Package 'mSigHdp'

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Title Mutational signature extraction using hdp (Hierarchical Dirichlet Process)
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AnalyzeAndPlotretval
BurninIteration
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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

the output from function CombinePosteriorChains retval 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 spectra.

ground.truth.exp

Optional. Ground truth exposure matrix or path to file with ground truth exposures. If \mathtt{NULL} skip checks that need this information.

If TRUE then message progress information. verbose

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

BurninIteration

Run hdp extraction and attribution on a spectra catalog file A function to do burn-in iteration only. This returns a list of hdp object. This needs to be converted to a hdpState object before hdp_posterior (hdpx:::as.hdpState(hdplist))

Description

Run hdp extraction and attribution on a spectra catalog file A function to do burn-in iteration only. This returns a list of hdp object. This needs to be converted to a hdpState object before hdp_posterior (hdpx:::as.hdpState(hdplist))

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Usage

```
BurninIteration(
  input.catalog,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  post.burnin = 4000,
  post.cpiter = 3,
  post.verbosity = 0,
  gamma.alpha = 1,
  gamma.beta = 1
)
```

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

Suggested initial value of the number of signatures, passed to ${\tt dp_activate}$

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.Kidney-RCC").

verbose

If TRUE then message progress information.

post.burnin Pass to hdp_posterior burnin.
post.cpiter Pass to hdp_posterior cpiter.
post.verbosity

Pass to hdp_posterior verbosity.

gamma.alpha

Shape parameter of gamma distribution from which the Dirichlet process concentration parameters are drawn; in this function the gamma distributions for all

Dirichlet processes are the same.

gamma.beta

Inverse scale parameter (rate parameter) of gamma distribution from which the Dirichlet process concentration parameters are drawn; in this function the gamma distributions for all Dirichlet processes are the same.

Value

A list with hdp object after burn-in iteration and likelihood of iteration

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ChainsDiagnosticPlot

Diagnostic plot for a hdpSampleMulti object

Description

Diagnostic plot for a hdpSampleMulti object

Usage

ChainsDiagnosticPlot(retval, out.dir, verbose)

Arguments

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 sig-
natures, 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.
Directory that will be created for the output; if overwrite is FALSE then
abort if out.dir already exits.
If TRUE then message progress information.
If the job of Gibbs sampling from
MultipleSetupAndPosterior has an error caught by R ,
the corresponding element of chlist has class try-error. If the job is

Description

If the job of Gibbs sampling from MultipleSetupAndPosterior has an error caught by R, the corresponding element of chlist has class try-error. If the job is stopped with, e.g. a segfault, the chlist element is NULL.

stopped with, e.g. a segfault, the chlist element is NULL.

Usage

```
CleanChlist(chlist, verbose = FALSE)
```

Arguments

chlist A list of hdpSampleChain-class objects.

Value

Invisibly, the clean, non-error chlist This is a list of hdpSampleChain-class objects.

CombinePosteriorChains 5

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.

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

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"

"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.

 $e.g. \; \texttt{c("SA.Syn.Ovary-AdenoCA","SA.Syn.Kidney-RCC")} \; .$

verbose

If TRUE then message progress information.

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.

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.

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,
  gamma.alpha = 1,
  gamma.beta = 1
)
```

Arguments

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

seedNumber A random seeds passed to dp_activate.

K. guess Suggested initial value of the number of signatures, passed to dp_activate

as initcc.

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

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.Kidney-RCC").

verbose If TRUE then message progress information.

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```
post.burnin Pass to hdp posterior burnin.
post.n
                 Pass to hdp_posterior n.
                 Pass to hdp_posterior space.
post.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.
gamma.alpha
                 Shape parameter of gamma distribution from which the Dirichlet process con-
                 centration parameters are drawn; in this function the gamma distributions for all
                 Dirichlet processes are the same.
                 Inverse scale parameter (rate parameter) of gamma distribution from which the
gamma.beta
                 Dirichlet process concentration parameters are drawn; in this function the gamma
                 distributions for all Dirichlet processes are the same.
```

Value

Invisibly, the clean chlist (output of CleanChlist). 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 <code>exp</code> sorted from largest to smallest use <code>SortExp</code>. 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 a manageable number of samples.

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,
  gamma.alpha = 1,
  gamma.beta = 1
```

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Arguments

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.Kidney-RCC").

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

verbose If TRUE then message progress information.

K. guess Suggested initial value of the number of signatures, passed to dp_activate

as initcc.

gamma.alpha Shape parameter of gamma distribution from which the Dirichlet process con-

centration parameters are drawn; in this function the gamma distributions for all

Dirichlet processes are the same.

gamma . beta Inverse scale parameter (rate parameter) of gamma distribution from which the

Dirichlet process concentration parameters are drawn; in this function the gamma

distributions for all Dirichlet processes are the same.

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,
```

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```
ground.truth.exp = NULL,
overwrite = TRUE,
out.dir = NULL,
gamma.alpha = 1,
gamma.beta = 1
)
```

Arguments

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

seedNumber A random seeds passed to dp_activate.

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, 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 ${\tt multi.types}$ is a character vector, then it should be of the same length as the number of columns in ${\tt input.catalog}$, and each value is the name of the

 $tumor\ type\ of\ the\ corresponding\ column\ in\ \verb"input.catalog".$

e.g. c("SA.Syn.Ovary-AdenoCA", "SA.Syn.Kidney-RCC").

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 exposures. If NULL skip checks that need this information.

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

abort if out . dir already exits.

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gamma.alpha	Shape parameter of gamma distribution from which the Dirichlet process concentration parameters are drawn; in this function the gamma distributions for all Dirichlet processes are the same.
gamma.beta	Inverse scale parameter (rate parameter) of gamma distribution from which the Dirichlet process concentration parameters are drawn; in this function the gamma distributions for all Dirichlet processes are the same.

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.

SetupAndActivate

Generate an HDP Gibbs sampling chain from a spectra catalog.

Description

Generate an HDP Gibbs sampling chain from a spectra catalog.

Usage

```
SetupAndActivate(
  input.catalog,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  gamma.alpha = 1,
  gamma.beta = 1
)
```

Arguments

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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.Kidney-RCC").

verbose If TRUE then message progress information.

gamma.alpha Shape parameter of gamma distribution from which the Dirichlet process concentration parameters are drawn; in this function the gamma distributions for all

Dirichlet processes are the same.

 ${\tt gamma.beta} \qquad {\tt Inverse\ scale\ parameter\ (rate\ parameter)\ of\ gamma\ distribution\ from\ which\ the}$

 $Dirichlet\ process\ concentration\ parameters\ are\ drawn;\ in\ this\ function\ the\ gamma$

distributions for all Dirichlet processes are the same.

Value

Invisibly, an hdpState-class object as returned from dp_activate.

SetupAndPosterior Generate an HDP Gibbs sampling chain from a spectra catalog.

Description

Generate an HDP Gibbs sampling chain from a spectra catalog.

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,
  gamma.alpha = 1,
  gamma.beta = 1)
```

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Arguments

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

seedNumber A random seeds passed to dp_activate.

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, 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.Kidney-RCC").

verbose If TRUE then message progress information.

post.burnin Pass to hdp_posterior burnin.

 $post.n \hspace{1cm} Pass \hspace{1cm} to \hspace{1cm} hdp_posterior \hspace{1cm} n.$

post.space Pass to hdp_posterior space.
post.cpiter Pass to hdp_posterior cpiter.

post.verbosity

Pass to hdp_posterior verbosity.

gamma.alpha Shape parameter of gamma distribution from which the Dirichlet process con-

centration parameters are drawn; in this function the gamma distributions for all

Dirichlet processes are the same.

gamma.beta Inverse scale parameter (rate parameter) of gamma distribution from which the

Dirichlet process concentration parameters are drawn; in this function the gamma

distributions for all Dirichlet processes are the same.

Value

Invisibly, an hdpSampleChain-class object as returned from hdp_posterior.

Sort Exp 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. decreasing If TRUE sort from largest to smallest.

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