# Package 'mSigHdp'

June 6, 2020
Title Mutational signature extraction using hdp (Hierarchical Dirichlet Process)
<b>Version</b> 0.0.0.9015
<b>Description</b> Calls hdp for mutational signature analysis, with performance issues in hdp:::stirling() corrected.
License GPL-3
Encoding UTF-8
LazyData true
Language en-US
biocViews
Imports hdpx (>= 0.1.5.0014), SynSigGen
<b>Roxygen</b> list(markdown = TRUE)
<b>Depends</b> R (>= 3.5)
RoxygenNote 7.1.0
Remotes github::steverozen/hdpx, github::steverozen/SynSigGen, github::WuyangFF95/SynSigEval
Suggests testthat, ICAMS, utils, SynSigEval
R topics documented:
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AnalyzeAndPlotretval Evaluate and plot retval from CombinePosteriorChains

# **Description**

Evaluate and plot retval from CombinePosteriorChains

# Usage

```
AnalyzeAndPlotretval(
  retval,
  out.dir = NULL,
  ground.truth.sig = NULL,
  ground.truth.exp = NULL,
  verbose = TRUE,
  overwrite = TRUE
)
```

### **Arguments**

retval the output from function CombinePosteriorChains

out.dir Directory that will be created for the output; if overwrite is FALSE then abort

if out.dir already exits.

ground.truth.sig

Optional. Either a string with the path to file with ground truth signatures or and ICAMS catalog with the ground truth signatures. These are the signatures used to construct the ground truth spectre.

construct the ground truth spectra.

ground.truth.exp

Optional.Ground truth exposure matrix or path to file with ground truth expo-

sures. If NULL skip checks that need this information.

verbose If TRUE then message progress information.

overwrite If TRUE overwrite out.dir if it exists, otherwise raise an error.

ChainsDiagnosticPlot Diagnostic plot for hdp multi sample chains (output from CombinePosteriorChains)

# **Description**

Diagnostic plot for hdp multi sample chains (output from CombinePosteriorChains)

# Usage

```
ChainsDiagnosticPlot(retval, out.dir, verbose)
```

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#### **Arguments**

retval output from CombinePosteriorChains. A list with the following elements:

**signature** The extracted signature profiles as a matrix; rows are mutation types, columns are samples (e.g. tumors).

**exposure** The inferred exposures as a matrix of mutation counts; rows are signatures, columns are samples (e.g. tumors).

multi.chains A hdpSampleMulti-class object. This object has the method chains which returns a list of hdpSampleChain-class objects. Each of these sample chains objects has a method final\_hdpState (actually the methods seems to be just hdp) that returns the hdpState from which it was generated.

out.dir Directory that will be created for the output; if overwrite is FALSE then abort

if out.dir already exits.

verbose If TRUE then message progress information.

CombinePosteriorChains

Extract components and exposures from multiple posterior sample chains

#### **Description**

Extract components and exposures from multiple posterior sample chains

# Usage

```
CombinePosteriorChains(
  clean.chlist,
  input.catalog,
  multi.types,
  verbose = TRUE,
  cos.merge = 0.9,
  min.sample = 1
)
```

### Arguments

clean.chlist It collects the output of multiple independent hdp\_posterior calls.

multi.types A logical scalar or a character vector. If FALSE, hdp will regard all input spectra

as one tumor type.

If TRUE, hdp will infer tumor types based on the string before "::" in their names. e.g. tumor type for "SA.Syn.Ovary-AdenoCA::S.500" would be "SA.Syn.Ovary-AdenoCA"

If multi.types is a character vector, then it should be of the same length as the number of columns in input.catalog, and each value is the name of the tumor

type of the corresponding column in input.catalog, e.g. c("SA.Syn.Ovary-AdenoCA", "SA.Syn.O

verbose If TRUE then message progress information.

cos.merge The cosine similarity threshold for merging raw clusters from the posterior sampling chains into "components" i.e. signatures; passed to hdp\_extract\_components.

A "component" (i.e. signature) must have at least this many samples; passed to hdp\_extract\_components.

#### Value

Invisibly, a list with the following elements:

**signature** The extracted signature profiles as a matrix; rows are mutation types, columns are samples (e.g. tumors).

**exposure** The inferred exposures as a matrix of mutation counts; rows are signatures, columns are samples (e.g. tumors).

multi.chains A hdpSampleMulti-class object. This object has the method chains which returns a list of hdpSampleChain-class objects. Each of these sample chains objects has a method final\_hdpState (actually the methods seems to be just hdp) that returns the hdpState from which it was generated.

#### ExtendIterationAndPosterior

Run hdp extraction and attribution on a spectra catalog file This repeats what Nicola do in her thesis. It starts four independent initial chains with post.burnin iterations, then pick up from the end of each initial chain, started another num.posterior MCMC chains for another post.burnin iterations and then collected post.n posterior samples at intervals of post.space iterations. In total, this collects 4 times num.posterior times post.n posterior samples from 4 times y separate chains.

# **Description**

Run hdp extraction and attribution on a spectra catalog file This repeats what Nicola do in her thesis. It starts four independent initial chains with post.burnin iterations, then pick up from the end of each initial chain, started another num.posterior MCMC chains for another post.burnin iterations and then collected post.n posterior samples at intervals of post.space iterations. In total, this collects 4 times num.posterior times post.n posterior samples from 4 times y separate chains.

#### Usage

```
ExtendIterationAndPosterior(
  input.catalog,
  CPU.cores = 1,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  num.posterior = 4,
  post.burnin = 4000,
  post.n = 50,
  post.space = 50,
  post.cpiter = 3,
```

```
post.verbosity = 0,
cos.merge = 0.9,
min.sample = 1,
checkpoint.aft.post = NULL
)
```

# **Arguments**

input.catalog Input spectra catalog as a matrix or in ICAMS format.

CPU.cores Number of CPUs to use in running hdp\_posterior; this is used to parallelize

running the posterior sampling chains, so there is no point in making this larger

than num.posterior.

seedNumber An integer that is used to generate separate random seeds for each call to dp\_activate,

and each call of hdp\_posterior; please see the code on how this is done. But repeated calls with same value of seedNumber and other inputs should produce

the same results.

K.guess Suggested initial value of the number of signatures, passed to dp\_activate as

initcc.

multi.types A logical scalar or a character vector. If FALSE, hdp will regard all input spectra

as one tumor type.

If TRUE, hdp will infer tumor types based on the string before "::" in their names. e.g. tumor type for "SA.Syn.Ovary-AdenoCA::S.500" would be "SA.Syn.Ovary-

AdenoCA"

If multi.types is a character vector, then it should be of the same length as the number of columns in input.catalog, and each value is the name of the tumor

type of the corresponding column in input.catalog, e.g. c("SA.Syn.Ovary-AdenoCA", "SA.Syn.O

verbose If TRUE then message progress information.

num.posterior Number of posterior sampling chains; can set to 1 for testing.

post.burnin Pass to hdp\_posterior burnin.

post.n Pass to hdp\_posterior n.

Pass to hdp\_posterior space.

post.space Pass to hdp\_posterior space.
post.cpiter Pass to hdp\_posterior cpiter.
post.verbosity Pass to hdp\_posterior verbosity.

cos.merge The cosine similarity threshold for merging raw clusters from the posterior sam-

pling chains into "components" i.e. signatures; passed to hdp\_extract\_components.

min.sample A "component" (i.e. signature) must have at least this many samples; passed to

hdp\_extract\_components.

checkpoint.aft.post

If non-NULL, a file path to checkpoint the list of values returned from the calls to

hdp\_posterior as a .Rdata file.

#### Value

A list with the following elements:

**signature** The extracted signature profiles as a matrix; rows are mutation types, columns are samples (e.g. tumors).

**exposure** The inferred exposures as a matrix of mutation counts; rows are signatures, columns are samples (e.g. tumors).

**exposure.p** exposure converted to proportions.

multi.chains A hdpSampleMulti-class object. This object has the method chains which returns a list of hdpSampleChain-class objects. Each of these sample chains objects has a method final\_hdpState (actually the methods seems to be just hdp) that returns the hdpState from which it was generated.

MultipleSetupAndPosterior

Activate hierarchical Dirichlet processes and run posterior sampling in parallel.

# **Description**

Activate hierarchical Dirichlet processes and run posterior sampling in parallel.

#### Usage

```
MultipleSetupAndPosterior(
  input.catalog,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  post.burnin = 4000,
  post.n = 50,
  post.space = 50,
  post.cpiter = 3,
  post.verbosity = 0,
  CPU.cores = 1,
  num.child.process = 4
)
```

#### **Arguments**

input.catalog Input spectra catalog as a matrix or in ICAMS format.

seedNumber An integer that is used to generate separate random seeds for each call to dp\_activate,

> and each call of hdp\_posterior; please see the code on how this is done. But repeated calls with same value of seedNumber and other inputs should produce

the same results.

K.guess Initial guess of the number of "raw clusters", which may be larger than the num-

ber of signatures (sometimes called "components" in the hdpx code); passed to

dp\_activate as initcc.

A logical scalar or a character vector. If FALSE, The HDP analysis will regard multi.types all input spectra as one tumor type.

> If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "SA.Syn.Ovary-AdenoCA::S.500" would be "SA.Syn.Ovary-AdenoCA"

> If multi. types is a character vector, then it should be of the same length as the number of columns in input.catalog, and each value is the name of the tumor

type of the corresponding column in input.catalog, e.g. c("SA.Syn.Ovary-AdenoCA", "SA.Syn.O

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verbose If TRUE then message progress information.

post.burnin Pass to hdp\_posterior burnin.

post.n Pass to hdp\_posterior n.

post.space Pass to hdp\_posterior space.

post.cpiter Pass to hdp\_posterior cpiter.

post.verbosity Pass to hdp\_posterior verbosity.

CPU. cores Number of CPUs to use; there is no point in making this larger than num. child. process.

num.child.process

Number of posterior sampling chains; can set to 1 for testing.

#### Value

Invisibly, the clean chlist (output of the hdp\_posterior calls). This is a list of hdpSampleChain-class objects.

PlotExposure Plot a single exposure plot

# Description

Plot a single exposure plot

#### Usage

```
PlotExposure(exposures, plot.proportion = FALSE, plot.legend = TRUE, ...)
```

# **Arguments**

exposures Exposures as a numerical matrix (or data frame) with signatures in rows and

samples in columns. Rownames are taken as the signature names and column names are taken as the sample IDs. If you want exp sorted from largest to smallest use SortExp. Do not use column names that start with multiple underscores. The exposures will often be mutation counts, but could also be e.g. mutations

per megabase.

plot.proportion

Plot exposure proportions rather than counts.

plot.legend If TRUE plot a legend.

... Parameters passed to barplot.

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PlotExposureByRange Plot exposures in multiple plots each with samples.	a manageable number of
---	------------------------

# **Description**

Plot exposures in multiple plots each with a manageable number of samples.

# Usage

```
PlotExposureByRange(exposures, num.per.line = 30, plot.proportion = FALSE, ...)
```

#### **Arguments**

exposures

Exposures as a numerical matrix (or data.frame) with signatures in rows and samples in columns. Rownames are taken as the signature names and column names are taken as the sample IDs. If you want exposures sorted from largest to smallest use SortExp. Do not use column names that start with multiple underscores. The exposures will often be mutation counts, but could also be e.g. mutations per megabase.

num.per.line

Number of samples to show in each plot.

plot.proportion

Plot exposure proportions rather than counts.

. . .

Other arguments passed to PlotExposure. If ylab is not included, it defaults to a value depending on plot.proportion. If col is not supplied the function tries to do something reasonable.

PrepInit

Initialize hdp object Allocate process index for hdp initialization. Prepare for hdp\_init

# **Description**

Initialize hdp object Allocate process index for hdp initialization. Prepare for hdp\_init

# Usage

```
PrepInit(multi.types, input.catalog, verbose, K.guess)
```

# **Arguments**

```
multi.types TODO
input.catalog TODO
verbose TODO
K.guess TODO
```

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RunHdpParallel	Extract mutational signatures and optionally compare them to existing
	signatures and exposures.

#### **Description**

Extract mutational signatures and optionally compare them to existing signatures and exposures.

# Usage

```
RunHdpParallel(
  input.catalog,
  seedNumber = 1,
 K.guess,
 multi.types = FALSE,
  verbose = TRUE,
 post.burnin = 4000,
 post.n = 50,
  post.space = 50,
 post.cpiter = 3,
 post.verbosity = 0,
 CPU.cores = 1,
  num.child.process = 4,
  cos.merge = 0.9,
 min.sample = 1,
 ground.truth.sig = NULL,
 ground.truth.exp = NULL,
 overwrite = TRUE,
  out.dir = NULL
)
```

#### **Arguments**

input.catalog	Input spectra	catalog as a ma	trix or in	ICAMS format.

seedNumber An integer that is used to generate separate random seeds for each call to dp\_activate,

and each call of hdp\_posterior; please see the code on how this is done. But repeated calls with same value of seedNumber and other inputs should produce

the same results.

K. guess Initial guess of the number of "raw clusters", which may be larger than the number of signatures (sometimes called "components" in the hdpy code); passed to

ber of signatures (sometimes called "components" in the hdpx code); passed to

dp\_activate as initcc.

multi.types A logical scalar or a character vector. If FALSE, The HDP analysis will regard all input spectra as one tumor type.

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "SA.Syn.Ovary-AdenoCA::S.500" would be "SA.Syn.Ovary-AdenoCA"

If multi.types is a character vector, then it should be of the same length as the number of columns in input.catalog, and each value is the name of the tumor

type of the corresponding column in input.catalog, e.g. c("SA.Syn.Ovary-AdenoCA", "SA.Syn.O

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verbose If TRUE then message progress information.

post.burnin Pass to hdp\_posterior burnin.

post.n Pass to hdp\_posterior n.

post.space Pass to hdp\_posterior space.

post.cpiter Pass to hdp\_posterior cpiter.

 $post.verbosity \ \ Pass\ to\ hdp\_posterior\ verbosity.$ 

CPU. cores Number of CPUs to use; there is no point in making this larger than num. child.process.

num.child.process

Number of posterior sampling chains; can set to 1 for testing.

cos.merge The cosine similarity threshold for merging raw clusters from the posterior sam-

pling chains into "components" i.e. signatures; passed to hdp\_extract\_components.

min.sample A "component" (i.e. signature) must have at least this many samples; passed to

hdp\_extract\_components.

ground.truth.sig

Optional. Either a string with the path to file with ground truth signatures or and ICAMS catalog with the ground truth signatures. These are the signatures used to construct the ground truth spectra.

ground.truth.exp

Optional.Ground truth exposure matrix or path to file with ground truth expo-

sures. If NULL skip checks that need this information.

overwrite If TRUE, overwrite out.dir if it is non-NULL and exists.

out.dir If not NULL, output including data and plots will be saved in out.dir.

#### Value

Invisibly, a list with the following elements:

**signature** The extracted signature profiles as a matrix; rows are mutation types, columns are samples (e.g. tumors).

**exposure** The inferred exposures as a matrix of mutation counts; rows are signatures, columns are samples (e.g. tumors).

multi.chains A hdpSampleMulti-class object. This object has the method chains which returns a list of hdpSampleChain-class objects. Each of these sample chains objects has a method final\_hdpState (actually the methods seems to be just hdp) that returns the hdpState from which it was generated.

SetupAndPosterior

Generate an HDP Gibbs sampling chain from a spectra catalog.

# **Description**

Generate an HDP Gibbs sampling chain from a spectra catalog.

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#### Usage

```
SetupAndPosterior(
  input.catalog,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  post.burnin = 4000,
  post.n = 50,
  post.space = 50,
  post.cpiter = 3,
  post.verbosity = 0
)
```

### **Arguments**

input.catalog Input spectra catalog as a matrix or in ICAMS format.

seedNumber An integer that is used to generate separate random seeds for each call to dp\_activate,

and each call of hdp\_posterior; please see the code on how this is done. But repeated calls with same value of seedNumber and other inputs should produce

the same results.

K. guess Initial guess of the number of "raw clusters", which may be larger than the num-

ber of signatures (sometimes called "components" in the hdpx code); passed to

dp\_activate as initcc.

multi.types A logical scalar or a character vector. If FALSE, The HDP analysis will regard

all input spectra as one tumor type.

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "SA.Syn.Ovary-AdenoCA::S.500" would be

"SA.Syn.Ovary-AdenoCA"

If multi.types is a character vector, then it should be of the same length as the

number of columns in input.catalog, and each value is the name of the tumor type of the corresponding column in input.catalog, e.g. c("SA.Syn.Ovary-AdenoCA", "SA.Syn.O

verbose If TRUE then message progress information.

post.burnin Pass to hdp\_posterior burnin.

post.n Pass to hdp\_posterior n.

post.space Pass to hdp\_posterior space.

post.cpiter Pass to hdp\_posterior cpiter.

post.verbosity Pass to hdp\_posterior verbosity.

#### Value

Invisibly, an hdpSampleChain-class object as returned from hdp\_posterior.

SortExp

SortExp	Sort columns of an exposure matrix from largest to smaller (or vice versa).

# Description

Sort columns of an exposure matrix from largest to smaller (or vice versa).

# Usage

```
SortExp(exposures, decreasing = TRUE)
```

# Arguments

exposures The exposures to sort; columns are samples.

 $\label{eq:continuous_decreasing} \qquad \quad \text{If TRUE sort from largest to smallest.}$ 

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