., Griffin, J. E. and Walker, S. G. (2011) Slice sampling mixture models, *Statistics and Computing*, 21(1): 93-105.

Fall, M. D. and Barat, E. (2014) Gibbs sampling methods for Pitman-Yor mixture models, *hal-00740770v2*.

#### See Also

mcmc\_IMIFA, G\_priorDensity, G\_moments, mixfaControl, mgpControl, storeControl

# **Examples**

coffee

Chemical composition of Arabica and Robusta coffee samples

### **Description**

Data on the chemical composition of coffee samples collected from around the world, comprising 43 samples from 29 countries. Each sample is either of the Arabica or Robusta variety. Twelve of the thirteen chemical constituents reported in the study are given. The omitted variable is total chlorogenic acid; it is generally the sum of the chlorogenic, neochlorogenic and isochlorogenic acid values.

#### Usage

```
data(coffee)
```

#### **Format**

A data frame with 43 observations and 14 columns. The first two columns contain Variety (either Arabica or Robusta) and Country, respectively, while the remaining 12 columns contain the chemical properties.

#### References

Streuli, H. (1973). Der heutige Stand der Kaffee-Chemie, *Association Scientifique International du Cafe, 6th International Colloquium on Coffee Chemistry*, Bogata, Columbia, pp. 61-72.

# **Examples**

```
data(coffee, package="IMIFA")
pairs(coffee[,-(1:2)], col=coffee$Variety)
```

get\_IMIFA\_results

Extract results, conduct posterior inference and compute performance metrics for MCMC samples of models from the IMIFA family

#### **Description**

This function post-processes simulations generated by mcmc\_IMIFA for any of the IMIFA family of models. This includes accounting for label switching, and accounting for rotational invariance via Procrustean methods. It can be re-ran at little computational cost in order to extract different models explored by the sampler used for sims, without having to re-run the model itself. New results objects using different numbers of clusters and different numbers of factors (if visited by the model in question), or using different model selection criteria (if necessary) can be generated with ease. Posterior predictive checking of the appropriateness of the fitted model is also facilitated.

### Usage

```
zlabels = NULL,
                   nonempty = TRUE,
                   . . . )
## S3 method for class 'Results_IMIFA'
print(x,
      ...)
## S3 method for class 'Results IMIFA'
summary(object,
        MAP = TRUE,
        ...)
```

# **Arguments**

sims An object of class "IMIFA" generated by mcmc\_IMIFA.

burnin Optional additional number of iterations to discard. Defaults to 0, corresponding

to no additional burnin. See mixfaControl for the default burnin settings used

previously by mcmc\_IMIFA.

Optional interval for extra thinning to be applied. Defaults to 1, corresponding thinning

to no additional thinning. See mixfaControl for the default thinning settings

used previously by mcmc\_IMIFA.

If this argument is not specified, results will be returned with the optimal number of clusters. If different numbers of clusters were explored in sims for the "MFA" or "MIFA" methods, supplying an integer value allows pulling out a specific

solution with G clusters, even if the solution is sub-optimal.

Similarly, this allows retrieval of samples corresponding to a solution, if visited,

with G clusters for the "OMFA", "OMIFA", "IMFA" and "IMIFA" methods.

If this argument is not specified, results will be returned with the optimal number of factors. If different numbers of factors were explored in sims for the "FA", "MFA", "OMFA" or "IMFA" methods, this allows pulling out a specific solution

with Q factors, even if the solution is sub-optimal.

Similarly, this allows retrieval of samples corresponding to a solution, if visited, with Q factors for the "IFA", "MIFA", "OMIFA" and "IMIFA" methods. Can be

supplied as a scalar or a vector of values for each cluster.

The criterion to use for model selection, where model selection is only required criterion if more than one model was run under the "FA", "MFA", "MIFA", "OMFA" or

"IMFA" methods when sims was created via mcmc\_IMIFA. Defaults to bicm, but note that these are all calculated; this argument merely indicates which one will

form the basis of the construction of the output.

Note that the first three options here might exhibit bias in favour of zero-factor models for the finite factor "FA", "MFA", "OMFA" and "IMFA" methods and might exhibit bias in favour of one-cluster models for the "MFA" and "MIFA" methods. The aic.mcmc and bic.mcmc criteria will only be returned for finite factor mod-

els.

G.meth If the object in sims arises from the "OMFA", "OMIFA", "IMFA" or "IMIFA" meth-

ods, this argument determines whether the optimal number of clusters is given

G

Q

by the mode or median of the posterior distribution of G. Defaults to "mode". Often the mode and median will agree in any case.

Q.meth

If the object in sims arises from the "IFA", "MIFA", "OMIFA" or "IMIFA" methods, this argument determines whether the optimal number of latent factors is given by the mode or median of the posterior distribution of Q. Defaults to "mode". Often the mode and median will agree in any case.

conf.level

The confidence level to be used throughout for credible intervals for all parameters of inferential interest, and error metrics if error.metrics=TRUE. Defaults to 0.95.

error.metrics

A logical activating or deactivating posterior predictive checking: i.e. controlling whether metrics quantifying a) the posterior predictive reconstruction error (PPRE) between bin counts of the data and bin counts of replicate draws from the posterior distribution & and b) the error between the empirical and estimated covariance matrices should be computed. These are computed for every *valid* retained iteration (see Details). Defaults to TRUE, but can be time-consuming for models which achieve clustering. These error metrics, and the uncertainty associated with them, can be visualised via plot.Results\_IMIFA. Depending on what parameters were stored when calling mcmc\_IMIFA, potentially not all error metrics will be available to compute.

The Frobenius norm is used in the computation of the PPRE, by default, but the type of norm can be changed via the ... construct below. So too can the breakpoints (dbreaks) used to bin the data and the posterior predictive replicate data sets. Some caution is advised in the latter case.

vari.rot

Logical indicating whether the loadings matrix/matrices template(s) should be varimax rotated first, prior to the Procrustes rotation steps. Defaults to FALSE. Not necessary at all for clustering purposes, or inference on the covariance matrix, but useful if interpretable inferences on the loadings matrix/matrices are desired. Arguments to varimax can be passed via the . . . construct, but note that the argument normalize here defaults to FALSE.

z.avgsim

Logical (defaults to FALSE) indicating whether the clustering should also be summarised with a call to <code>Zsimilarity</code> by the clustering with minimum mean squared error to the similarity matrix obtained by averaging the stored adjacency matrices, in addition to the MAP estimate.

Note that the MAP clustering is computed *conditional* on the estimate of the number of clusters (whether that be the modal estimate or the estimate according to criterion) and other parameters are extracted conditional on this estimate of G: however, in contrast, the number of distinct clusters in the summarised labels obtained by specifying z.avgsim=TRUE may not necessarily coincide with the MAP estimate of G, but it may provide a useful alternative summary of the partitions explored during the chain, and the user is free to call get\_IMIFA\_results again with the new suggested G value.

Please be warned that this feature requires loading the mcclust package. This is liable to take considerable time to compute, and may not even be possible if the number of observations &/or number of stored iterations is large and the resulting matrix isn't sufficiently sparse. When z.avgsim=TRUE, both the summarised clustering and the similarity matrix are stored: the latter can be visualised as part of a call to plot.Results\_IMIFA.

zlabels For any method that performs clustering, the true labels can be supplied if they

are known in order to compute clustering performance metrics. This also has the effect of ordering the MAP labels (and thus the ordering of cluster-specific

parameters) to most closely correspond to the true labels if supplied.

nonempty For "MFA" and "MIFA" models ONLY: a logical indicating whether only iterations with non-empty components should be retained. Defaults to TRUE, but

may lead to empty chains - conversely, FALSE may lead to empty components

and related errors.

x, object, MAP, ...

Arguments required for the print.Results\_IMIFA and summary.Results\_IMIFA functions: x and object are objects of class "Results\_IMIFA" resulting from a call to get\_IMIFA\_results. MAP is a logical which governs whether a table of the MAP classification is printed, while . . . gathers additional arguments to those functions.

Users can also pass the type argument to the norm function when isTRUE(error.metrics) and the posterior predictive reconstruction error (PPRE) is calculated. By default the Frobenius norm (type="F") is employed.

Finally, the ... construct also allows arguments to varimax to be passed to get\_IMIFA\_results itself, when isTRUE(vari.rot), or arguments to hist when isTRUE(error.metrics), in order to guide construction of the bins. Additionally, by passing the argument dbreaks via the ... construct, the bins can be specified directly. However, caution is advised in doing so; in particular, the bins must be constructed on data which has been standardised in the same way as the data modelled within mcmc\_IMIFA.

### **Details**

The function also performs post-hoc corrections for label switching, as well as post-hoc Procrustes rotation of loadings matrices and scores, in order to ensure sensible posterior parameter estimates, computes error metrics, constructs credible intervals, and generally transforms the raw sims object into an object of class "Results\_IMIFA" in order to prepare the results for plotting via plot.Results\_IMIFA.

For the infinite factor methods, iterations where the maximum number of factors was greater than or equal to the maximum of the estimated cluster-specific factors are retained for posterior summaries of the scores, in order to preserve the estimated dimension of the scores matrices. Similarly, these are also the *valid* iterations used for the computation of the averages and credible intervals for the error metrics. For the finite factor models, *all* retained iterations are used in both instances (i.e. both for the scores and the error metrics).

In all cases, only iterations with G non-empty components are retained.

### Value

An object of class "Results\_IMIFA" to be passed to plot.Results\_IMIFA for visualising results. Dedicated print and summary functions also exist for objects of this class. The object, say x, is a list of lists, the most important components of which are:

Clust Everything pertaining to clustering performance can be found here for all but the "FA" and "IFA" methods (or models where the estimate number of clusters

is 1), in particular x\$Clust\$MAP, the MAP summary of the posterior clustering, the last valid sample of cluster labels x\$Clust\$last.z, the matrix of posterior cluster membership probabilities x\$Clust\$post.prob, and the posterior confusion matrix x\$Clust\$PCM.

More detail is given if known zlabels are supplied: performance is always evaluated against the MAP clustering, with additional evaluation against the alternative clustering computed if z.avgsim=TRUE. Posterior summaries of the mixing proportions, and the concentration/discount parameters, if necessary, are also included here, as well as the last valid samples of each.

Error

Everything pertaining the model fit assessment can be found here, incl. the distribution of the PPRE values and associated bin counts for the replicate draws, as well as average error metrics (e.g. MSE, RMSE), and credible intervals quantifying the associated uncertainty, between the empirical and estimated covariance matrix/matrices, both of which are also included.

GQ.results

Everything pertaining to model choice can be found here, incl. posterior summaries for the estimated number of clusters and estimated number of factors, if applicable to the method employed. Model selection criterion values are also accessible here.

Means

Posterior summaries for the means, after conditioning on G.

Loadings

Posterior summaries for the factor loadings matrix/matrices, after conditioning on G and Q. Posterior mean loadings given by x\$Loadings\$post.load are given the loadings class for printing purposes and thus the manner in which they are displayed can be modified.

The number of iterations retained for posterior summaries of the loadings may vary for different clusters for the infinite factor methods, corresponding to iterations where the cluster-specific number of factors was greater than or equal to the modal estimate of the cluster-specific number of factors.

Scores

Posterior summaries for the latent factor scores, after conditioning on the maximum of the estimated number of cluster-specific factors. Summaries are given for the *single* matrix of factor scores. See scores\_MAP to decompose these summaries into sub-matrices according to the MAP partition (for models which achieve clustering).

For the infinite factor methods, iterations where the maximum number of factors was greater than or equal to the maximum of the estimated cluster-specific factors are retained for posterior summaries of the scores, in order to preserve the estimated dimension of the scores matrices.

Uniquenesses

Posterior summaries for the uniquenesses, after conditioning on G.

The objects Means, Loadings, Scores and Uniquenesses (if stored when calling mcmc\_IMIFA!) also contain, as well as the posterior summaries, the entire chain of valid samples of each, as well as, for convenience, the last valid samples of each (after conditioning on the modal G and Q values, and accounting for label switching, and rotational invariance via Procrustes rotation).

# Note

For the "IMIFA", "IMFA", "OMIFA", and "OMFA" methods, the retained mixing proportions are renormalised after conditioning on the modal G. This is especially necessary for the computation of the

error.metrics, just note that the values on which posterior inference are conducted will ever so slightly differ from the actually sampled values.

Due to the way the offline label-switching correction is performed, different runs of this function may give *very slightly* different results in terms of the cluster labellings (and by extension the parameters, which are permuted in the same way), but only if the chain was run for an extremely small number of iterations, well below the number required for convergence, and samples of the cluster labels match poorly across iterations (particularly if the number of clusters suggested by those sampled labels is high).

#### Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

#### See Also

plot.Results\_IMIFA, mcmc\_IMIFA, Zsimilarity, scores\_MAP, sim\_IMIFA\_model, Procrustes, varimax, norm

```
# data(coffee)
# data(olive)
# Run a MFA model on the coffee data over a range of clusters and factors.
# simMFAcoffee <- mcmc_IMIFA(coffee, method="MFA", range.G=2:3, range.Q=0:3, n.iters=1000)
# Accept all defaults to extract the optimal model.
# resMFAcoffee <- get_IMIFA_results(simMFAcoffee)</pre>
# Instead let's get results for a 3-cluster model, allowing Q be chosen by aic.mcmc.
# resMFAcoffee2 <- get_IMIFA_results(simMFAcoffee, G=3, criterion="aic.mcmc")</pre>
# Run an IMIFA model on the olive data, accepting all defaults.
# simIMIFAolive <- mcmc_IMIFA(olive, method="IMIFA", n.iters=10000)</pre>
# Extract optimum results
# Estimate G & Q by the median of their posterior distributions
# Construct 90% credible intervals and try to return the similarity matrix.
# resIMIFAolive <- get_IMIFA_results(simIMIFAolive, G.meth="median", Q.meth="median",
                                     conf.level=0.9, z.avgsim=TRUE)
# summary(resIMIFAolive)
# Simulate new data from the above model
# newdata
               <- sim_IMIFA_model(resIMIFAolive)
```

gumbel\_max 15

gumbel_max	Simulate Cluster Labels from Unnormalised Log-Probabilities using the Gumbel-Max Trick

### **Description**

Samples cluster labels for N observations from G clusters efficiently using log-probabilities and the so-called Gumbel-Max trick, without requiring that the log-probabilities be normalised; thus redundant computation can be avoided.

### Usage

### **Arguments**

probs An N x G matrix of unnormalised probabilities on the log scale, where N is he

number of observations that require labels to be sampled and G is the number of

active clusters s.t. sampled labels can take values in 1:G. Typically N > G.

slice A logical indicating whether or not the indicator correction for slice sampling

has been applied to probs. Defaults to FALSE but is TRUE for the "IMIFA" and "IMFA" methods under mcmc\_IMIFA. Details of this correction are given in Murphy et. al. (2020). When set to TRUE, this results in a speed-improvement when probs contains non-finite values (e.g. -Inf, corresponding to zero on the prob-

ability scale).

# **Details**

Computation takes place on the log scale for stability/underflow reasons (to ensure negligible probabilities won't cause computational difficulties); in any case, many functions for calculating multivariate normal densities already output on the log scale.

#### Value

A vector of N sampled cluster labels, with the largest label no greater than G.

#### Note

Though the function is available for standalone use, note that no checks take place, in order to speed up repeated calls to the function inside mcmc\_IMIFA.

If the normalising constant is required for another reason, e.g. to compute the log-likelihood, it can be calculated by summing the output obtained by calling rowLogSumExps on probs.

# Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

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#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

Yellott, J. I. Jr. (1977) The relationship between Luce's choice axiom, Thurstone's theory of comparative judgment, and the double exponential distribution, *Journal of Mathematical Psychology*, 15(2): 109-144.

### See Also

```
mcmc_IMIFA, rowLogSumExps
```

### **Examples**

```
# Create weights for 3 components
            <- 3
 weights
            <- seq_len(G)
# Call gumbel_max() repeatedly to obtain samples of the labels, zs
 iters
            <- 10000
            <- vapply(seq_len(iters), function(i)</pre>
 zs
               gumbel_max(probs=log(weights)), numeric(1L))
# Compare answer to the normalised weights
 tabulate(zs, nbins=G)/iters
 (normalised <- as.numeric(weights/sum(weights)))</pre>
# Simulate a matrix of Dirichlet weights & the associated vector of N labels
          <- 400
 G
          <- 8
         <- seq(from=85, to=15, by=-10)
 sizes
 weights <- matrix(rDirichlet(N * G, alpha=1, nn=sizes), byrow=TRUE, nrow=N, ncol=G)</pre>
          <- gumbel_max(probs=log(weights)))
```

**G\_moments** 

1st & 2nd Moments of the Pitman-Yor / Dirichlet Processes

### **Description**

Calculate the *a priori* expected number of clusters (G\_expected) or the variance of the number of clusters (G\_variance) under a PYP or DP prior for a sample of size N at given values of the concentration parameter alpha and optionally also the Pitman-Yor discount parameter. Useful for soliciting sensible priors (or fixed values) for alpha or discount under the "IMFA" and "IMIFA" methods for mcmc\_IMIFA. Additionally, for a given sample size N and given expected number of clusters EG, G\_calibrate elicits a value for the concentration parameter alpha **or** the discount parameter.

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### Usage

### **Arguments**

	TT1 1	
N	The sample	C176
11	The sample	DIZC.

alpha The concentration parameter. Must be specified (though not for G\_calibrate)

and must be strictly greater than -discount. The case alpha=0 is accommodated. When discount is negative alpha must be a positive integer multiple of

abs(discount). See **Details** for behaviour for G\_calibrate.

discount The discount parameter for the Pitman-Yor process. Must be less than 1, but typ-

ically lies in the interval [0, 1). Defaults to 0 (i.e. the Dirichlet process). When discount is negative alpha must be a positive integer multiple of abs(discount).

See **Details** for behaviour for G\_calibrate.

MPFR Logical indicating whether the high-precision libraries Rmpfr and gmp are in-

voked, at the expense of run-time. Defaults to TRUE and **must** be TRUE for G\_expected when alpha=0 or G\_variance when discount is non-zero. For G\_calibrate, it is *strongly recommended* to use MPFR=TRUE when discount is

non-zero and strictly necessary when alpha=0 is supplied. See Note.

EG The prior expected number of clusters. Must exceed 1 and be less than N.

... Additional arguments passed to uniroot, e.g. maxiter.

## **Details**

All arguments are vectorised. Users can also consult G\_priorDensity in order to solicit sensible priors.

For G\_calibrate, **only one** of alpha or discount can be supplied, and the function elicits a value for the opposing parameter which achieves the desired expected number of clusters EG for the given sample size N. By default, a value for alpha subject to discount=0 (i.e. the Dirichlet process) is elicited. Note that alpha may not be a positive integer multiple of discount as it should be if discount is negative. See **Examples** below.

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#### Value

The expected number of clusters under the specified prior conditions (G\_expected), or the variance of the number of clusters (G\_variance), or the concentration parameter alpha **or** discount parameter achieving a particular expected number of clusters (G\_calibrate).

### Note

G\_variance requires use of the Rmpfr and gmp libraries for non-zero discount values. G\_expected requires these libraries only for the alpha=0 case. These libraries are *strongly recommended* (but they are not required) for G\_calbirate when discount is non-zero, but they are required when alpha=0 is supplied. Despite the high precision arithmetic used, the functions can still be unstable for large N and/or extreme values of alpha and/or discount. See the argument MPFR.

### Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

#### References

De Blasi, P., Favaro, S., Lijoi, A., Mena, R. H., Prunster, I., and Ruggiero, M. (2015) Are Gibbstype priors the most natural generalization of the Dirichlet process?, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 37(2): 212-229.

Yamato, H. and Shibuya, M. (2000) Moments of some statistics of Pitman sampling formula, *Bulletin of Informatics and Cybernetics*, 32(1): 1-10.

#### See Also

```
G_priorDensity, Rmpfr, uniroot
```

G\_priorDensity 19

```
# G_variance(N=50, alpha=c(27.1401, 0), discount=c(-27.1401/100, 0.8054448))
# Elicit values for alpha under a DP prior
G_calibrate(N=50, EG=25)
# Elicit values for alpha under a PYP prior
# require("Rmpfr")
# G_calibrate(N=50, EG=25, discount=c(-27.1401/100, 0.25, 0.7300045))
# Elicit values for discount under a PYP prior
# G_calibrate(N=50, EG=25, alpha=c(12.21619, 1, 0), maxiter=2000)
```

G\_priorDensity

Plot Pitman-Yor / Dirichlet Process Priors

# **Description**

Plots the prior distribution of the number of clusters under a Pitman-Yor / Dirichlet process prior, for a sample of size N at given values of the concentration parameter alpha and optionally also the discount parameter. Useful for soliciting sensible priors (or fixed values) for alpha or discount under the "IMFA" and "IMIFA" methods for mcmc\_IMIFA.

# Usage

# **Arguments**

N	The sample size.
alpha	The concentration parameter. Must be specified and must be strictly greater than -discount. The case alpha=0 is accommodated. When discount is negative alpha must be a positive integer multiple of abs(discount).
discount	The discount parameter for the Pitman-Yor process. Must be less than 1, but typically lies in the interval [0, 1). Defaults to 0 (i.e. the Dirichlet process). When discount is negative alpha must be a positive integer multiple of abs(discount).
show.plot	Logical indicating whether the plot should be displayed (default = TRUE).
type	The type of plot to be drawn, as per plot. Defaults to "h": histogram-like vertical lines.

### **Details**

All arguments are vectorised. Users can also consult G\_expected, G\_variance, and G\_calibrate in order to solicit sensible priors.

 $G_{prior}$   $G_{prior}$   $G_{prior}$ 

#### Value

A plot of the prior distribution if show.plot is TRUE. Density values are returned invisibly. Note that the density values may not strictly sum to one in certain cases, as values small enough to be represented as zero may well be returned.

#### Note

The actual density values are returned invisibly. Therefore, they can be visualised as desired by the user even if show.plot is FALSE.

Requires use of the Rmpfr and gmp libraries; may encounter difficulty and slowness for large N, especially with non-zero discount values. Despite the high precision arithmetic used, the functions can be unstable for small values of discount.

### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### References

De Blasi, P., Favaro, S., Lijoi, A., Mena, R. H., Prunster, I., and Ruggiero, M. (2015) Are Gibbstype priors the most natural generalization of the Dirichlet process?, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 37(2): 212-229.

# See Also

```
G_moments, Rmpfr
```

heat\_legend 21

heat_legend	Add a colour key legend to heatmap plots	
-------------	--	--

# Description

Using only base graphics, this function appends a colour key legend for heatmaps produced by, for instance, plot\_cols or image.

# Usage

# Arguments

data	Either the data with which the heatmap was created or a vector containing its minimum and maximum values. Missing values are ignored.
cols	The colour palette used when the heatmap was created. By default, the same viridis default as in mat2cols is used. Will be checked for validity by is.cols.
breaks	Optional argument giving the break-points for the axis labels
cex.lab	Magnification of axis annotation, indicating the amount by which plotting text and symbols should be scaled relative to the default of 1.
	Catches unused arguments.

# Value

Modifies an existing plot by adding a colour-key legend.

### See Also

```
image, plot_cols, mat2cols, is.cols
```

```
# Generate a matrix and plot it with a legend
data <- matrix(rnorm(50), nrow=10, ncol=5)
cols <- heat.colors(12)[12:1]
par(mar=c(5.1, 4.1, 4.1, 3.1))

plot_cols(mat2cols(data, col=cols))
heat_legend(data, cols); box(lwd=2)</pre>
```

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IMIFA\_news

Show the NEWS file

# Description

Show the NEWS file of the IMIFA package.

# Usage

```
IMIFA_news()
```

# Value

The IMIFA NEWS file, provided the session is interactive.

# **Examples**

```
IMIFA_news()
```

is.cols

Check for Valid Colours

# Description

Checks if the supplied vector contains valid colours.

# Usage

```
is.cols(cols)
```

# **Arguments**

cols

A vector of colours, usually as a character string.

# Value

A logical vector of length length(cols) which is TRUE for entries which are valid colours and FALSE otherwise.

```
all(is.cols(1:5))
all(is.cols(heat.colors(30)))
any(!is.cols(c("red", "green", "aquamarine")))
```

is.posi\_def 23

is.posi_def	Check Positive-(Semi)definiteness of a matrix
	· · · · · · · · · · · · · · · · · · ·

### **Description**

Tests whether all eigenvalues of a symmetric matrix are positive (or strictly non-negative) to check for positive-definiteness and positive-semidefiniteness, respectively. If the supplied matrix doesn't satisfy the test, the nearest matrix which does can optionally be returned.

# Usage

# Arguments

Χ	A matrix, assumed to be real and symmetric.
---	---

tol Tolerance for singular values and for absolute eigenvalues - only those with

values larger than tol are considered non-zero.

(default: tol = max(dim(x))\*max(E)\*.Machine\$double.eps, where E is the

vector of absolute eigenvalues).

semi Logical switch to test for positive-semidefiniteness when TRUE or positive-definiteness

when FALSE (the default).

make Logical switch to return the nearest matrix which satisfies the test - if the test

has been passed, this is of course just x itself, otherwise the nearest positive-(semi)definite matrix. Note that for reasons due to finite precision arithmetic, finding the nearest positive-definite and nearest positive-semidefinite matrices

are effectively equivalent tasks.

# Value

If isTRUE(make), a list with two components:

check A logical value indicating whether the matrix satisfies the test.

X. new The nearest matrix which satisfies the test (which may just be the input matrix

itself.)

Otherwise, only the logical value indicating whether the matrix satisfies the test is returned.

```
x <- cov(matrix(rnorm(100), nrow=10, ncol=10))
is.posi_def(x) #FALSE
is.posi_def(x, semi=TRUE) #TRUE</pre>
```

24 Itrgamma

```
Xnew <- is.posi_def(x, semi=FALSE, make=TRUE)$X.new
identical(x, Xnew) #FALSE
identical(x, is.posi_def(x, semi=TRUE, make=TRUE)$X.new) #TRUE</pre>
```

Ledermann

Ledermann Bound

# **Description**

Returns the maximum number of latent factors in a factor analysis model for data of dimension P which actually achieves dimension reduction in terms of the number of covariance parameters. This Ledermann bound is given by the largest integer smaller than or equal to the solution k of  $(M-k)^2 \ge M+k$ .

# Usage

# **Arguments**

P Integer number of variables in data set. This argument is vectorised.

isotropic Logical indicating whether uniquenesses are constrained to be isotropic, in which

case the bound is simply P-1. Defaults to FALSE.

#### Value

The Ledermann bound, a non-negative integer, or a vector of length(P) such bounds.

# **Examples**

```
Ledermann(c(25, 50, 100))
data(olive)
Ledermann(ncol(olive[,-c(1,2)]))
```

1trgamma

Left Truncated Gamma Distributions

# **Description**

Functions to draw pseudo-random numbers from, or calculate the expectation of, left-truncated gamma distributions (see Details below).

Itrgamma 25

# Usage

### Arguments

n	Number of observations to generate.
shape	Shape parameter for the desired gamma distribution. Must be strictly positive
rate	Rate parameter for the desired gamma distribution. Must be strictly positive.
trunc	The point of left truncation (corresponding to $\tau$ below). Defaults to 1. Must be non-negative. When inverse is TRUE, this becomes the point of <i>right</i> truncation.
inverse	A logical indicating whether to calculate the expectation for a right-truncated <i>inverse</i> gamma distribution instead of a left-truncated gamma distribution. Defaults to FALSE.

#### **Details**

The left-truncated gamma distribution has PDF:

$$f(x|\alpha,\beta) = \frac{\beta^{\alpha}}{(\Gamma(\alpha) - \Gamma(\alpha,\tau\beta))} x^{\alpha-1} e^{-x\beta}$$

for  $0 \le \tau \le x$ , and  $\min(\tau, \beta) > 0$ , where  $\alpha$  and  $\beta$  are the shape and rate parameters, respectively,  $\tau$  is the cutoff point at which truncation occurs, and  $\Gamma(\alpha, \tau\beta)$  is the upper incomplete gamma function.

# Value

For rltrgamma, a vector of length n giving draws from the left-truncated gamma distribution with the specified shape and rate parameters, and truncation point trunc.

For exp\_ltrgamma, the expected value of a left-truncated (inverse) gamma distribution.

## Note

rltrgamma is invoked internally for the "IFA", "MIFA", "OMIFA", and "IMIFA" models to draw column shrinkage parameters for all but the first loadings column under the MGP prior when truncated=TRUE (which is **not** the default) is supplied to mgpControl, at the expense of slightly longer run times. exp\_ltrgamma is used within MGP\_check to check the validity of the MGP hyperparameters when truncated=TRUE (which is again, **not** the default). Both functions always assume trunc=1 for these internal usages.

Note also that no arguments are recycled, i.e. all arguments must be of length 1.

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### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### References

Dagpunar, J. S. (1978) Sampling of variates from a truncated gamma distribution, *Statistical Computation and Simulation*, 8(1): 59-64.

### See Also

```
mgpControl, MGP_check
```

# **Examples**

```
# Generate left-truncated Ga(3.1, 2.1, 1) variates
rltrgamma(n=10, shape=3.1, rate=2.1)

# Calculate the expectation of a Ga(3.1, 2.1, 1) distribution
exp_ltrgamma(shape=3.1, rate=2.1)

# Calculate the expectation of an inverse gamma distribution right-truncated at 2
exp_ltrgamma(shape=3.1, rate=2.1, trunc=2, inverse=TRUE)
```

mat2cols

Convert a numeric matrix to colours

# **Description**

Converts a matrix to a hex colour code representation for plotting using plot\_cols. Used internally by plot.Results\_IMIFA for plotting posterior mean loadings heatmaps.

# Usage

# **Arguments**

mat Either a matrix or, when compare is TRUE, a list of matrices.

The colour palette to be used. The default palette uses viridis. Will be checked

for validity by is.cols.

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compare	Logical switch used when desiring comparable colour representations (usually for comparable heat maps) across multiple matrices. Ensures plots will be calibrated to a common colour scale so that, for instance, the colour on the heat map of an entry valued at 0.7 in Matrix A corresponds exactly to the colour of a similar value in Matrix B. When TRUE, mat must be supplied as a list of matrices, which must have either the same number of rows, or the same number of columns.
byrank	Logical indicating whether to convert the matrix itself or the sample ranks of the values therein. Defaults to FALSE.
breaks	Number of gradations in colour to use. Defaults to length(cols). Alternatively, a vector of breakpoints for use with cut.
na.col	Colour to be used to represent missing data. Will be checked for validity by is.cols.
transparency	A factor in [0, 1] modifying the opacity for overplotted lines. Defaults to 1 (i.e. no transparency). Only relevant when cols is not supplied, otherwise the supplied cols must already be adjusted for transparency.
	Catches unused arguments.

#### Value

A matrix of hex colour code representations, or a list of such matrices when compare is TRUE.

### See Also

```
plot_cols, heat_legend, is.cols, cut
```

```
# Generate a colour matrix using mat2cols()
mat <- matrix(rnorm(100), nrow=10, ncol=10)</pre>
mat[2,3] \leftarrow NA
cols
        <- heat.colors(12)[12:1]
(matcol <- mat2cols(mat, cols=cols))</pre>
# Use plot_cols() to visualise the colours matrix
par(mar=c(5.1, 4.1, 4.1, 3.1))
plot_cols(matcol)
# Add a legend using heat_legend()
heat_legend(mat, cols=cols); box(lwd=2)
# Try comparing heat maps of multiple matrices
        <- cbind(matrix(rnorm(100, sd=c(4,2)), nr=50, nc=2, byrow=TRUE), 0.1)</pre>
mat2
         <- cbind(matrix(rnorm(150, sd=c(7,5,3)), nr=50, nc=3, byrow=TRUE), 0.1)</pre>
mat3
        <- cbind(matrix(rnorm(50, sd=1), nr=50, nc=1, byrow=TRUE), 0.1)
         <- list(mat1, mat2, mat3)
colmats <- mat2cols(mats, cols=cols, compare=TRUE)</pre>
par(mfrow=c(2, 3), mar=c(1, 2, 1, 2))
```

```
# Use common palettes (top row)
plot_cols(colmats[[1]]); heat_legend(range(mats), cols=cols); box(lwd=2)
plot_cols(colmats[[2]]); heat_legend(range(mats), cols=cols); box(lwd=2)
plot_cols(colmats[[3]]); heat_legend(range(mats), cols=cols); box(lwd=2)

# Use uncommon palettes (bottom row)
plot_cols(mat2cols(mat1, cols=cols)); heat_legend(range(mat1), cols=cols); box(lwd=2)
plot_cols(mat2cols(mat2, cols=cols)); heat_legend(range(mat2), cols=cols); box(lwd=2)
plot_cols(mat2cols(mat3, cols=cols)); heat_legend(range(mat3), cols=cols); box(lwd=2)
```

mcmc\_IMIFA

Adaptive Gibbs Sampler for Nonparametric Model-based Clustering using models from the IMIFA family

# **Description**

Carries out Gibbs sampling for all models from the IMIFA family, facilitating model-based clustering with dimensionally reduced factor-analytic covariance structures, with automatic estimation of the number of clusters and cluster-specific factors as appropriate to the method employed. Factor analysis with one group (FA/IFA), finite mixtures (MFA/MIFA), overfitted mixtures (OMFA/OMIFA), infinite factor models which employ the multiplicative gamma process (MGP) shrinkage prior (IFA/MIFA/OMIFA/IMIFA), and infinite mixtures which employ Pitman-Yor / Dirichlet Process Mixture Models (IMFA/IMIFA) are all provided.

# Usage

```
mcmc_IMIFA(dat,
           method = c("IMIFA", "IMFA",
                       "OMIFA", "OMFA",
                       "MIFA", "MFA",
                       "IFA", "FA",
                       "classifv").
           range.G = NULL,
           range.Q = NULL,
           MGP = mgpControl(...),
           BNP = bnpControl(...),
           mixFA = mixfaControl(...),
           alpha = NULL,
            storage = storeControl(...),
            ...)
## S3 method for class 'IMIFA'
print(x,
      . . . )
## S3 method for class 'IMIFA'
summary(object,
        ...)
```

#### **Arguments**

dat

A matrix or data frame such that rows correspond to observations (N) and columns correspond to variables (P). Non-numeric variables will be discarded if they are explicitly coded as factors or ordinal factors; otherwise they will be treated as though they were continuous. Rows with missing entries will be also be automatically removed.

method

An acronym for the type of model to fit where:

"FA" Factor Analysis

"IFA" Infinite Factor Analysis

"MFA" Mixtures of Factor Analysers

"MIFA" Mixtures of Infinite Factor Analysers

"OMFA" Overfitted Mixtures of Factor Analysers

"OMIFA" Overfitted Mixtures of Infinite Factor Analysers

"IMFA" Infinite Mixtures of Factor Analysers

"IMIFA" Infinite Mixtures of Infinite Factor Analysers

In principle, of course, one could overfit the "MFA" or "MIFA" models, but it is recommend to use the corresponding model options which begin with 'O' instead. Note that the "classify" method is not yet implemented.

range.G

Depending on the method employed, either the range of values for the number of clusters, or the conservatively high starting value for the number of clusters. Defaults to (and must be!) 1 for the "FA" and "IFA" methods. For the "MFA" and "MIFA" models this is to be given as a range of candidate models to explore. For the "OMFA", "OMIFA", "IMFA", and "IMIFA" models, this is the conservatively high number of clusters with which the chain is to be initialised (default =  $\max(25, \text{ceiling}(3 * \log(N)))$ ) for large N, or  $\min(N-1, \text{ceiling}(3 * \log(N)))$  for small N<=50).

For the "OMFA", and "OMIFA" models this upper limit remains fixed for the entire length of the chain; the upper limit for the for the "IMFA" and "IMIFA" models can be specified via trunc.G (see bnpControl), which must satisfy range.G <= trunc.G < N.

If length(range.G) \* length(range.Q) is large, consider not storing unnecessary parameters (via storeControl), or breaking up the range of models to be explored into chunks and sending each chunk to get\_IMIFA\_results separately.

range.Q

Depending on the method employed, either the range of values for the number of latent factors or, for methods ending in IFA, the conservatively high starting value for the number of cluster-specific factors, in which case the default starting value is round(3 \* log(P)).

For methods ending in IFA, different clusters can be modelled using different numbers of latent factors (incl. zero); for methods not ending in IFA it is possible to fit zero-factor models, corresponding to simple diagonal covariance structures. For instance, fitting the "IMFA" model with range .Q=0 corresponds to a vanilla Pitman-Yor / Dirichlet Process Mixture Model.

If length(range.G) \* length(range.Q) is large, consider not storing unnecessary parameters (via storeControl), or breaking up the range of models to be explored into chunks and sending each chunk to get\_IMIFA\_results.

See Ledermann for bounds on range. Q; this is useful in both the finite factor and infinite factor settings, as one may wish to ensure the fixed number of factors, or upper limits on the number of factors, respectively, respects this bound to yield indentifiable solutions, particularly in low-dimensional settings.

MGP

A list of arguments pertaining to the multiplicative gamma process (MGP) shrinkage prior and adaptive Gibbs sampler (AGS). For use with the infinite factor models "IFA", "MIFA", "OMIFA", and "IMIFA" only. Defaults are set by a call to mgpControl, with further checking of validity by MGP\_check (though arguments can also be supplied here directly).

BNP

A list of arguments pertaining to the Bayesian Nonparametric Pitman-Yor / Dirichlet process priors, for use with the infinite mixture models "IMFA" and "IMIFA", or select arguments related to the Dirichlet concentration parameter for the overfitted mixtures "OMFA" and "OMIFA". Defaults are set by a call to bnpControl (though arguments can also be supplied here directly).

mixFA

A list of arguments pertaining to *all other* aspects of model fitting, e.g. MCMC settings, cluster initialisation, and hyperparameters common to every method in the IMIFA family. Defaults are set by a call to mixfaControl (though arguments can also be supplied here directly).

alpha

Depending on the method employed, either the hyperparameter of the Dirichlet prior for the cluster mixing proportions, or the Pitman-Yor / Dirichlet process concentration parameter. Defaults to 1 for the finite mixture models "MFA" and "MIFA", and must be a strictly positive scalar. Not relevant for the "FA" and "IFA" methods.

Under the "IMFA" and "IMIFA" models: alpha defaults to a simulation from the prior if learn. alpha is TRUE, otherwise alpha *must* be specified. Must be positive, unless non-zero discount is supplied or learn.d=TRUE (the default), in which case it must be greater than -discount. Under certain conditions, alpha can remain fixed at 0 (see bnpControl). Additionally, when discount is negative, alpha must be a positive integer multiple of abs(discount) (default=range.G \* abs(discount)).

**Under the** "OMFA" **and** "OMIFA" **models:** alpha defaults to a simulation from the prior if learn. alpha is TRUE, otherwise alpha defaults to 0.5/range.G. If supplied, alpha must be positive, and you are supplying the numerator of alpha/range.G.

If alpha remains fixed (i.e. learn.alpha=FALSE), alpha should be less than half the dimension (per cluster!) of the free parameters of the smallest model considered in order to ensure superfluous clusters are emptied (for "OMFA", this corresponds to the smallest range.Q; for "OMIFA", this corresponds to a zero-factor model) [see: PGMM\_dfree and Rousseau and Mengersen (2011)].

See bnpControl for further details of specifying alpha or specifying a prior for alpha under the "IMFA", "IMIFA", "OMFA", or "OMIFA" methods.

storage

A vector of named logical indicators governing storage of parameters of interest for all models in the IMIFA family. Defaults are set by a call to storeControl. It may be useful not to store certain parameters if memory is an issue.

... An alternative means of passing control parameters directly via the named arguments of mixfaControl, mgpControl, bnpControl, and storeControl. Do not pass the output from calls to those functions here!

x, object Object of class "IMIFA", for the print.IMIFA and summary.IMIFA functions, respectively.

#### **Details**

Creates a raw object of class "IMIFA" from which the optimal/modal model can be extracted by get\_IMIFA\_results. Dedicated print and summary functions exist for objects of class "IMIFA".

#### Value

A list of lists of lists of class "IMIFA" to be passed to get\_IMIFA\_results. If the returned object is x, candidate models are accessible via subsetting, where x is of the following form:

```
x[[1:length(range.G)]][[1:length(range.Q)]].
```

However, these objects of class "IMIFA" should rarely if ever be manipulated by hand - use of the get\_IMIFA\_results function is *strongly* advised.

#### Note

Further control over the specification of advanced function arguments can be obtained with recourse to the following functions:

- mgpControl Supply arguments (with defaults) pertaining to the multiplicative gamma process (MGP) shrinkage prior and adaptive Gibbs sampler (AGS). For use with the infinite factor models "IFA", "MIFA", "OMIFA", and "IMIFA" only.
- bnpControl Supply arguments (with defaults) pertaining to the Bayesian Nonparametric Pitman-Yor / Dirichlet process priors, for use with the infinite mixture models "IMFA" and "IMIFA". Certain arguments related to the Dirichlet concentration parameter for the overfitted mixtures "OMFA" and "OMIFA" can be supplied in this manner also.
- mixfaControl Supply arguments (with defaults) pertaining to *all other* aspects of model fitting (e.g. MCMC settings, cluster initialisation, and hyperparameters common to every method in the IMIFA family.
- storeControl Supply logical indicators governing storage of parameters of interest for all models in the IMIFA family. It may be useful not to store certain parameters if memory is an issue (e.g. for large data sets or for a large number of MCMC iterations after burnin and thinning).

Note however that the named arguments of these functions can also be supplied directly. Parameter starting values are obtained by simulation from the relevant prior distribution specified in these control functions, though initial means and mixing proportions are computed empirically.

#### Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

Bhattacharya, A. and Dunson, D. B. (2011) Sparse Bayesian infinite factor models, *Biometrika*, 98(2): 291-306.

Kalli, M., Griffin, J. E. and Walker, S. G. (2011) Slice sampling mixture models, *Statistics and Computing*, 21(1): 93-105.

Rousseau, J. and Mengersen, K. (2011) Asymptotic Behaviour of the posterior distribution in over-fitted mixture models, *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 73(5): 689-710.

McNicholas, P. D. and Murphy, T. B. (2008) Parsimonious Gaussian mixture models, *Statistics and Computing*, 18(3): 285-296.

#### See Also

get\_IMIFA\_results, mixfaControl, mgpControl, bnpControl, storeControl, Ledermann

```
# data(olive)
# data(coffee)
# Fit an IMIFA model to the olive data. Accept all defaults.
# simIMIFA <- mcmc_IMIFA(olive, method="IMIFA")</pre>
# summary(simIMIFA)
# Fit an IMIFA model assuming a Pitman-Yor prior.
# Control the balance between the DP and PY priors using the kappa parameter.
# simPY
           <- mcmc_IMIFA(olive, method="IMIFA", kappa=0.75)</pre>
# summary(simPY)
# Fit a MFA model to the scaled olive data, with isotropic uniquenesses (i.e. MPPCA).
# Allow diagonal covariance as a special case where range 0 = 0.
# Don't store the scores. Accept all other defaults.
# simMFA <- mcmc_IMIFA(olive, method="MFA", n.iters=10000, range.G=3:6, range.Q=0:3,
                         score.switch=FALSE, centering=FALSE, uni.type="isotropic")
# Fit a MIFA model to the centered & scaled coffee data, w/ cluster labels initialised by K-Means.
# Note that range.Q doesn't need to be specified. Allow IFA as a special case where range.G=1.
# simMIFA <- mcmc_IMIFA(coffee, method="MIFA", n.iters=10000, range.G=1:3, z.init="kmeans")
# Fit an IFA model to the centered and pareto scaled olive data.
# Note that range.G doesn't need to be specified. We can optionally supply a range.Q starting value.
# Enforce additional shrinkage using alpha.d1, alpha.d2, prop, and eps (via mgpControl()).
# simIFA <- mcmc_IMIFA(olive, method="IFA", n.iters=10000, range.Q=4, scaling="pareto",
                         alpha.d1=2.5, alpha.d2=4, prop=0.6, eps=0.12)
# Fit an OMIFA model to the centered & scaled coffee data.
# Supply a sufficiently small alpha value. Try varying other hyperparameters.
# Accept the default value for the starting number of factors,
```

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```
# but supply a value for the starting number of clusters.
# Try constraining uniquenesses to be common across both variables and clusters.
# simOMIFA <- mcmc_IMIFA(coffee, method="OMIFA", range.G=10, psi.alpha=3,
# phi.hyper=c(2, 1), alpha=0.8, uni.type="single")</pre>
```

mgpControl

Control settings for the MGP prior and AGS for infinite factor models

# **Description**

Supplies a list of arguments for use in mcmc\_IMIFA pertaining to the use of the multiplicative gamma process (MGP) shrinkage prior and adaptive Gibbs sampler (AGS) for use with the infinite factor models "IFA", "MIFA", "OMIFA", and "IMIFA".

### Usage

```
mgpControl(alpha.d1 = 2.1,
           alpha.d2 = 3.1,
           phi.hyper = c(3, 2),
           sigma.hyper = c(3, 2),
           prop = 0.7,
           eps = 0.1,
           adapt = TRUE,
           forceQg = FALSE,
           cluster.shrink = TRUE,
           truncated = FALSE,
           b0 = 0.1
           b1 = 5e-05,
           beta.d1 = 1,
           beta.d2 = 1,
           start.AGS = 2L,
           stop.AGS = Inf,
           delta0g = FALSE,
           ...)
```

# **Arguments**

alpha.d1

Shape hyperparameter of the column shrinkage on the first column of the loadings according to the MGP shrinkage prior. Passed to MGP\_check to ensure validity. Defaults to 2.1.

alpha.d2

Shape hyperparameter of the column shrinkage on the subsequent columns of the loadings according to the MGP shrinkage prior. Passed to MGP\_check to ensure validity. Defaults to 3.1.

phi.hyper

A vector of length 2 giving the shape and rate hyperparameters for the gamma prior on the local shrinkage parameters. Passed to MGP\_check to ensure validity. Defaults to c(3,2). It is suggested that the rate be <= shape minus 1 to induce local shrinkage, though the cumulative shrinkage property is unaffected by these

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> hyperparameters. Excessively small values may lead to critical numerical issues and should thus be avoided; indeed it is *suggested* that the shape be >=1.

sigma.hyper

A vector of length 2 giving the shape and rate hyperparameters for the gamma prior on the cluster shrinkage parameters. Passed to MGP\_check to ensure validity. Defaults to c(3,2). Again, it is *suggested* that the shape be  $\geq 1$ . Only relevant for the "IMIFA", "OMIFA", and "MIFA" methods when isTRUE(cluster.shrink).

prop

Proportion of loadings elements within the neighbourhood eps of zero necessary to consider a loadings column redundant. Defaults to floor (0.7 \* P)/P, where P is the number of variables in the data set. However, if the data set is univariate or bivariate, the default is 0.5 (see Note).

eps

Neighbourhood epsilon of zero within which a loadings entry is considered negligible according to prop. Defaults to 0.1. Must be positive.

adapt

A logical value indicating whether adaptation of the number of cluster-specific factors is to take place when the MGP prior is employed. Defaults to TRUE. Specifying FALSE and supplying range. Q within mcmc\_IMIFA provides a means to either approximate the infinite factor model with a fixed high truncation level, or to use the MGP prior in a finite factor context, however this is NOT recommended for the "OMIFA" and "IMIFA" methods.

forceQg

A logical indicating whether the upper limit on the number of cluster-specific factors Q is also cluster-specific. Defaults to FALSE: when TRUE, the number of factors in each cluster is kept below the number of observations in each cluster, in addition to the bound defined by range.Q. Only relevant for the "IMIFA", "OMIFA", and "MIFA" methods, and only invoked when adapt is TRUE. May be useful for low-dimensional data sets for which identifiable solutions are desired.

cluster.shrink A logical value indicating whether to place the prior specified by sigma.hyper on the cluster shrinkage parameters. Defaults to TRUE. Specifying FALSE is equivalent to fixing all cluster shrinkage parameters to 1. Only relevant for the "IMIFA", "OMIFA", and "MIFA" methods. If invoked, the posterior mean cluster shrinkage factors will be reported.

truncated

A logical value indicating whether the version of the MGP prior based on lefttruncated gamma distributions is invoked (see Zhang et al. reference below and additional relevant documentation in ltrgamma and MGP\_check). Defaults to FALSE. Note that, when TRUE, only the shrinkage parameters for the first loadings column are affected and the conditions needed to pass MGP\_check are much less strict. Moreover, more desirable shrinkage properties are easily obtained, at the expense of slightly longer run times.

b0, b1

Intercept & slope parameters for the exponentially decaying adaptation probability:

p(iter) = 1/exp(b0 + b1 \* (iter - start.AGS)).

Defaults to 0.1 & 0.00005, respectively. Must be non-negative and strictly positive, respectively, to ensure diminishing adaptation.

beta.d1

Rate hyperparameter of the column shrinkage on the first column of the loadings according to the MGP shrinkage prior. Passed to MGP\_check to ensure validity. Defaults to 1.

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beta.d2	Rate hyperparameter of the column shrinkage on the subsequent columns of the loadings according to the MGP shrinkage prior. Passed to MGP_check to ensure validity. Defaults to 1.
start.AGS	The iteration at which adaptation under the AGS is to begin. Defaults to burnin for the "IFA" and "MIFA" methods, defaults to 2 for the "OMIFA" and "IMIFA" methods, and defaults to 2 for all methods if the data set is univariate or bivariate. Cannot exceed burnin; thus defaults to the same value as burnin if necessary.
stop.AGS	The iteration at which adaptation under the AGS is to stop completely. Defaults to Inf, such that the AGS is never explicitly forced to stop (thereby overriding the diminishing adaptation probability after stop.AGS). Must be greater than start.AGS. The diminishing adaptation probability prior to stop.AGS is still governed by the arguments b0 and b1.
delta0g	Logical indicating whether the alpha.d1 and alpha.d2 hyperparameters can be cluster-specific. Defaults to FALSE. Only relevant for the "MIFA" method and only allowed when z.list is supplied within mcmc_IMIFA.
	Catches unused arguments.

#### Value

A named list in which the names are the names of the arguments related to the MGP and AGS and the values are the values supplied to the arguments.

### Note

Certain supplied arguments will be subject to further checks by MGP\_check to ensure the cumulative shrinkage property of the MGP prior holds according to the given parameterisation.

The adaptive Gibbs sampler (AGS) monitors the prop of loadings elements within the neighbour-hood eps of 0 and discards columns or simulates new columns on this basis. However, if at any stage the number of group-specific latent factors reaches zero, the decision to add columns is instead based on a simple binary trial with probability 1-prop, as there are no loadings entries to monitor.

#### Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

Durante, D. (2017). A note on the multiplicative gamma process, *Statistics & Probability Letters*, 122: 198-204.

Bhattacharya, A. and Dunson, D. B. (2011) Sparse Bayesian infinite factor models, *Biometrika*, 98(2): 291-306.

Zhang, X., Dunson, D. B., and Carin, L. (2011) Tree-structured infinite sparse factor model. In Getoor, L. and Scheffer, T. (Eds.), *Proceedings of the 28th International Conference on Machine Learning*, ICML'11, Madison, WI, USA, pp. 785-792. Omnipress.

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### See Also

```
mcmc_IMIFA, MGP_check, ltrgamma, mixfaControl, bnpControl, storeControl
```

# **Examples**

MGP\_check

Check the validity of Multiplicative Gamma Process (MGP) hyperparameters

### **Description**

Checks the hyperparameters for the multiplicative gamma process (MGP) shrinkage prior in order to ensure that the property of cumulative shrinkage (in expectation) holds, i.e. checks whether growing mass is assigned to small neighbourhoods of zero as the column index increases.

### Usage

# **Arguments**

ad1, ad2 Shape hyperparameters for  $\delta_1$  and  $\delta_k \forall k \geq 2$ , respectively.

Q

Number of latent factors. Defaults to 3, which is enough to check if the cumulative shrinkage property holds. Supply Q if the actual *a priori* expected shrinkage factors are of interest.

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phi.shape, phi.rate

The shape and rate hyperparameters for the gamma prior on the local shrinkage parameters. Not necessary for checking if the cumulative shrinkage property holds, but worth supplying both if the actual a priori expected shrinkage factors are of interest. The default value(s) depends on the value of inverse, but are chosen in such a way that the local shrinkage has no effect on the expectation unless both are supplied. Cannot be incorporated into the expectation if phi.shape < 1 and isTRUE(inverse).</pre>

sigma.shape, sigma.rate

The shape and rate hyperparameters for the gamma prior on the cluster shrinkage parameters. Not necessary for checking if the cumulative shrinkage property holds, but worth supplying both if the actual a priori expected shrinkage factors are of interest. The default value(s) depends on the value of inverse, but are chosen in such a way that the cluster shrinkage has no effect on the expectation unless both are supplied. Cannot be incorporated into the expectation if sigma.shape < 1 and isTRUE(inverse).</pre>

Rate hyperparameters for  $\delta_1$  and  $\delta_k \forall k \geq 2$ , respectively. Both default to 1. bd1, bd2

> A logical value indicating whether the version of the MGP prior based on lefttruncated gamma distributions is invoked (see ltrgamma and the Zhang et al. reference below). Defaults to FALSE. Note that, when TRUE, only the shrinkage parameters for the first loadings column are affected and the conditions needed to pass this check are much less strict. Moreover, more desirable shrinkage

properties are easily obtained.

Logical indicator for whether the cumulative shrinkage property is assessed against the induced Inverse Gamma prior, the default, or in terms of the Gamma prior (which is incorrect). This is always TRUE when used inside mcmc\_IMIFA:

the FALSE option exists only for demonstration purposes.

#### **Details**

truncated

inverse

This is called inside mcmc\_IMIFA for the "IFA", "MIFA", "OMIFA" and "IMIFA" methods. This function is vectorised with respect to the arguments ad1, ad2, phi.shape, phi.rate, sigma.shape, sigma.rate, bd1 and bd2.

#### Value

A list of length 2 containing the following objects:

- expectation The vector (or list of vectors) of actual expected a priori shrinkage factors.
- valid A logical (or vector of logicals) indicating whether the cumulative shrinkage property holds (in expectation).

### Note

It is recommended that ad2 be moderately large relative to ad1, even if valid can sometimes be TRUE when this is not the case (e.g. when truncated=TRUE). Similarly, satisfying this condition is no guarantee that valid will be TRUE, unless truncated=TRUE. Therefore, a warning is returned if ad1 <= ad2, regardless of the value taken by valid, when truncated=FALSE (the default).

### Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

Durante, D. (2017). A note on the multiplicative gamma process, *Statistics & Probability Letters*, 122: 198-204.

Bhattacharya, A. and Dunson, D. B. (2011). Sparse Bayesian infinite factor models, *Biometrika*, 98(2): 291-306.

Zhang, X., Dunson, D. B., and Carin, L. (2011) Tree-structured infinite sparse factor model. In Getoor, L. and Scheffer, T. (Eds.), *Proceedings of the 28th International Conference on Machine Learning*, ICML'11, Madison, WI, USA, pp. 785-792. Omnipress.

#### See Also

mcmc\_IMIFA, ltrgamma

### **Examples**

# Check if expected shrinkage under the MGP increases with the column index (WRONG approach!).  $MGP\_check(ad1=1.5, ad2=1.8, Q=10, phi.shape=3, inverse=FALSE)$valid #TRUE$ 

# Check if the induced IG prior on the MGP column shrinkage parameters # is stochastically increasing, thereby inducing cumulative shrinkage (CORRECT approach!). MGP\_check(ad1=1.5, ad2=1.8, Q=10, phi.shape=3, inverse=TRUE)\$valid #FALSE

# Check again with a parameterisation that IS valid and examine the expected shrinkage values (shrink <- MGP\_check(ad1=1.5, ad2=2.8, Q=10, phi.shape=2, phi.rate=0.5, inverse=TRUE))

# Check previously invalid parameterisation again using truncated version of the MGP prior  $MGP\_check(ad1=1.5, ad2=1.8, Q=10, phi.shape=3, truncated=FALSE)$ \$valid # TRUE

mixfaControl

Control settings for the IMIFA family of factor analytic mixtures

# **Description**

Supplies a list of arguments for use in mcmc\_IMIFA pertaining to *ALL* methods in the IMIFA family: e.g. MCMC settings, cluster initialisation, generic hyperparameters for factor-analytic mixtures, etc.

### Usage

```
mixfaControl(n.iters = 25000L,
             burnin = n.iters/5L,
             thinning = 2L,
             centering = TRUE,
             scaling = c("unit", "pareto", "none"),
             uni.type = c("unconstrained", "isotropic",
                           "constrained", "single"),
             psi.alpha = 2.5,
             psi.beta = NULL,
             mu.zero = NULL,
             sigma.mu = 1L,
             prec.mu = 0.01,
             sigma.l = 1L,
             z.init = c("hc", "kmeans", "list", "mclust", "priors"),
             z.list = NULL,
             equal.pro = FALSE,
             uni.prior = c("unconstrained", "isotropic"),
             mu0g = FALSE,
             psi0g = FALSE,
             drop@sd = TRUE,
             verbose = interactive(),
             ...)
```

# **Arguments**

n.iters The number of iterations to run the sampler for. Defaults to 25000.

burnin The number of burn-in iterations for the sampler. Defaults to n. iters/5. Note

that chains can also be burned in later, using get\_IMIFA\_results.

The thinning interval used in the simulation. Defaults to 2. No thinning correthinning sponds to 1. Note that chains can also be thinned later, using get\_IMIFA\_results.

> A logical value indicating whether mean centering should be applied to the data, defaulting to TRUE.

> The scaling to be applied - one of "unit", "none" or "pareto". Defaults to "unit".

> This argument specifies the type of constraint, if any, to be placed on the uniquenesses/idiosyncratic variances, i.e. whether a general diagonal matrix or isotropic diagonal matrix is to be assumed, and in turn whether these matrices are constrained to be equal across clusters. The default "unconstrained" corresponds to factor analysis (and mixtures thereof), whereas "isotropic" corresponds to probabilistic principal components analysers (and mixtures thereof).

> Constraints may be particularly useful when N <= P, though caution is advised when employing constraints for any of the infinite factor models, especially "isotropic" and "single", which may lead to overestimation of the number of clusters &/or factors if this specification is inappropriate. The four options correspond to the following 4 parsimonious Gaussian mixture models:

centering

scaling

uni.type

> "unconstrained" (UUU) - variable-specific and cluster-specific:  $\Psi_g = \Psi_g$ . "isotropic" (UUC) - cluster-specific, equal across variables:  $\Psi_g = \psi \mathcal{I}_p$ . "constrained" (UCU) - variable-specific, equal across clusters:  $\Psi_q = \Psi$ . "single" (UCC) - single value equal across clusters and variables:  $\Psi_g = \psi \mathcal{I}_p$ .

The first letter U here corresponds to constraints on loadings (not yet implemented), the second letter corresponds to uniquenesses constrained/unconstrained across clusters, and the third letter corresponds to the isotropic constraint on the uniquenesses. Of course, only the third letter is of relevance for the singlecluster "FA" and "IFA" models, such that "unconstrained" and "constrained" are equivalent for these models, and so too are "isotropic" and "single".

psi.alpha

The shape of the inverse gamma prior on the uniquenesses. Defaults to 2.5. Must be greater than 1 if psi.beta is *not* supplied. Otherwise be warned that values less than or equal to 1 may not bound uniquenesses sufficiently far away from 0, and the algorithm may therefore terminate. Also, excessively small values may lead to critical numerical issues and should thus be avoided.

psi.beta

The scale of the inverse gamma prior on the uniquenesses. Can be either a single parameter, a vector of variable specific scales, or (if psi0g is TRUE) a matrix of variable and cluster-specific scales. If this is not supplied, psi\_hyper is invoked to choose sensible values, depending on the value of uni.prior and the data size and dimension, for the "MFA" and "MIFA" models only, the value of psi0g. Excessively small values may lead to critical numerical issues and should thus be avoided.

Note that optional arguments to psi\_hyper can be supplied via the . . . construct here.

mu.zero

The mean of the prior distribution for the mean parameter. Either a scalar of a vector of appropriate dimension. Defaults to the sample mean of the data.

sigma.mu

The covariance of the prior distribution for the cluster mean parameters. Always assumed to be a diagonal matrix, and set to the identity matrix by default. Can also be a scalar by which the identity is multiplied, a vector of appropriate dimension; if supplied as a matrix, only the diagonal elements will be extracted. Specifying sigma.mu=NULL will use the diagonal entries of the sample covariance matrix: for unit-scaled data this is simply the identity again. See prec.mu for further control over the hypercovariance in the prior for the means.

A scalar controlling the degree of flatness of the prior for the cluster means by scaling sigma.mu (i.e. multiplying every element of sigma.mu by 1/prec.mu). Lower values lead to a more diffuse prior. Defaults to 0.01, such that the prior is relatively non-informative by default. Of course, prec.mu=1 nullifies any effect of this argument. The user can supply a scaled sigma.mu directly, but this argument is especially useful when specifying sigma.mu=NULL, such that the diagonal entries of the sample covariance matrix are used.

sigma.l

A scalar controlling the diagonal covariance of the prior distribution for the loadings. Defaults to 1, i.e. the identity; otherwise a diagonal matrix with non-zero entries all equal to sigma. 1 Only relevant for the finite factor methods.

z.init

The method used to initialise the cluster labels. Defaults to model-based agglomerative hierarchical clustering via "hc". Other options include "kmeans"

prec.mu

> (with 10 random starts, by default), Mclust via "mclust", random initialisation via "priors", and a user-supplied "list" (z.list). Not relevant for the "FA" and "IFA" methods. Arguments for the relevant functions can be passed via the . . . construct. For "hc", VVV is used by default, unless the data is highdimensional, in which case the default is EII. The option "priors" may lead to empty components at initialisation, which will return an error.

> In any case, unless z.list is explicitly supplied, or verbose is FALSE, the initial cluster sizes will be printed to the screen to alert users to potentially bad initialisiations (e.g. heavily imbalanced initial cluster sizes).

z.list A user supplied list of cluster labels. Only relevant if z.init == "z.list".

equal.pro Logical variable indicating whether or not the mixing mixing proportions are to be equal across clusters in the model (default = FALSE). Only relevant for the "MFA" and "MIFA" methods.

> A switch indicating whether uniquenesses scale hyperparameters are to be "unconstrained" or "isotropic", i.e. variable-specific or not. "uni.prior" must be "isotropic" if the last letter of uni. type is C, but can take either value otherwise. Defaults to correspond to the last letter of uni. type if that is supplied and uni.prior is not, otherwise defaults to "unconstrained" (though "isotropic" is recommended when N <= P). Only relevant when psi.beta is not supplied and psi\_hyper is therefore invoked (with optional arguments passable via the . . . construct).

Logical indicating whether the mu.zero hyperparameter can be cluster-specific. Defaults to FALSE. Only relevant for the "MFA" and "MIFA" methods when z.list is supplied.

Logical indicating whether the psi. beta hyperparameter(s) can be cluster-specific. Defaults to FALSE. Only relevant for the "MFA" and "MIFA" methods when z.list is supplied, and only allowable when uni.type is one of unconstrained or isotropic.

Logical indicating whether to drop variables with no standard deviation (defaults to TRUE). This is strongly recommended, especially a) when psi.beta is not supplied &/or sigma.mu=NULL, and either/both are therefore estimated using the empirical covariance matrix, &/or b) if some form of posterior predictive checking is subsequently desired when calling get\_IMIFA\_results.

Logical indicating whether to print output (e.g. run times) and a progress bar to the screen while the sampler runs. By default is TRUE if the session is interactive, and FALSE otherwise. If FALSE, warnings and error messages will still be printed to the screen, but everything else will be suppressed.

Also catches unused arguments. A number of optional arguments can be also supplied here:

- The additional psi\_hyper argument beta0, especially when N <= P.
- Additional arguments to be passed to hc (modelName & use only), to Mclust (modelNames, and the arguments for hc with which Mclust is itself initialised - modelName & use), or to kmeans (iter.max and nstart only), depending on the value of z.init.
- Additionally, when z.init="mclust", criterion can be passed here (can be "icl" or "bic", the default) to control how the optimum Mclust model to initialise with is determined.

uni.prior

mu0g

psi0g

drop0sd

verbose

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#### Value

A named list in which the names are the names of the arguments and the values are the values of the arguments.

#### Note

Users should be careful to note that data are mean-centered (centering=TRUE) and unit-scaled (scaling="unit") by default when supplying other parameters among the list above, especially those related in any way to psi.hyper, or to the other control functions mgpControl and bnpControl.

### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

McNicholas, P. D. and Murphy, T. B. (2008) Parsimonious Gaussian mixture models, *Statistics and Computing*, 18(3): 285-296.

#### See Also

```
mcmc_IMIFA, psi_hyper, hc, kmeans, Mclust, mgpControl, bnpControl, storeControl
```

# **Examples**

olive

Fatty acid composition of Italian olive oils

# Description

Data on the percentage composition of eight fatty acids found by lipid fraction of 572 Italian olive oils. The data come from three areas; within each area there are a number of constituent regions, of which there are 9 in total.

# Usage

```
data(olive)
```

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#### **Format**

A data frame with 572 observations and 10 columns. The first columns gives the area (one of Southern Italy, Sardinia, and Northern Italy), the second gives the region, and the remaining 8 columns give the variables. Southern Italy comprises the North Apulia, Calabria, South Apulia, and Sicily regions, Sardinia is divided into Inland Sardinia and Coastal Sardinia and Northern Italy comprises the Umbria, East Liguria, and West Liguria regions.

#### References

Forina, M., Armanino, C., Lanteri, S. and Tiscornia, E. (1983). Classification of olive oils from their fatty acid composition, In Martens, H. and Russrum Jr., H. (Eds.), *Food Research and Data Analysis*, Applied Science Publishers, London, pp. 189-214.

Forina, M. and Tiscornia, E. (1982). Pattern recognition methods in the prediction of Italian olive oil origin by their fatty acid content, *Annali di Chimica*, 72:143-155.

### **Examples**

pareto\_scale

Pareto Scaling

# **Description**

Pareto scaling of a numeric matrix, with or without centering. Observations are scaled by the square-root of their column-wise standard deviations.

# Usage

#### **Arguments**

x A numeric matrix-like object.

centering A logical vector indicating whether centering is to be applied (default=TRUE).

#### Value

The Pareto scaled version of the matrix x.

# Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

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#### References

van den Berg, R.A., Hoefsloot, H.C.J, Westerhuis, J.A. and Smilde, A.K. and van der Werf, M.J. (2006) Centering, scaling, and transformations: improving the biological information content of metabolomics data. *BMC Genomics*, 7(142).

# **Examples**

```
dat <- pareto_scale(olive[,-c(1,2)])</pre>
```

PGMM\_dfree

Estimate the Number of Free Parameters in Finite Factor Analytic Mixture Models (PGMM)

# Description

Estimates the dimension of the 'free' parameters in fully finite factor analytic mixture models, otherwise known as Parsimonious Gaussian Mixture Models (PGMM), typically necessary for the penalty term of various model selection criteria.

### Usage

### **Arguments**

Q	The number of latent factors (which can be 0, corresponding to a model with
	diagonal covariance). This argument is vectorised.

P The number of variables. Must be a single strictly positive integer.

G The number of clusters. This defaults to 1. Must be a single strictly positive

integer.

method By default, calculation assumes the UUU model with unconstrained loadings and

unconstrained diagonal uniquesseses (i.e. the factor analysis model). The seven other models detailed in McNicholas and Murphy (2008) are given too (of which currently the first four are accommodated within mcmc\_IMIFA). The first letter denotes whether loadings are constrained/unconstrained across clusters; the second letter denotes the same for the uniquenesses; the final letter denotes whether uniquenesses are in turn constrained to be isotropic. Finally, the 4 extra 4-letter models from the EPGMM family (McNicholas and Murphy, 2010), are also in-

cluded.

equal.pro Logical variable indicating whether or not the mixing mixing proportions are

equal across clusters in the model (default = FALSE).

#### Value

A vector of length length(Q) giving the total number of parameters, including means and mixing proportions, and not only covariance parameters. Set equal.pro to FALSE and subtract G \* P from the result to determine the number of covariance parameters only.

### Note

This function is used to calculate the penalty terms for the aic.mcmc and bic.mcmc model selection criteria implemented in get\_IMIFA\_results for *finite* factor models (though mcmc\_IMIFA currently only implements the UUU, UUC, UCU, and UCC covariance structures). The function is vectorised with respect to the argument Q.

Though the function is available for standalone use, note that no checks take place, in order to speed up repeated calls to the function inside mcmc\_IMIFA.

#### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### References

McNicholas, P. D. and Murphy, T. B. (2008) Parsimonious Gaussian mixture models, *Statistics and Computing*, 18(3): 285-296.

McNicholas, P. D. and Murphy, T. B. (2010) Model-Based clustering of microarray expression data via latent Gaussian mixture models, *Bioinformatics*, 26(21): 2705-2712.

# See Also

```
get_IMIFA_results, mcmc_IMIFA
```

### **Examples**

```
(UUU <- PGMM_dfree(Q=0:5, P=50, G=3, method="UUU"))
(CCC <- PGMM_dfree(Q=0:5, P=50, G=3, method="CCC", equal.pro=TRUE))</pre>
```

plot.Results\_IMIFA Plotting output and parameters of inferential interest for IMIFA and related models

### **Description**

Plotting output and parameters of inferential interest for IMIFA and related models

### Usage

```
## S3 method for class 'Results_IMIFA'
plot(x,
     plot.meth = c("all", "correlation", "density", "errors", "GQ",
                   "means", "parallel.coords", "trace", "zlabels"),
     param = c("means", "scores", "loadings", "uniquenesses",
               "pis", "alpha", "discount"),
     g = NULL,
     mat = TRUE,
     zlabels = NULL,
     heat.map = TRUE
     show.last = FALSE,
     palette = NULL,
     ind = NULL,
     fac = NULL
     by.fac = FALSE,
     type = c("h", "n", "p", "l"),
     intervals = TRUE,
     common = TRUE,
     partial = FALSE,
     titles = TRUE,
     transparency = 0.75,
     ...)
```

### **Arguments**

X

An object of class "Results\_IMIFA" generated by get\_IMIFA\_results.

plot.meth

The type of plot to be produced for the param of interest, where correlation refers to ACF/PACF plots, means refers to posterior means, density, trace and parallel.coords are self-explanatory. "all" in this case, the default, refers to "trace", "density", "means", and "correlation". "parallel.coords" is only available when param is one of "means", "loadings" or "uniquenesses" - note that this method applies a small amount of horizontal jitter to avoid overplotting.

Special types of plots which don't require a param are:

- "GQ" for plotting the posterior summaries of the numbers of clusters/factors, if available.
- "zlabels" for plotting clustering uncertainties in four different ways (incl. the posterior confusion matrix) if clustering has taken place, with or without the clustering labels being supplied via the zlabels argument. If available, the average similarity matrix, reordered according to the MAP labels, is shown as a 5-th plot.
- "errors" for conducting posterior predictive checking of the appropriateness of the fitted model by visualising the posterior predictive reconstruction error (PPRE) &/or histograms comparing the data to replicate draws from the posterior distribution &/or error metrics quantifying the difference between the estimated and empirical covariance matrices. The type of plot(s)

produced depends on how the error.metrics argument was supplied to get\_IMIFA\_results and what parameters were stored.

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The argument g can be used to cycle through the available plots in each case. ind can also be used to govern which variable is shown for the 2-nd plot.

param

The parameter of interest for any of the following plot.meth options: all, trace, density, means, correlation. The param must have been stored when mcmc\_IMIFA was initially ran. Includes pis for methods where clustering takes place, and allows posterior inference on alpha (for the "IMFA", "IMIFA", "OMFA", and "OMIFA" methods) and discount (for the "IMFA" and "IMIFA" methods). Otherwise "means", "scores", "loadings", and "uniquenesses" can be plotted

g

Optional argument that allows specification of exactly which cluster the plot of interest is to be produced for. If not supplied, the user will be prompted to cycle through plots for all clusters. Also functions as an index for which plot to return when plot.meth is GQ, zlabels, or errors in much the same way.

mat

Logical indicating whether a matplot is produced (defaults to TRUE). If given as FALSE, ind is invoked.

zlabels

The true labels can be supplied if they are known. If this is not supplied, the function uses the labels that were supplied, if any, to <code>get\_IMIFA\_results</code>. Only relevant when plot.meth = "zlabels". When explicitly supplied, misclassified observations are highlighted in the first type of uncertainty plot (otherwise observations whose uncertainty exceed the inverse of the number of clusters are highlighted). For the second type of uncertainty plot, when zlabels are explicitly supplied, the uncertainty of misclassified observations is marked by vertical lines on the profile plot.

heat.map

A logical which controls plotting posterior mean loadings or posterior mean scores as a heatmap, or else as something akin to link{plot(...,type="h")}. Only relevant if param = "loadings" (in which case the default is TRUE) or param = "scores" (in which case the default is FALSE). Heatmaps are produced with the aid of mat2cols and plot\_cols.

show.last

A logical indicator which defaults to FALSE, but when TRUE replaces any instance of the posterior mean with the last valid sample. Only relevant when param is one of "means" "scores", "loadings", "uniquenesses", or "pis" and plot.meth is one of "all" or "means". Also relevant for "means", "loadings" and "uniquenesses" when plot.meth is "parallel.coords". When TRUE, this has the effect of forcing intervals to be FALSE.

palette

An optional colour palette to be supplied if overwriting the default palette set inside the function by viridis is desired. It makes little sense to a supply a palette when plot.meth="all" and param is one of "scores" or "loadings".

ind

Either a single number indicating which variable to plot when param is one of means or uniquenesses (or plot.meth="errors"), or which cluster to plot if param is pis. If scores are plotted, a vector of length two giving which observation and factor to plot; if loadings are plotted, a vector of length two giving which variable and factor to plot. Will be recycled to length 2 if necessary. Also governs which two factors are displayed on posterior mean plots of the "scores" when heat.map is FALSE; otherwise only relevant when mat is FALSE.

fac Optional argument that provides an alternative way to specify ind[2] when mat is FALSE and param is one of scores or loadings. by.fac Optionally allows (mat)plotting of scores and loadings by factor - i.e. observation(s) (scores) or variable(s) (loadings) for a given factor, respectively, controlled by ind or fac) when set to TRUE. Otherwise all factor(s) are plotted for a given observation or variable when set to FALSE (the default), again controlled by ind or fac. Only relevant when paramis one of scores or loadings. The manner in which the plot is to be drawn, as per the type argument to plot. type Logical indicating whether credible intervals around the posterior mean(s) are intervals to be plotted when is.element(plot.meth,c("all", "means")). Defaults to TRUE, but can only be TRUE when show.last is FALSE. Logical indicating whether plots with plot.meth="means" (or the correspondcommon ing plots for plot.meth="all") when param is one of "means", "scores", "loadings", or "uniquenesses" are calibrated to a common scale based on the range of the param parameters across all clusters (defaults to TRUE, and only relevant when there are clusters). Otherwise, the only the range corresponding to the image being plotted is used to determine the scale. Note that this affects the "loadings" and "scores" plots regardless of the value of heat.map. An exception is the "scores" plots when plot.meth="means" and heat.map is FALSE, in which case common defaults to FALSE. Logical indicating whether plots of type "correlation" use the PACF. The departial fault, FALSE, ensures the ACF is used. Only relevant when plot.meth = "all", otherwise both plots are produced when plot.meth = "correlation". titles Logical indicating whether default plot titles are to be used (TRUE), or suppressed (FALSE). transparency A factor in [0, 1] modifying the opacity for overplotted lines. Defaults to 0.75, unless semi-transparency is not supported. Only relevant when palette is not supplied, otherwise the supplied palette must already be adjusted for transparency. Other arguments typically passed to plot or the breaks argument to mat2cols

# Value

The desired plot with appropriate output and summary statistics printed to the console screen.

and heat\_legend when heatmaps are plotted.

# Note

Supplying the argument zlabels does **not** have the same effect of reordering the sampled parameters as it does if supplied directly to get\_IMIFA\_results.

When mat is TRUE and by. fac is FALSE (both defaults), the convention for dealing with overplotting for trace and density plots when paramis either scores or loadings is to plot the last factor first, such that the first factor appears 'on top'.

# Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

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### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

### See Also

```
mcmc_IMIFA, get_IMIFA_results, mat2cols, plot_cols
```

```
# See the vignette associated with the package for more graphical examples:
# vignette("IMIFA", package = "IMIFA")
# data(olive)
# simIMIFA <- mcmc_IMIFA(olive, method="IMIFA")</pre>
# resIMIFA <- get_IMIFA_results(simIMIFA, z.avgsim=TRUE)</pre>
# Examine the posterior distribution(s) of the number(s) of clusters (G) &/or latent factors (Q)
# For the IM(I)FA and OM(I)FA methods, this also plots the trace of the active/non-empty clusters
# plot(resIMIFA, plot.meth="GQ")
# plot(resIMIFA, plot.meth="GQ", g=2)
# Plot clustering uncertainty (and, if available, the similarity matrix)
# plot(resIMIFA, plot.meth="zlabels", zlabels=olive$area)
# Visualise the posterior predictive reconstruction error
# plot(resIMIFA, plot.meth="errors", g=1)
# Compare histograms of the data vs. replicate draw from the posterior for the 1st variable
# plot(resIMIFA, plot.meth="errors", g=2, ind=1)
# Visualise empirical vs. estimated covariance error metrics
# plot(resIMIFA, plot.meth="errors", g=3)
# Look at the trace, density, posterior mean, and correlation of various parameters of interest
# plot(resIMIFA, plot.meth="all", param="means", g=1)
# plot(resIMIFA, plot.meth="all", param="means", g=1, ind=2)
# plot(resIMIFA, plot.meth="trace", param="scores")
# plot(resIMIFA, plot.meth="trace", param="scores", by.fac=TRUE)
# plot(resIMIFA, plot.meth="mean", param="loadings", g=1)
# plot(resIMIFA, plot.meth="mean", param="loadings", g=1, heat.map=FALSE)
# plot(resIMIFA, plot.meth="parallel.coords", param="uniquenesses")
# plot(resIMIFA, plot.meth="density", param="pis", intervals=FALSE, partial=TRUE)
# plot(resIMIFA, plot.meth="all", param="alpha")
# plot(resIMIFA, plot.meth="all", param="discount")
```

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# **Description**

Plots a matrix of colours as a heat map type image or as points. Intended for joint use with mat2cols.

# Usage

# Arguments

cmat A	matrix of valid colours,	with missing values	coded as NA allowed.	Vectors
--------	--------------------------	---------------------	----------------------	---------

should be supplied as matrices with 1 row or column, as appropriate.

na.col Colour used for missing NA entries in cmat.

ptype Switch controlling output as either a heat map "image" (the default) or as "points".

border.col Colour of border drawn around the plot.

dlabels, rlabels, clabels

Vector of labels for the diagonals, rows, and columns, respectively.

pch Point type used when ptype="points".

cex Point cex used when ptype="points".

label.cex Govens cex parameter used for labels.

... Further graphical parameters.

### Value

Either an "image" or "points" type plot of the supplied colours.

#### See Also

```
mat2cols, image, heat_legend, is.cols
```

```
# Generate a colour matrix using mat2cols()
mat     <- matrix(rnorm(100), nrow=10, ncol=10)
mat[2,3] <- NA
cols     <- heat.colors(12)[12:1]
(matcol     <- mat2cols(mat, cols=cols))</pre>
```

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```
# Use plot_cols() to visualise the colours matrix
par(mar=c(5.1, 4.1, 4.1, 3.1))
plot_cols(matcol)

# Add a legend using heat_legend()
heat_legend(mat, cols=cols); box(lwd=2)

# Replace colour of exact zero entries:
# Often important to call mat2cols() first (to include 0 in the cuts),
# then replace relevant entries with NA for plot_cols(), i.e.
mat[2,3] <- 0
matcol2 <- mat2cols(mat, cols=cols)
plot_cols(replace(matcol2, mat == 0, NA), na.col="blue")
heat_legend(mat, cols=cols); box(lwd=2)</pre>
```

post\_conf\_mat

Posterior Confusion Matrix

# **Description**

For a (N \* G) matrix of posterior cluster membership probabilities, this function creates a (G \* G) posterior confusion matrix, whose hk-th entry gives the average probability that observations with maximum posterior allocation h will be assigned to cluster k.

# Usage

```
post\_conf\_mat(z, scale = TRUE)
```

# **Arguments**

Z

A (N  $\star$  G) matrix of posterior cluster membership probabilities whose (ig)-th entry gives the posterior probability that observation i belongs to cluster g. Entries must be valid probabilities in the interval [0,1]; missing values are not allowed. Otherwise, a list of such matrices can be supplied, where each matrix in the list has the same dimensions.

scale

A logical indicator whether the PCM should be rescaled by its row sums. When TRUE (the default), the benchmark matrix for comparison is the identity matrix of order G, corresponding to a situation with no uncertainty in the clustering. When FALSE, the row sums give the number of observations in each cluster.

# Value

A (G \* G) posterior confusion matrix, whose hk-th entry gives the average probability that observations with maximum posterior allocation h will be assigned to cluster k. When scale=TRUE, the benchmark matrix for comparison is the identity matrix of order G, corresponding to a situation with no uncertainty in the clustering.

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### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### References

Ranciati, S., Vinciotti, V. and Wit, E., (2017) Identifying overlapping terrorist cells from the No-ordin Top actor-event network, *to appear*. <arXiv:1710.10319v1>.

#### See Also

```
get_IMIFA_results
```

# **Examples**

```
# data(olive)
# sim <- mcmc_IMIFA(olive, n.iters=1000)
# res <- get_IMIFA_results(sim)
# (PCM <- post_conf_mat(res$Clust$post.prob))

# par(mar=c(5.1, 4.1, 4.1, 3.1))
# PCM <- replace(PCM, PCM == 0, NA)
# plot_cols(mat2cols(PCM, col=heat.colors(30, rev=TRUE), na.col=par()$bg)); box(lwd=2)
# heat_legend(PCM, cols=heat.colors(30, rev=TRUE))
# par(mar=c(5.1, 4.1, 4.1, 2.1))</pre>
```

Procrustes

**Procrustes Transformation** 

# **Description**

This function performs a Procrustes transformation on a matrix X to minimize the squared distance between X and another comparable matrix Xstar.

# Usage

# **Arguments**

X The matrix to be transformed.

Xstar The target matrix.

translate Logical value indicating whether X should be translated (defaults to FALSE).

Logical value indicating whether X should be dilated (defaults to FALSE).

sumsq Logical value indicating whether the sum of squared differences between X and

Xstar should be calculated and returned.

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### **Details**

R, tt, and d are chosen so that:

$$d \times \mathbf{XR} + \mathbb{1}\underline{t}^{\top} \approx X^{\star}$$

X. new is given by:

$$X_{\text{new}} = d \times \mathbf{X}\mathbf{R} + \mathbb{1}\underline{t}^{\top}$$

# Value

A list containing:

X.new	The matrix that is the Procrustes transformed version of X.
R	The rotation matrix.
t	The translation vector (if $isTRUE(translate)$ ).
d	The scaling factor (is isTRUE(dilate)).
SS	The sum of squared differences (if isTRUE(sumsq)).

#### Note

X is padded out with columns containing 0 if it has fewer columns than Xstar.

### References

Borg, I. and Groenen, P. J. F. (1997) *Modern Multidimensional Scaling*. Springer-Verlag, New York, pp. 340-342.

```
# Match two matrices, allowing translation and dilation
mat1
         <- diag(rnorm(10))
         <- 0.05 * matrix(rnorm(100), 10, 10) + mat1
mat2
         <- Procrustes(X=mat1, Xstar=mat2, translate=TRUE, dilate=TRUE, sumsq=TRUE)</pre>
proc
# Extract the transformed matrix, rotation matrix, translation vector and scaling factor
mat_new <- proc$X.new</pre>
mat_rot <- proc$R</pre>
mat_t
         <- proc$t
mat_d
         <- proc$d
# Compare the sum of squared differences to a Procrustean transformation with rotation only
mat_ss <- proc$ss</pre>
mat_ss2 <- Procrustes(X=mat1, Xstar=mat2, sumsq=TRUE)$ss</pre>
```

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psi_hyper	Find	sensible	inverse	gamma	hyperparameters	for	vari-
	ance/ı	ıniqueness	parametei	rs			

### **Description**

Takes an inverse-Gamma shape hyperparameter, and an inverse covariance matrix (or estimate thereof), and finds data-driven scale hyperparameters in such a way that Heywood problems are avoided for factor analysis or probabilistic principal components analysis (and mixtures thereof).

# Usage

# **Arguments**

shape	A positive shape hyperparameter.
dat	The data matrix for which the inverse covariance matrix is to be estimated. If data are to be centered &/or scaled within mcmc_IMIFA, then dat must also be standardised in the same way.
type	A switch indicating whether a single scale (isotropic) or variable-specific scales (unconstrained) are to be derived. Both options are allowed under models in mcmc_IMIFA with "constrained" or "unconstrained" uniquenesses, but only a single scale can be specified for models with "isotropic" or "single" uniquenesses.
beta0	See Note below. Must be a strictly positive numeric scalar. Defaults to 3, but is only invoked when explicitly supplied or when the number of observations N is not greater than the number of variables P (or when inverting the sample covariance matrix somehow otherwise fails). In some cases, beta0 should not be so small as to render the estimate of the inverse unstable.
• • •	Catches unused arguments. Advanced users can also supply the sample covariance matrix of dat, if available, through via the argument covar.

# **Details**

Constraining uniquenesses to be isotropic provides the link between factor analysis and the probabilistic PCA model. When used in conjunction with mcmc\_IMIFA with "isotropic" or "single" uniquenesses, type must be isotropic, but for "unconstrained" or "constrained" uniquenesses, it's possible to specify either a single scale (type="isotropic") or variable-specific scales (type="unconstrained").

Used internally by mcmc\_IMIFA when its argument psi\_beta is not supplied.

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#### Value

Either a single scale hyperparameter or ncol(dat) variable-specific scale hyperparameters.

#### Note

When N > P, where N is the number of observations and P is the number of variables, the inverse of the sample covariance matrix is used by default.

When N <= P, the inverse either does not exist or the estimate thereof is highly unstable. Thus, an estimate of the form  $\left(\beta_0 + \frac{N}{2}\right) \left(\beta_0 \mathcal{I}_p + 0.5 \sum_{i=1}^N x_i x_i^\top\right)^{-1}$  is used instead.

For unstandardised data, the estimate is instead constructed using a standardised version of the data, and the resulting inverse *correlation* matrix estimate is scaled appropriately by the diagonal entries of the sample covariance matrix of the original data.

This estimate can also be used in N > P cases by explicitly supplying beta0. It will also be used if inverting the sample covariance matrix fails in N > P cases.

The optional argument beta0 can be supplied to mcmc\_IMIFA via the control function mixfaControl.

#### Author(s)

Keefe Murphy - <<keefe.murphy@mu.ie>>

#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

Fruwirth-Schnatter, S. and Lopes, H. F. (2010). Parsimonious Bayesian factor analysis when the number of factors is unknown, *Technical Report*. The University of Chicago Booth School of Business.

Fruwirth-Schnatter, S. and Lopes, H. F. (2018). Sparse Bayesian factor analysis when the number of factors is unknown, *to appear*. <arXiv:1804.04231>.

Tipping, M. E. and Bishop, C. M. (1999). Probabilistic principal component analysis, *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 61(3): 611-622.

#### See Also

```
mcmc_IMIFA, mixfaControl
```

```
data(olive)
olive2 <- olive[,-(1:2)]
shape <- 2.5
(scale1 <- psi_hyper(shape=shape, dat=olive2))

# Try again with scaled data
olive_S <- scale(olive2, center=TRUE, scale=TRUE)

# Use the inverse of the sample covariance matrix</pre>
```

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```
(scale2 <- psi_hyper(shape=shape, dat=olive_S))

# Use the estimated inverse covariance matrix
(scale3 <- psi_hyper(shape=shape, dat=olive_S, beta0=3))

# In the normalised example, the mean uniquenesses (given by scale/(shape - 1)),
# can be interpreted as the prior proportion of the variance that is idiosyncratic
(prop1 <- scale1/(shape - 1))
(prop2 <- scale2/(shape - 1))</pre>
```

rDirichlet

Simulate Mixing Proportions from a Dirichlet Distribution

# **Description**

Generates samples from the Dirichlet distribution with parameter alpha efficiently by simulating Gamma(alpha, 1) random variables and normalising them.

# Usage

```
rDirichlet(G,
alpha,
nn = 0L)
```

#### **Arguments**

G The number of clusters for which weights need to be sampled.

alpha The Dirichlet hyperparameter, either of length 1 or G. When the length of alpha

is 1, this amounts to assuming an exchangeable prior, which doesn't favour one component over another. Be warned that this will be recycled if necessary.

Larger values have the effect of making the returned samples more equal.

nn A vector giving the number of observations in each of G clusters so that Dirich-

let posteriors rather than priors can be sampled from. This defaults to 0, i.e. simulation from the prior. Must be non-negative. Be warned that this will be

recycled if necessary.

# Value

A Dirichlet vector of G weights which sum to 1.

#### Note

Though the function is available for standalone use, note that few checks take place, in order to speed up repeated calls to the function inside mcmc\_IMIFA. In particular, alpha and nn may be invisibly recycled.

While small values of alpha have the effect of increasingly concentrating the mass onto fewer components, note that this function may return NaN for excessively small values of alpha, when nn=0; see the details of rgamma for small shape values.

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#### References

Devroye, L. (1986) Non-Uniform Random Variate Generation, Springer-Verlag, New York, p. 594.

### **Examples**

```
(prior <- rDirichlet(G=5, alpha=1))
(posterior <- rDirichlet(G=5, alpha=1, nn=c(20, 41, 32, 8, 12)))
(asymmetric <- rDirichlet(G=5, alpha=c(3,4,5,1,2), nn=c(20, 41, 32, 8, 12)))</pre>
```

scores\_MAP

Decompose factor scores by cluster

# **Description**

Takes posterior summaries of the overall factor scores matrix and returns lists of sub-matrices corresponding to the G-cluster MAP partition.

# Usage

```
scores_MAP(res,
dropQ = FALSE)
```

# **Arguments**

res

An object of class "Results\_IMIFA" generated by get\_IMIFA\_results.

dropQ

A logical indicating whether columns of the factor scores matrix should be dropped such that the number of columns in each sub-matrix corresponds to the cluster-specific number of factors (if the number of factors is indeed cluster-specific). When FALSE (the default), the number of columns instead remains common to all sub-matrices - given by the largest of the cluster-specific numbers of latent factors.

Note that this argument is irrelevant (i.e. always FALSE) for the finite factor methods ("FA", "MFA", "OMFA", and "IMFA").

# **Details**

Under the models in the IMIFA family, there exists only one factor scores matrix. For the finite factor methods, this has dimensions N \* Q.

For the infinite factor methods ("IFA", "MIFA", "OMIFA", and "IMIFA"), the factor scores matrix has dimensions N  $\star$  Qmax, where Qmax is the largest of the cluster-specific numbers of latent factors  $q_1, \ldots, q_g$ . Entries of this matrix thus may have been padded out with zero entries, as appropriate, prior to the Procrustes rotation-based correction applied within get\_IMIFA\_results (thus now these entries will be near-zero).

In partitioning rows of the factor scores matrix into the same clusters the corresponding observations themselves belong to according to the MAP clustering, the number of columns *may* vary according to the cluster-specific numbers of latent factors (depending on the value of dropQ and the method employed).

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#### Value

For models which achieve clustering, a list of lists (say x) decomposing the posterior mean scores (x\$post.eta), the associated variance estimates (x\$var.eta) and credible intervals (x\$ci.eta), and the last valid sample of the scores (x\$last.eta) into lists of length G, corresponding to the MAP clustering, with varying or common numbers of cluster-specific factors (depending on the value of dropQ and the method employed).

For models with only one component, or the "FA" and "IFA" methods, scores cannot be decomposed, and posterior summaries of the scores will be returned unchanged.

### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### See Also

```
get_IMIFA_results
```

# **Examples**

```
data(coffee)
sim <- mcmc_IMIFA(coffee, n.iters=1000)
res <- get_IMIFA_results(sim)

# Examine the single posterior mean scores matrix
res$Scores$post.eta

# Decompose into G matrices, common numbers of columns
eta <- scores_MAP(res)
eta$post.eta

# Allow the number of columns be cluster-specific
scores_MAP(res, dropQ=TRUE)$post.eta</pre>
```

shift\_GA

Moment Matching Parameters of Shifted Gamma Distributions

### **Description**

This function takes shape and rate parameters of a Gamma distribution and modifies them to achieve the same expected value and variance when the left extent of the support of the distribution is shifted up or down.

### Usage

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# **Arguments**

shape, rate	Shape and rate parameters a and b, respectively, of a Gamma(a, b) distribution.
	Both must be strictly positive.
shift	Modifier, such that the Gamma distribution has support on (shift, $\infty$ ). Can be positive or negative, though typically negative and small.
param	Switch controlling whether the supplied rate parameter is indeed a rate, or actually a scale parameter. Also governs whether the output is given in terms of rate or scale. Defaults to "rate".

# Value

A named vector of length 2, containing the modified shape and rate parameters, respectively.

### Note

This function is invoked within mcmc\_IMIFA when discount is *fixed* at a non-zero value and learn.alpha=TRUE.

# Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

# **Examples**

```
# Shift a Ga(shape=4, rate=2) distribution to the left by 1; # achieving the same expected value of 2 and variance of 1. shift_GA(4, 2, -1)
```

show\_digit

Show image of grayscale grid

# Description

Plots an image of a grayscale grid representation of a digit.

# Usage

# **Arguments**

dat	A matrix or data.frame with the same number of rows and columns (or a vector which can be coerced to such a format), representing a grayscale map of a single digit.
col	The colour scale to be used. Defaults to grey( $seq(1,0,length = ncol(dat))$ ).
	Additional arguments to be passed to mat2cols and/or plot_cols (e.g. na.col)
	when dat is a matrix or image when dat is a vector.

show\_IMIFA\_digit

# Value

The desired image representation of the digit.

# Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

### See Also

```
USPSdigits, show_IMIFA_digit, mat2cols, plot_cols
```

# **Examples**

```
data(USPSdigits)
# Plot the first digit
show_digit(USPSdigits$train[1,-1])
# Visualise the overall mean
show_digit(colMeans(USPSdigits$train[,-1]))
```

show\_IMIFA\_digit

Plot the posterior mean image

# Description

Plots the posterior mean of a given cluster from an "IMIFA"-related model fit to a digit data set in the form of a square grayscale grid.

### Usage

### **Arguments**

res	An object of class "Results_IMIFA" generated by get_IMIFA_results.
G	The index of the cluster for which the posterior mean digit is to be represented.
what	A switch controlling whether the "mean" or "last" valid sample is to be plotted.
dat	The full grayscale grid data set (prior to centering and scaling). Necessary when ind is supplied or if pixels with standard deviation of 0 exist in the data set (which will have been automatically removed by mcmc_IMIFA).

show\_IMIFA\_digit 61

ind The index of	columns of dat which v	were discarded prior to	fitting the "IMIFA"-
------------------	------------------------	-------------------------	----------------------

related model via mcmc\_IMIFA. Can be a vector of column indices of dat or an equivalent vector of logicals. The discarded pixels are replaced by the column-means corresponding to ind among images assigned to the given cluster G.

... Additional arguments to be passed, via show\_digit, to mat2cols and/or plot\_cols.

#### **Details**

This function is a wrapper to show\_digit which supplies the posterior mean digit of a given cluster from a "IMIFA" model.

#### Value

The desired image representation of the posterior mean digit (or the last valid sample) from the desired cluster.

#### Note

Note that both centering and scaling of the original data prior to modelling is accounted for in reconstructing the means, but dat, if necessary, must be the raw data prior to pre-processing.

### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### See Also

```
USPS digits, show\_digit, get\_IMIFA\_results, mcmc\_IMIFA, mat2cols, plot\_cols
```

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sim\_IMIFA

Simulate Data from a Mixture of Factor Analysers Structure

# **Description**

Functions to simulate data of any size and dimension from a (infinite) mixture of (infinite) factor analysers parameterisation or fitted object.

### Usage

```
sim_IMIFA_data(N = 300L,
               G = 3L
               P = 50L
               Q = rep(floor(log(P)), G),
               pis = rep(1/G, G),
               mu = NULL,
               psi = NULL,
               loadings = NULL,
               scores = NULL,
               nn = NULL,
               loc.diff = 2,
               non.zero = P,
               forceQg = TRUE,
               method = c("conditional", "marginal"))
sim_IMIFA_model(res,
                method = c("conditional", "marginal"))
```

# **Arguments**

N, G, P	Desired overall number of observations, number of clusters, and number of variables in the simulated data set. All must be a single integer.
Q	Desired number of cluster-specific latent factors in the simulated data set. Can be specified either as a single integer if all clusters are to have the same number of factors, or a vector of length G. Defaults to floor(log(P)) in each cluster. Should be less than the associated Ledermann bound and the number of observations in the corresponding cluster. The argument forceQg can be used to enforce this upper limit.
pis	Mixing proportions of the clusters in the data set if $G > 1$ . Must sum to 1. Defaults to rep(1/G,G).
mu	True values of the mean parameters, either as a single value, a vector of length $G$ , a vector of length $P$ , or a $G \star P$ matrix. If $mu$ is missing, $loc.diff$ is invoked to simulate distinct means for each cluster by default.
psi	True values of uniqueness parameters, either as a single value, a vector of length $G$ , a vector of length $P$ , or a $G \star P$ matrix. As such the user can specify unique-

nesses as a diagonal or isotropic matrix, and further constrain uniquenesses

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across clusters if desired. If psi is missing, uniquenesses are simulated via 1/rgamma(P, 2, 1) within each cluster by default. loadings True values of the loadings matrix/matrices. Must be supplied in the form of a list of numeric matrices when G > 1, otherwise a single matrix. Matrices must contain P rows and the number of columns must correspond to the values in Q. If loadings are not supplied, such matrices are populated with standard normal random variates by default (see non.zero). scores True values of the latent factor scores, as a N \* max(Q) numeric matrix. If scores are not supplied, such a matrix is populated with standard normal random variates by default. Only relevant when method="conditional". An alternative way to specify the size of each cluster, by giving the exact number nn of observations in each cluster explicitly. Must sum to N. loc.diff A parameter to control the closeness of the clusters in terms of the difference in their location vectors. Only relevant if mu is NOT supplied. Defaults to 2. More specifically, loc.diff (if invoked) is invoked as follows: means are simulated with the vector of cluster-specific hypermeans given by: scale(1:G,center=TRUE,scale=FALSE) \* loc.diff. Controls the number of non-zero entries in each loadings column (per cluster) non.zero only when loadings is not explicitly supplied. Values must be integers in the interval [1,P]. Defaults to P. The positions of the zeros are randomised, and non-zero entries are drawn from a standard normal. Must be given as a list of length G of vectors of length corresponding to Q when G>1. Can be given either as such a list or simply a vector of length Q when G=1. Alternatively, a single integer can be supplied, common across all loadings columns across all clusters. In any case, non.zero will be affected by forceQg=TRUE by default (see below). A logical indicating whether the upper limit on the number of cluster-specific forceQg factors Q is enforced. Defaults to TRUE for sim\_IMIFA\_data, but is always FALSE for sim\_IMIFA\_model. Note that when forceQg=TRUE is invoked, non.zero (see above) is also affected. method A switch indicating whether the mixture to be simulated from is the conditional distribution of the data given the latent variables (default), or simply the

#### **Details**

res

sim\_IMIFA\_model is a simple wrapper to sim\_IMIFA\_data which uses the estimated parameters of a fitted IMIFA related model, as generated by get\_IMIFA\_results. The necessary parameters must have been originally stored via storeControl in the creation of res.

An object of class "Results\_IMIFA" generated by get\_IMIFA\_results.

marginal distribution of the data.

### Value

Invisibly returns a data. frame with N observations (rows) of P variables (columns). The true values of the parameters which generated these data are also stored as attributes.

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#### Note

N, G, P & Q will **NOT** be inferred from the supplied parameters pis, mu, psi, loadings, scores & nn - rather, the parameters' length/dimensions must adhere to the supplied values of N, G, P & Q.

Missing values are not allowed in any of pis, mu, psi, loadings, scores & nn.

# Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### References

Murphy, K., Viroli, C., and Gormley, I. C. (2020) Infinite mixtures of infinite factor analysers, *Bayesian Analysis*, 15(3): 937-963. <a href="https://doi.org/10.1214/19-BA1179">doi:10.1214/19-BA1179</a>>.

#### See Also

```
mcmc_IMIFA for fitting an IMIFA related model to the simulated data set.
```

```
get_IMIFA_results for generating input for sim_IMIFA_model.
```

Ledermann for details on the upper-bound for Q. Note that this function accounts for isotropic uniquenesses, if psi is supplied in that manner, in computing this bound.

```
# Simulate 100 observations from 3 balanced clusters with cluster-specific numbers of latent factors
# Specify isotropic uniquenesses within each cluster
# Supply cluster means directly
sim_data <- sim_IMIFA_data(N=100, G=3, P=20, Q=c(2, 2, 5), psi=1:3,
                          mu=matrix(rnorm(60, -2 + 1:3, 1), nrow=20, ncol=3, byrow=TRUE))
names(attributes(sim_data))
labels
         <- attr(sim_data, "Labels")
# Visualise the data in two-dimensions
plot(cmdscale(dist(sim_data), k=2), col=labels)
# Examine the overlap with a pairs plot of 5 randomly chosen variables
pairs(sim_data[,sample(1:20, 5)], col=labels)
# Fit a MIFA model to this data
          <- mcmc_IMIFA(sim_data, method="MIFA", range.G=3, n.iters=5000)</pre>
# tmp
# Simulate from this model
         <- get_IMIFA_results(tmp, zlabels=labels)</pre>
# sim_mod <- sim_IMIFA_model(res)</pre>
```

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Set storage values for use with the IMIFA family of models

### **Description**

Supplies a list of values for logical switches indicating whether parameters of interest (means, scores, loadings, uniquenesses, and mixing proportions) should be stored when running models from the IMIFA family via mcmc\_IMIFA. It may be useful not to store certain parameters if memory is an issue.

### Usage

### **Arguments**

mu.switch	Logical indicating whether the means are to be stored (defaults to TRUE).  Logical indicating whether the factor scores are to be stored.
	As the array containing each sampled scores matrix tends to be amongst the largest objects to be stored, this defaults to FALSE inside mcmc_IMIFA when length(range.G) * length(range.Q) > 10, otherwise the default is TRUE. For the "MIFA", "OMIFA", and "IMIFA" methods, setting this switch to FALSE also offers a slight speed-up.
	Unlike other parameters, the scores need not be stored for posterior predictive checking (see Note below).
load.switch	Logical indicating whether the factor loadings are to be stored (defaults to TRUE).
psi.switch	Logical indicating whether the uniquenesses are to be stored (defaults to TRUE).
pi.switch	Logical indicating whether the mixing proportions are to be stored (defaults to TRUE).
	Catches unused arguments.

# **Details**

storeControl is provided for assigning values for IMIFA models within mcmc\_IMIFA. It may be useful not to store certain parameters if memory is an issue (e.g. for large data sets or for a large number of MCMC iterations after burnin and thinning).

# Value

A named vector in which the names are the names of the storage switches and the values are logicals indicating whether that parameter is to be stored. The list also contains as an attribute a logical for each switch indicating whether it was actually supplied (TRUE) or the default was accepted (FALSE).

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### Note

Posterior inference and plotting won't be possible for parameters not stored.

Non-storage of parameters will almost surely prohibit the computation of posterior predictive checking error metrics within <code>get\_IMIFA\_results</code> also. In particular, if such error metrics are desired, <code>mu.switch</code> and <code>psi.switch</code> must be TRUE for all but the "FA" and "IFA" models, load.switch must be TRUE for all but the entirely zero-factor models, and <code>pi.switch</code> must be TRUE for models with clustering structure and unequal mixing proportions for all but the PPRE metric. <code>score.switch=TRUE</code> is not required for any posterior predictive checking.

Finally, if loadings are not stored but scores are, caution is advised when examining posterior scores as Procrustes rotation will not occur within get\_IMIFA\_results.

### Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

#### See Also

```
mcmc_IMIFA, get_IMIFA_results, mixfaControl, mgpControl, bnpControl
```

# **Examples**

```
stctrl <- storeControl(score.switch=FALSE)

# data(olive)
# sim <- mcmc_IMIFA(olive, "IMIFA", n.iters=5000, storage=stctrl)

# Alternatively specify these arguments directly
# sim <- mcmc_IMIFA(olive, "IMIFA", n.iters=5000, score.switch=FALSE)</pre>
```

USPSdigits

USPS handwritten digits

# **Description**

Training and test sets for the United States Postal Service (USPS) handwritten digits data, with 8-bit 16x16 grayscale grid representations of image scans of the digits "0" through "9".

### Usage

```
data(USPSdigits)
```

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### **Format**

A list of length 2 with the following elements, each one a data. frame:

train The training set of 7,291 digits.

test The test set of 2,007 digits.

Each data. frame contains the known digit labels in its first column.

The remaining 256 columns give the concatenation of the 16x16 grid.

Pixels are scaled such that [-1,1] corresponds to [white,black].

#### References

Hastie, T., Tibshirani, R., and Friedman, J. (2001). *The Elements of Statistical Learning*. Springer Series in Statistics. New York, NY, USA: Spring New York Inc., 2<sup>nd</sup> edition.

### See Also

```
show_digit, show_IMIFA_digit
```

### **Examples**

```
# Load the data and record the labels
data(USPSdigits, package="IMIFA")
ylab <- USPSdigits$train[,1]
train <- USPSdigits$train[,-1]

# Examine the effect of discarding peripheral pixels
SDs <- apply(train, 2, sd)
ind <- SDs > 0.7
dat <- train[,ind]
hist(SDs, breaks=200, xlim=c(0, 1))
rect(0.7, 0, 1, 12, col=2, density=25)
show_digit(ind) # retained pixels are shown in black</pre>
```

Zsimilarity

Summarise MCMC samples of clustering labels with a similarity matrix and find the 'average' clustering

# Description

This function takes a Monte Carlo sample of cluster labels, computes an average similarity matrix and returns the clustering with minimum mean squared error to this average. The mcclust package **must** be loaded.

# Usage

```
Zsimilarity(zs)
```

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#### **Arguments**

zs

A matrix containing samples of clustering labels where the columns correspond to the number of observations (N) and the rows correspond to the number of iterations (M).

#### **Details**

This function takes a Monte Carlo sample of cluster labels, converts them to adjacency matrices, and computes a similarity matrix as an average of the adjacency matrices. The dimension of the similarity matrix is invariant to label switching and the number of clusters in each sample, desirable features when summarising partitions of Bayesian nonparametric models such as IMIFA. As a summary of the posterior clustering, the clustering with minimum mean squared error to this 'average' clustering is reported.

A heatmap of z.sim may provide a useful visualisation, if appropriately ordered. The user is also invited to perform hierarchical clustering using hclust after first converting this similarity matrix to a distance matrix - "complete" linkage is recommended. Alternatively, hc could be used.

### Value

A list containing three elements:

z.avg	The 'average' clustering, with minimum squared distance to z.sim.
z.sim	The N x N similarity matrix, in a sparse format (see $simple\_triplet\_matrix$ ).
MSE.z	A vector of length M recording the MSEs between each clustering and the 'average' clustering.

### Note

The mcclust package must be loaded.

This is liable to take quite some time to run, especially if the number of observations &/or number of iterations is large. Depending on how distinct the clusters are, z.sim may be stored better in a non-sparse format. This function can optionally be called inside get\_IMIFA\_results.

# Author(s)

```
Keefe Murphy - <<keefe.murphy@mu.ie>>
```

### References

Carmona, C., Nieto-barajas, L. and Canale, A. (2018) Model based approach for household clustering with mixed scale variables. *Advances in Data Analysis and Classification*, 13(2): 559-583.

#### See Also

```
get_IMIFA_results, simple_triplet_matrix, hclust, hc, comp.psm, cltoSim
```

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```
# Run a IMIFA model and extract the sampled cluster labels
# data(olive)
         <- mcmc_IMIFA(olive, method="IMIFA", n.iters=5000)</pre>
# zs
         <- sim[[1]][[1]]$z.store
# Get the similarity matrix and visualise it
# zsimil <- Zsimilarity(zs)</pre>
# z.sim <- as.matrix(zsimil$z.sim)</pre>
# z.col <- mat2cols(z.sim, cols=heat.colors(30, rev=TRUE))</pre>
# z.col[z.sim == 0] <- NA
# plot_cols(z.col, na.col=par()$bg); box(lwd=2)
# Extract the clustering with minimum squared distance to this
# 'average' and evaluate its performance against the true labels
# table(zsimil$z.avg, olive$area)
# Perform hierarchical clustering on the distance matrix
         <- hclust(as.dist(1 - z.sim), method="complete")
# plot(Hcl)
# table(cutree(Hcl, k=3), olive$area)
```

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