Package 'mSigHdp'

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AnalyzeAndPlotretval

Evaluate and plot retval from CombinePosteriorChains or CombineChainsAndExtractSigs This function now works for both NR's pipeline and Mo's pipeline

Description

Evaluate and plot retval from CombinePosteriorChains or CombineChainsAndExtractSigs This function now works for both NR's pipeline and Mo's pipeline

Usage

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

Arguments

```
the output from function CombinePosteriorChains or CombineChainsAndExtractSigs
retval
input.catalog
                 input catalog matrix or path to file with input catalog
                 Directory that will be created for the output; if overwrite is FALSE then
out.dir
                 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 expo-
                 sures. If NULL skip checks that need this information.
                 If TRUE then message progress information.
verbose
                 If TRUE overwrite out .dir if it exists, otherwise raise an error.
overwrite
```

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```
diagnostic.plot
```

If TRUE plot diagnostic plot. This is optional because there are cases having error

ChainBurnin

Prepare an hdpState-class object and run the Gibbs sampling burnin.

Description

Prepare an hdpState-class object and run the Gibbs sampling burnin.

Usage

```
ChainBurnin(
  hdp.state,
  seedNumber = 1,
  burnin = 4000,
  cpiter = 3,
  burnin.verbosity = 0,
  burnin.multiplier = 1,
  burnin.checkpoint = FALSE
)
```

Arguments

An hdpState-class object or a list representation of an hdpState-class object.

seedNumber An integer that is used to generate separate random seeds for the call to dp_activate, and before the call of hdp_burnin.

burnin Pass to hdp_burnin burnin.

cpiter Pass to hdp_burnin cpiter.

burnin.verbosity

Pass to hdp_burnin verbosity.

burnin.multiplier

A checkpoint setting. burnin.multiplier rounds of burnin iterations will be run. After each round, a burn-in chain will be save for checkpoint.

Default is False. If True, a checkpoint for burnin will be created.

Value

A list with 2 elements:

burnin.checkpoint

hdplist A list representation of an hdpState-class object.

likelihood A numeric vector with the likelihood at each iteration.

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ChainsDiagnosticPlot

Diagnostic plot for a hdpSampleMulti object

Description

Diagnostic plot for a hdpSampleMulti object

Usage

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

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.

input.catalog

ground truth catalog

out.dir Directory the

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.

CleanChlist

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.

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.

Usage

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

Arguments

```
chlist A list of hdpSampleChain-class objects.

verbose If TRUE then message progress information.
```

Value

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

```
CombineChainsAndExtractSigs
```

Extract components and exposures from multiple posterior sample chains This function returns signatures with high confidence (found in more than 90% #' posterior samples)

Description

Extract components and exposures from multiple posterior sample chains This function returns signatures with high confidence (found in more than 90% #' posterior samples)

Usage

```
CombineChainsAndExtractSigs(
  clean.chlist,
  input.catalog,
  multi.types,
  verbose = TRUE,
  cos.merge = 0.9,
  confident.prop = 0.9,
  noise.prop = 0.1,
  hc.cutoff = 0.12
)
```

Arguments

clean.chlist A list of hdpSampleChain-class objects. Each element is the result of one posterior sample chain.

```
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"

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.

6 CombinePosteriorChains

The cosine similarity threshold for merging raw clusters from the posterior sampling chains into "components" i.e. signatures; passed to extract_components_from_clusters confident.prop

Passed to interpret_components. clusters with at least confident.prop of posterior samples are high confident signatures

noise.prop

Passed to interpret_components. Clusters with less than noise.prop of posterior samples are noise signatures

hc.cutoff

passed to extract_components_from_clusters. The cutoff of height of hierarchical clustering dendrogram

Value

Invisibly, a list with the following elements:

signature The extracted signature profiles as a matrix; rows are mutation types, columns are signatures including high confident signatures -'hdp' signatures and moderate confident signatures - 'potential hdp' signatures.

signature.post.samp.number A dataframe with two columns. The first column corresponds to each signature in signature and the second columns contains the number of posterior samples that found the raw clusters contributing to the signature.

signature.cdc A comp_dp_counts like dataframe. Each column corresponds to the sum of all comp_dp_counts matrices of the raw clusters contributing to each signature in codesignature

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

noise.signature The extracted signature profiles as a matrix; rows are mutation types, columns are signatures with less than noise.prop of posterior samples

noise.post.samp.number A data frame with two columns. The first column corresponds to each signature in noise.signature and the second columns contains the number of posterior samples that found the raw clusters contributing to the signature.

noise.cdc A comp_dp_counts like data frame. Each column corresponds to the sum of all comp_dp_counts matrices of the raw clusters contributing to each signature in codenoise.signature

extracted.retval A list object returned from codeinterpret_components.

CombinePosteriorChains

Extract components and exposures from multiple posterior sample chains

Description

Extract components and exposures from multiple posterior sample chains

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Usage

```
CombinePosteriorChains(
  clean.chlist,
  input.catalog,
  multi.types,
  verbose = TRUE,
  cos.merge = 0.9,
  categ.CI = 0.95,
  exposure.CI = 0.95,
  min.sample = 1,
  diagnostic.folder = NULL
)
```

Arguments

clean.chlist A list of hdpSampleChain-class objects. Each element is the result of one posterior sample chain.

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"

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.

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.

categ.CI

A number the range [0, 1]. The level of the confidence interval used in step 4 of hdp_merge_and_extract_components. This governs when "averaged raw cluster" get assigned to component 0, i.e. if the the confidence interval overlaps 0. Lower values make it less likely that an averaged raw cluster will be assigned to component 0. The CI in question is for the number of mutations in a given mutation class (e.g. ACA > AAA, internally called a "category"). If, for every mutation class, this CI overlaps 0, then the averaged raw cluster goes to component 0.

exposure.CI

A number in the range [0,1]. The level of the confidence interval used in step 5 of hdp_merge_and_extract_components. The CI in question here for the total number of mutations assigned to an averaged raw cluster.

min.sample

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

diagnostic.folder

If provided, diagnostic plots for hdp.0 components are provided

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.
- **sum_raw_clusters_after_cos_merge** A matrix containing aggregated spectra of raw clusters after cosine similarity merge step in hdp_merge_and_extract_components.
- **sum_raw_clusters_after_nonzero_categ** A matrix containing aggregated spectra of raw clusters after non-zero category selecting step in hdp_merge_and_extract_components.
- clust_hdp0_ccc4 A matrix containing aggregated spectra of raw clusters moving to hdp.0 after non-zero category selection step in hdp_merge_and_extract_components.
- clust_hdp0_ccc5 A matrix containing aggregated spectra of raw clusters moving to hdp.0 after non-zero observation selection step in hdp_merge_and_extract_components.

ComponentDiagnosticPlotting

Diagnostic plot for a hdpSampleMulti object. This function is compatible with the return object from Liu's extract_components_from_clusters

Description

Diagnostic plot for a hdpSampleMulti object. This function is compatible with the return object from Liu's extract_components_from_clusters

Usage

ComponentDiagnosticPlotting(retval, input.catalog, out.dir, verbose)

Arguments

retval output from CombineChainsAndExtractSigs
input.catalog
ground truth catalog

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.

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ExtendBurnin	Extend Burn in iteration for a list representation of an
	$\begin{tabular}{ll} $hdpState-class \it object. \it This \it list is an \it output from \it hdp_burnin \\ \it or \it Activate \it and \it Burnin. \end{tabular}$

Description

Extend Burn in iteration for a list representation of an hdpState-class object. This list is an output from hdp_burnin or ActivateandBurnin.

Usage

```
ExtendBurnin(hdplist, seedNumber = 1, burnin = 4000, cpiter = 3, verbosity = 0)
```

Arguments

hdplist A list representation of an hdpState-class object seedNumber A random seed for setting the environment of hdp_burnin.

burnin Pass to hdp_posterior burnin.

cpiter Pass to hdp_posterior cpiter.

verbosity Pass to hdp_posterior verbosity.

Value

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

GenerateAverageCluster

Generate average pattern of clusters of each posterior chain from combined list of multiple posterior sample chains

Description

Generate average pattern of clusters of each posterior chain from combined list of multiple posterior sample chains

Usage

```
GenerateAverageCluster(clean.chlist)
```

Arguments

clean.chlist A list of multiple (or one) posterior sample chains.

Value

A list of matrices containing the average pattern of clusters within each posterior chain and a list of matrices containing the sum of each cluster in each posterior chain

Generateppindex

Generate index for a HDP structure and num.tumor.types for other functions

Description

Generate index for a HDP structure and num.tumor.types for other functions

Usage

```
Generateppindex (multi.types, input.catalog)
```

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.

GeneratePriorppindex

Generate index for a HDP structure and num.tumor.types for other functions for hdp_prior_init

Description

Generate index for a HDP structure and num.tumor.types for other functions for hdp_prior_init

Usage

```
GeneratePriorppindex(multi.types, input.catalog, nps)
```

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.

nps

Number of prior signatures

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,
  gamma0.alpha = gamma.alpha,
  gamma0.beta = gamma.beta,
  checkpoint.chlist = TRUE,
  checkpoint.1.chain = TRUE,
  prior.sigs = NULL,
  prior.pseudoc = NULL,
  burnin.multiplier = 1,
  burnin.checkpoint = FALSE
)
```

Arguments

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

 ${\tt seedNumber} \qquad A \ random \ seeds \ passed \ to \ {\tt dp_activate}.$

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.

post.burnin Pass to hdp_posterior_sample burnin.

post.n Pass to hdp_posterior_sample n.

post.space Pass to hdp_posterior_sample space.

post.cpiter Pass to hdp_posterior_sample cpiter.

post.verbosity

Pass to hdp_posterior_sample 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.

Shape parameter of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same.

Inverse scale parameter (rate parameter) of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same

gamma 0.alpha See figure B.1 from Nicola Robert's thesis. The shape parameter (α_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

gamma 0 . beta See figure B.1 from Nicola Robert's thesis. Inverse scale parameter (rate parameter, β_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

checkpoint.chlist

If TRUE, checkpoint the (unclean) chlist to "initial.chlist.Rdata" in the current working directory. and checkpoint the clean chlist to "clean.chlist.Rdata" in the current working directory.

checkpoint.1.chain

If TRUE checkpoint the sample chain to current working directory, in a file called sample.chain.seed number.Rdata.

prior.sigs A matrix containing prior signatures.

prior.pseudoc

A numeric list. Pesudo counts of each prior signature. Recommended is 1000. In practice, it may be advisable to put lower weights on prior signatures that you do not expect to be present in your dataset, or even exclude some priors entirely.

burnin.multiplier

A checkpoint setting. burnin.multiplier rounds of burnin iterations will be run. After each round, a burn-in chain will be save for checkpoint.

burnin.checkpoint

Default is False. If True, a checkpoint for burnin will be created.

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Value

Invisibly, the clean chlist (output of CleanChlist). This is a list of hdpSampleChain-class objects.

NewRunHdpParallel 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

```
NewRunHdpParallel(
  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,
  confident.prop = 0.9,
  noise.prop = 0.5,
  hc.cutoff = 0.1,
  ground.truth.sig = NULL,
  ground.truth.exp = NULL,
  overwrite = TRUE,
  out.dir = NULL,
  gamma.alpha = 1,
  gamma.beta = 1,
  gamma0.alpha = gamma.alpha,
  gamma0.beta = gamma.beta,
  checkpoint.chlist = TRUE,
  checkpoint.1.chain = TRUE,
  prior.sigs = NULL,
  prior.pseudoc = NULL,
 burnin.multiplier = 1,
  burnin.checkpoint = FALSE
)
```

Arguments

```
input.catalog
```

Input spectra catalog as a matrix or in ICAMS format.

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seedNumber A random seeds passed to dp activate. Suggested initial value of the number of signatures, passed to dp_activate K.guess 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. Pass to hdp_posterior_sample burnin. post.burnin Pass to hdp_posterior_sample n. post.n Pass to hdp_posterior_sample space. post.space Pass to hdp_posterior_sample cpiter. post.cpiter post.verbosity Pass to hdp_posterior_sample verbosity. Number of CPUs to use; there is no point in making this larger than num.child.process. CPU.cores 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 sampling chains into "components" i.e. signatures; passed to extract_components_from_cluste confident.prop Passed to interpret_components. clusters with at least confident.prop of posterior samples are high confident signatures Passed to interpret components. Clusters with less than noise.prop noise.prop of posterior samples are noise signatures passed to extract_components_from_clusters. The cutoff of height hc.cutoff of hierarchical clustering dendrogram 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. overwrite If TRUE overwrite out . dir if it exists, otherwise raise an error. Directory that will be created for the output; if overwrite is FALSE then out.dir abort if out . dir already exits. gamma.alpha Shape parameter of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same. Inverse scale parameter (rate parameter) of the gamma distribution prior for the gamma.beta Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same.

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gamma0.alpha See figure B.1 from Nicola Robert's thesis. The shape parameter (α_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

gamma 0.beta See figure B.1 from Nicola Robert's thesis. Inverse scale parameter (rate parameter, β_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

checkpoint.chlist

If TRUE, checkpoint the (unclean) chlist to "initial.chlist.Rdata" in the current working directory. and checkpoint the clean chlist to "clean.chlist.Rdata" in the current working directory.

checkpoint.1.chain

If TRUE checkpoint the sample chain to current working directory, in a file called sample.chain.seed_number.Rdata.

prior.sigs A matrix containing prior signatures.

prior.pseudoc

A numeric list. Pesudo counts of each prior signature. Recommended is 1000. In practice, it may be advisable to put lower weights on prior signatures that you do not expect to be present in your dataset, or even exclude some priors entirely.

burnin.multiplier

A checkpoint setting. burnin.multiplier rounds of burnin iterations will be run. After each round, a burn-in chain will be save for checkpoint.

burnin.checkpoint

Default is False. If True, a checkpoint for burnin will be created.

Value

Invisibly, a list with the following elements:

- **signature** The extracted signature profiles as a matrix; rows are mutation types, columns are signatures including high confident signatures -'hdp' signatures and moderate confident signatures 'potential hdp' signatures.
- **signature.post.samp.number** A dataframe with two columns. The first column corresponds to each signature in signature and the second columns contains the number of posterior samples that found the raw clusters contributing to the signature.
- **signature.cdc** A comp_dp_counts like dataframe. Each column corresponds to the sum of all comp_dp_counts matrices of the raw clusters contributing to each signature in codesignature
- **exposureProbs** The inferred exposures as a matrix of mutation probabilities; rows are signatures, columns are samples (e.g. tumors).
- **noise.signature** The extracted signature profiles as a matrix; rows are mutation types, columns are signatures with less than noise.prop of posterior samples
- **noise.post.samp.number** A data frame with two columns. The first column corresponds to each signature in noise.signature and the second column contains the number of posterior samples that found the raw clusters contributing to the signature.
- **noise.cdc** A comp_dp_counts like data frame. Each column corresponds to the sum of all comp_dp_counts matrices of the raw clusters contributing to each signature in codenoise.signature

extracted.retval A list object returned from codeinterpret_components.

```
PlotSamplesHighSigExp
```

Plot hdp signature exposure in each sample. This function returns the plot of top 5 samples with the highest exposure to a signature. Each spectrum's title is in the form of: SampleName(Proportion of Signature Assginment) This function is here because it is specific for signature extraction application.

Description

Plot hdp signature exposure in each sample. This function returns the plot of top 5 samples with the highest exposure to a signature. Each spectrum's title is in the form of: SampleName(Proportion of Signature Assginment) This function is here because it is specific for signature extraction application.

Usage

```
PlotSamplesHighSigExp(
  retval,
  hdpsample,
  input.catalog,
  col_comp = NULL,
  incl_numdata_plot = TRUE,
  ylab_numdata = "Number of data items",
  ylab_exp = "Component exposure",
  leg.title = "Component",
  cex.names = 0.6,
  cex.axis = 0.7,
  mar = c(1, 4, 2, 0.5),
  oma = c(1.5, 1.5, 1, 1)
)
```

Arguments

```
retval
                 an object return from extract_ccc_cdc_from_hdp
hdpsample
                 A hdpSampleChain-class or hdpSampleMulti-class object includ-
                 ing output from extract_components_from_clusters
input.catalog
                 input catalog for samples
                 Colours of each component, from 0 to the max number. If NULL, default colors
col_comp
                 will be used
incl_numdata_plot
                 Logical - should an upper barplot indicating the number of data items per DP be
                 included? (Default TRUE)
ylab_numdata Vertical axis label for numdata plot
                 Vertical exis label for exposure plot
ylab_exp
leg.title
                 Legend title
cex.names
                 Expansion factor for bar labels (dpnames) in exposure plot
                 Expansion factor for vertical-axis annotation
cex.axis
```

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mar	See ?par
oma	See ?par

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 = TRUE,
  K.guess,
  gamma.alpha = 1,
  gamma.beta = 1,
  gamma0.alpha = gamma.alpha,
  gamma0.beta = gamma.beta
)
```

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 the gamma distribution prior for the Dirichlet process con-

centration parameters; in this function the gamma distributions for all Dirichlet

processes, except possibly the top level process, are the same.

gamma .beta Inverse scale parameter (rate parameter) of the gamma distribution prior for the

Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the

same.

```
gamma0.alpha See figure B.1 from Nicola Robert's thesis. The shape parameter (\alpha_0) of the gamma distribution priors for the Dirichlet process concentration parameters (\gamma_0) for G_0.
```

gamma 0.beta See figure B.1 from Nicola Robert's thesis. Inverse scale parameter (rate parameter, β_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

PriorSetupAndActivate

Generate an HDP Gibbs sampling chain from a spectra catalog.

Description

Generate an HDP Gibbs sampling chain from a spectra catalog.

Usage

```
PriorSetupAndActivate(
   prior.sigs,
   prior.pseudoc,
   gamma.alpha = 1,
   gamma.beta = 1,
   K.guess,
   gamma0.alpha = gamma.alpha,
   gamma0.beta = gamma.beta,
   multi.types = F,
   input.catalog,
   verbose = TRUE,
   seedNumber = 1
)
```

Arguments

prior.sigs	A matrix containing prior signatures.
prior.pseudo	C
	A numeric list. Pesudo counts of each prior signature. Recommended is 1000. In practice, it may be advisable to put lower weights on prior signatures that you do not expect to be present in your dataset, or even exclude some priors entirely.
gamma.alpha	Shape parameter of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same.
gamma.beta	Inverse scale parameter (rate parameter) of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same.
K.guess	Suggested initial value of the number of signatures, passed to ${\tt dp_activate}$ as initcc.
gamma0.alpha	See figure B.1 from Nicola Robert's thesis. The shape parameter (α_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

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gamma0.beta See figure B.1 from Nicola Robert's thesis. Inverse scale parameter (rate parameter, β_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 . 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.

Value

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

A random seeds passed to dp_activate.

RunHdpParallel

seedNumber

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.quess,
 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,
  categ.CI = 0.95,
 exposure.CI = 0.95,
  ground.truth.sig = NULL,
  ground.truth.exp = NULL,
```

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```
overwrite = TRUE,
out.dir = NULL,
gamma.alpha = 1,
gamma.beta = 1,
gamma0.alpha = gamma.alpha,
gamma0.beta = gamma.beta,
checkpoint.chlist = TRUE,
checkpoint.1.chain = TRUE,
prior.sigs = NULL,
prior.pseudoc = NULL,
burnin.multiplier = 1,
burnin.checkpoint = FALSE
```

Arguments

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

seedNumber A random seeds passed to dp_activate.

 $\textbf{K.guess} \qquad \qquad \textbf{Suggested initial value of the number of signatures, passed to } \\ \textbf{dp_activate}$

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

 $tumor\ type\ of\ the\ corresponding\ column\ in\ {\tt input.catalog}.$

 $e.g. \verb| c("SA.Syn.Ovary-AdenoCA", "SA.Syn.Kidney-RCC")|.$

verbose If TRUE then message progress information.

post.burnin Pass to hdp_posterior_sample burnin.

post.n Pass to hdp_posterior_sample n.
post.space Pass to hdp posterior sample space.

post.verbosity

num.child.process

Pass to hdp_posterior_sample verbosity.

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

 $\verb|categ.CI| \qquad \text{A number the range } [0,1]. \text{ The level of the confidence interval used in step 4 of}$

hdp_merge_and_extract_components. This governs when "averaged raw cluster" get assigned to component 0, i.e. if the confidence interval overlaps 0. Lower values make it less likely that an averaged raw cluster will be

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assigned to component 0. The CI in question is for the number of mutations in a given mutation class (e.g. ACA > AAA, internally called a "category"). If, for every mutation class, this CI overlaps 0, then the averaged raw cluster goes to component 0.

exposure.CI A number in the range [0, 1]. The level of the confidence interval used in step 5 of hdp_merge_and_extract_components. The CI in question here for the total number of mutations assigned to an averaged raw cluster.

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.

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

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

Shape parameter of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same.

Inverse scale parameter (rate parameter) of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same.

gamma 0.alpha See figure B.1 from Nicola Robert's thesis. The shape parameter (α_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

gamma 0 . beta See figure B.1 from Nicola Robert's thesis. Inverse scale parameter (rate parameter, β_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

checkpoint.chlist

If TRUE, checkpoint the (unclean) chlist to "initial.chlist.Rdata" in the current working directory. and checkpoint the clean chlist to "clean.chlist.Rdata" in the current working directory.

checkpoint.1.chain

If TRUE checkpoint the sample chain to current working directory, in a file called sample.chain.seed_number.Rdata.

prior.sigs A matrix containing prior signatures.

prior.pseudoc

A numeric list. Pesudo counts of each prior signature. Recommended is 1000. In practice, it may be advisable to put lower weights on prior signatures that you do not expect to be present in your dataset, or even exclude some priors entirely.

burnin.multiplier

A checkpoint setting. burnin.multiplier rounds of burnin iterations will be run. After each round, a burn-in chain will be save for checkpoint.

burnin.checkpoint

Default is False. If True, a checkpoint for burnin will be created.

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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.
- **sum_raw_clusters_after_cos_merge** A matrix containing aggregated spectra of raw clusters after cosine similarity merge step in hdp_merge_and_extract_components.
- **sum_raw_clusters_after_nonzero_categ** A matrix containing aggregated spectra of raw clusters after non-zero category selecting step in hdp_merge_and_extract_components.
- clust_hdp0_ccc4 A matrix containing aggregated spectra of raw clusters moving to hdp.0 after non-zero category selection step in hdp_merge_and_extract_components.
- clust_hdp0_ccc5 A matrix containing aggregated spectra of raw clusters moving to hdp.0 after non-zero observation selection step in hdp_merge_and_extract_components.

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,
  gamma0.alpha = gamma.alpha,
  gamma0.beta = gamma.beta
)
```

Arguments

```
input.catalog
```

Input spectra catalog as a matrix or in ICAMS format.

 ${\tt seedNumber} \qquad A \ random \ seeds \ passed \ to \ {\tt dp_activate}.$

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

as initcc.

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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"). If TRUE then message progress information. verbose gamma.alpha Shape parameter of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same. Inverse scale parameter (rate parameter) of the gamma distribution prior for the gamma.beta Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the same. gamma 0.alpha See figure B.1 from Nicola Robert's thesis. The shape parameter (α_0) of the

gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

gamma 0.beta See figure B.1 from Nicola Robert's thesis. Inverse scale parameter (rate parameter, β_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

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,
```

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```
gamma.beta = 1,
gamma0.alpha = gamma.alpha,
gamma0.beta = gamma.beta,
checkpoint.1.chain = TRUE,
burnin.multiplier = 1,
burnin.checkpoint = FALSE,
prior.sigs = NULL,
prior.pseudoc = NULL)
```

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 tumo of the corresponding column in input.gatalog

tumor type of the corresponding column in input.catalog.

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

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post.burnin Pass to hdp_posterior_sample burnin.

post.n Pass to hdp_posterior_sample n.

post.space Pass to hdp_posterior_sample space.

 $\verb"post.cpiter" Pass to \verb"hdp_posterior_sample cpiter".$

post.verbosity

Pass to hdp_posterior_sample verbosity.

gamma.alpha Shape parameter of the gamma distribution prior for the Dirichlet process con-

centration parameters; in this function the gamma distributions for all Dirichlet

processes, except possibly the top level process, are the same.

gamma .beta Inverse scale parameter (rate parameter) of the gamma distribution prior for the

Dirichlet process concentration parameters; in this function the gamma distributions for all Dirichlet processes, except possibly the top level process, are the

same.

gamma 0.alpha See figure B.1 from Nicola Robert's thesis. The shape parameter (α_0) of the

gamma distribution priors for the Dirichlet process concentration parameters

 (γ_0) for G_0 .

gamma0.beta See figure B.1 from Nicola Robert's thesis. Inverse scale parameter (rate param-

eter, β_0) of the gamma distribution priors for the Dirichlet process concentration

parameters (γ_0) for G_0 .

checkpoint.1.chain

If TRUE checkpoint the sample chain to current working directory, in a file called sample.chain.seed_number.Rdata.

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burnin.multiplier

A checkpoint setting. burnin.multiplier rounds of burnin iterations will be run. After each round, a burn-in chain will be save for checkpoint.

burnin.checkpoint

Default is False. If True, a checkpoint for burnin will be created.

 ${\tt prior.sigs} \quad \ \, A \ matrix \ containing \ prior \ signatures.$

prior.pseudoc

A numeric list. Pesudo counts of each prior signature. Recommended is 1000. In practice, it may be advisable to put lower weights on prior signatures that you do not expect to be present in your dataset, or even exclude some priors entirely.

Value

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

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