Package 'mSigHdp'

October 30, 2020
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AnalyzeAndPlotretval

Index		29
	test.spectra	28
	test.ground.truth.sig	27
	SetupAndPosterior	25
	SetupAndActivate	24
	RunHdpxParallel	20
	PriorSetupAndActivate	19
	PrepInit	18
	PlotSamplesHighSigExp	17
	OldRunHdpParallel	13
	MultipleSetupAndPosterior	11
	GeneratePriorppindex	10
	Generateppindex	10
	Generate Average Cluster	9
	ExtendBurnin	9

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

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

Arguments

retval the output from function CombinePosteriorChains or CombineChainsAndExtractSigs
input.catalog
input catalog and input catalog input catalog
out.dir Directory that will be created for the output; if overwrite is FALSE then abort if out.dir already exits.

ground.truth.sig
Ontional Fither a string with the path to file with ground truth signatures or and

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.

ChainBurnin 3

```
ground.truth.exp
```

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

sures. If ${\tt NULL}$ 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.

diagnostic.plot

If ${\tt TRUE}$ 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 = 5000,
  cpiter = 3,
  burnin.verbosity = 0,
  burnin.multiplier = 2,
  burnin.checkpoint = TRUE
)
```

Arguments

 $\verb| hdp.state-class| \textbf{Object or a list representation of an hdpState-class}|$

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. The number of burn-in iterations

cpiter Pass to hdp burnin cpiter. The number of iterations of concentration

parameter sampling to perform after each iteration.

burnin.verbosity

Pass to hdp_burnin verbosity. Verbosity of debugging statements.

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. A total number of 10,000 iterations is recommended for most analysis. However, number of iterations can be adjusted based on the size of dataset. According to our experience, 20,000 iterations are needed when analyzing all PCAWG7 genomes (2,780 samples). The burnin can be continued from a checkpoint file with ExtendBurnin.

burnin.checkpoint

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

4 CleanChlist

Value

A list with 2 elements:

hdplist A list representation of an hdpState-class object.

likelihood A numeric vector with the likelihood at each iteration.

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 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. Return from MultipleSetupAndPosterior. 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 = 0.1
)
```

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. HDP structure as one parent node for all tumors

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" HDP structure as a grandparent node for whole data and one parent node for each tumor type

6 CombinePosteriorChains

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 sam-

pling chains into "components" i.e. signatures; passed to extract_components_from_cluste

confident.prop

 $Pass\ to\ interpret_components.\ clusters\ with\ at\ least\ \texttt{confident.prop}$

of posterior samples are high confident signatures

noise.prop Pass to interpret_components. Clusters with less than noise.prop of

posterior samples are noise signatures

hc.cutoff Pass 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

CombinePosteriorChains 7

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

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.

ExtendBurnin 9

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. HDP structure as one parent node for all tumors

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "Ovary-AdenoCA::S.500" would be "Ovary-AdenoCA" HDP structure as a grandparent node for whole data and one parent node for each tumor type

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.

If not FALSE, HDP will give a parent node for each tumor type and a grandparent node for the whole dataset.

```
e.g. c("Ovary-AdenoCA", "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.

MultipleSetupAndPosterior

Activate hierarchical Dirichlet processes and run posterior sampling in parallel.

Description

nps

Activate hierarchical Dirichlet processes and run posterior sampling in parallel.

Number of prior signatures

Usage

```
MultipleSetupAndPosterior(
  input.catalog,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  burnin = 5000,
  burnin.multiplier = 2,
  burnin.checkpoint = TRUE,
  post.n = 200,
  post.space = 100,
  post.cpiter = 3,
  post.verbosity = 0,
  CPU.cores = 20,
  num.child.process = 20,
  gamma.alpha = 1,
  gamma.beta = 20,
  gamma0.alpha = gamma.alpha,
  gamma0.beta = gamma.beta,
  checkpoint.chlist = TRUE,
  checkpoint.1.chain = TRUE,
  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 clusters. Usually, the number of clusters is two times of the number of extracted signatures. Passed to dp_activate as initco.

multi.types

A logical scalar or a character vector. If FALSE, The HDP analysis will regard all input spectra as one tumor type. HDP structure as one parent node for all tumors

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "Ovary-AdenoCA::S.500" would be "Ovary-AdenoCA" HDP structure as a grandparent node for whole data and one parent node for each tumor type

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.

If not FALSE, HDP will give a parent node for each tumor type and a grandparent node for the whole dataset.

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

verbose

If TRUE then message progress information.

burnin Pass to hdp_burnin burnin. The number of burn-in iterations 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. A total number of 10,000 iterations is recommended for most analysis. However, number of iterations can be adjusted based on the size of dataset. According to our experience, 20,000 iterations are needed when analyzing all PCAWG7

genomes (2,780 samples). The burnin can be continued from a checkpoint file

with ExtendBurnin.

burnin.checkpoint

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

post.n Pass to hdp_posterior_sample n. The number of posterior samples to col-

lect

post.space Pass to hdp_posterior_sample space. The number of iterations be-

tween collected samples.

post.cpiter Pass to hdp_posterior_sample and hdp_burnin cpiter.The number

of iterations of concentration parameter sampling to perform after each iteration

post.verbosity

CPU.cores

Pass to hdp_posterior_sample verbosity. Verbosity of debugging

Number of CPUs to use; this should be no more than num.child.process.

statements. No need to change unless for development purpose

num.child.process

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

20 for real data analysis

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.

We recommend gamma.alpha = 1 and gamma.beta = 20 for single-base-substitution signatures extraction; gamma.alpha = 1 and gamma.beta = 50 for doublet-basesubstitution/INDEL signature extraction

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 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.

Value

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

OldRunHdpParallel

Deprecated, extract mutational signatures and optionally compare them to existing signatures and exposures.

Description

Deprecated, This functions uses the original method of combining raw clusters into "components". Use RunHdpxParallel instead.

Usage

```
OldRunHdpParallel(
  input.catalog,
  seedNumber = 1,
 K.quess,
 multi.types = FALSE,
  verbose = TRUE,
 post.burnin = 5000,
```

```
post.n = 200,
 post.space = 100,
 post.cpiter = 3,
 post.verbosity = 0,
 CPU.cores = 20,
 num.child.process = 20,
 cos.merge = 0.9,
 min.sample = 1,
 cateq.CI = 0.95,
 exposure.CI = 0.95,
 ground.truth.sig = NULL,
 ground.truth.exp = NULL,
 overwrite = TRUE,
 out.dir = NULL,
 gamma.alpha = 1,
 gamma.beta = 20,
 gamma0.alpha = gamma.alpha,
 gamma0.beta = gamma.beta,
 checkpoint.chlist = TRUE,
 checkpoint.1.chain = TRUE,
 prior.sigs = NULL,
 prior.pseudoc = NULL,
 burnin.multiplier = 2,
 burnin.checkpoint = TRUE
)
```

Arguments

input.catalog

Input spectra catalog as a matrix or in ICAMS format.

seedNumber

A random seeds passed to dp_activate.

K.quess

Suggested initial value of the number of clusters. Usually, the number of clusters is two times of the number of extracted signatures. Passed to dp_activate as initco.

multi.types

A logical scalar or a character vector. If FALSE, The HDP analysis will regard all input spectra as one tumor type. HDP structure as one parent node for all tumors

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "Ovary-AdenoCA::S.500" would be "Ovary-AdenoCA" HDP structure as a grandparent node for whole data and one parent node for each tumor type

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.

If not FALSE, HDP will give a parent node for each tumor type and a grandparent node for the whole dataset.

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

verbose

If TRUE then message progress information.

post.n

Pass to hdp_posterior_sample n. The number of posterior samples to collect.

post.space Pass to hdp posterior sample space. The number of iterations between collected samples. Pass to hdp_posterior_sample and hdp_burnin cpiter. The number post.cpiter of iterations of concentration parameter sampling to perform after each iteration post.verbosity Pass to hdp_posterior_sample verbosity. Verbosity of debugging statements. No need to change unless for development purpose Number of CPUs to use; this should be no more than num.child.process. CPU.cores num.child.process Number of posterior sampling chains; can set to 1 for testing. We recommend 20 for real data analysis The cosine similarity threshold for merging raw clusters from the posterior samcos.merge pling 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 min.sample hdp_merge_and_extract_components. cateq.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. A number in the range [0,1]. The level of the confidence interval used in step exposure.CI 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. If TRUE overwrite out .dir if it exists, otherwise raise an error. overwrite 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 congamma.alpha 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. We recommend gamma.alpha = 1 and gamma.beta = 20 for single-base-substitution signatures extraction; gamma.alpha = 1 and gamma.beta = 50 for doublet-basesubstitution/INDEL signature extraction 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. A total number of 10,000 iterations is recommended for most analysis. However, number of iterations can be adjusted based on the size of dataset. According to our experience, 20,000 iterations are needed when analyzing all PCAWG7 genomes (2,780 samples). The burnin can be continued from a checkpoint file with ExtendBurnin.

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 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.

```
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

```
An object return from extract_ccc_cdc_from_hdp
retval
hdpsample
                 A hdpSampleChain-class or hdpSampleMulti-class object includ-
                 ing output from extract_components_from_clusters
input.catalog
                 Input spectra catalog as a matrix or in ICAMS format.
                 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
```

18 PrepInit

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. HDP structure as one parent node for all tumors

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "Ovary-AdenoCA::S.500" would be "Ovary-AdenoCA" HDP structure as a grandparent node for whole data and one parent node for each tumor type

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.

If not FALSE, HDP will give a parent node for each tumor type and a grandparent node for the whole dataset.

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

input.catalog

K.guess

Input spectra catalog as a matrix or in ICAMS format.

verbose If TRUE then message progress information.

Suggested initial value of the number of clusters. Usually, the number of clusters is two times of the number of extracted signatures. Passed to dp_activate

as initcc.

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.

We recommend gamma.alpha = 1 and gamma.beta = 20 for single-base-substitution signatures extraction; gamma.alpha = 1 and gamma.beta = 50 for doublet-basesubstitution/INDEL signature extraction

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 .

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 .

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.quess,
  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.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.

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

Value

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

RunHdpxParallel

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

```
RunHdpxParallel(
  input.catalog,
  seedNumber = 123,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  burnin = 5000,
  burnin.multiplier = 2,
  burnin.checkpoint = FALSE,
```

```
post.n = 200,
 post.space = 100,
 post.cpiter = 3,
 post.verbosity = 0,
 CPU.cores = 20,
 num.child.process = 20,
 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 = 20,
 gamma0.alpha = gamma.alpha,
 gamma0.beta = gamma.beta,
 checkpoint.chlist = TRUE,
 checkpoint.1.chain = TRUE,
 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.quess

Suggested initial value of the number of clusters. Usually, the number of clusters is two times of the number of extracted signatures. Passed to dp_activate as initco.

multi.types

A logical scalar or a character vector. If FALSE, The HDP analysis will regard all input spectra as one tumor type. HDP structure as one parent node for all tumors

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "Ovary-AdenoCA::S.500" would be "Ovary-AdenoCA" HDP structure as a grandparent node for whole data and one parent node for each tumor type

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.

If not FALSE, HDP will give a parent node for each tumor type and a grandparent node for the whole dataset.

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

verbose

If TRUE then message progress information.

burnin

Pass to hdp burnin burnin. The number of burn-in iterations

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. A total number of 10,000 iterations is recommended for most analysis. However,

number of iterations can be adjusted based on the size of dataset. According to our experience, 20,000 iterations are needed when analyzing all PCAWG7 genomes (2,780 samples). The burnin can be continued from a checkpoint file with ExtendBurnin.

burnin.checkpoint

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

post.n Pass to hdp_posterior_sample n. The number of posterior samples to col-

lect.

post.space Pass to hdp_posterior_sample space. The number of iterations be-

tween collected samples.

of iterations of concentration parameter sampling to perform after each iteration

post.verbosity

Pass to hdp_posterior_sample verbosity. Verbosity of debugging

statements. No need to change unless for development purpose

CPU.cores Number of CPUs to use; this should be no more than num.child.process.

num.child.process

Number of posterior sampling chains; can set to 1 for testing. We recommend 20 for real data analysis

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

pling chains into "components" i.e. signatures; passed to extract_components_from_cluste

confident.prop

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

noise.prop Pass to interpret_components. Clusters with less than noise.prop of

posterior samples are noise signatures

hc.cutoff Pass to extract_components_from_clusters. The cutoff of height 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.

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

abort if out .dir already exits.

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.

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

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

same.

We recommend gamma.alpha = 1 and gamma.beta = 20 for single-base-substitution signatures extraction; gamma.alpha = 1 and gamma.beta = 50 for doublet-base-substitution/INDEL signature extraction

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.

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.

24 SetupAndActivate

SetupAndActivate General

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.

seedNumber

A random seeds passed to dp_activate.

K.guess

Suggested initial value of the number of clusters. Usually, the number of clusters is two times of the number of extracted 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. HDP structure as one parent node for all tumors

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "Ovary-AdenoCA::S.500" would be "Ovary-AdenoCA" HDP structure as a grandparent node for whole data and one parent node for each tumor type

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.

If not FALSE, HDP will give a parent node for each tumor type and a grandparent node for the whole dataset.

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

verbose

If TRUE then message progress information.

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.

SetupAndPosterior 25

gamma.beta Inverse scale parameter (rate parameter) of the gamma distribution prior for the Dirichlet process concentration parameters; in this function the gamma distri-

butions for all Dirichlet processes, except possibly the top level process, are the

same.

We recommend gamma.alpha = 1 and gamma.beta = 20 for single-base-substitution signatures extraction; gamma.alpha = 1 and gamma.beta = 50 for doublet-base-substitution/INDEL signature extraction

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 .

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.quess,
 multi.types = FALSE,
 verbose = TRUE,
 burnin = 5000,
 post.n = 50,
 post.space = 50,
 cpiter = 3,
 post.verbosity = 0,
 gamma.alpha = 1,
 gamma.beta = 20,
 gamma0.alpha = gamma.alpha,
 gamma0.beta = gamma.beta,
 checkpoint.1.chain = TRUE,
 burnin.multiplier = 2,
 burnin.checkpoint = TRUE,
 prior.sigs = NULL,
 prior.pseudoc = NULL
)
```

26 SetupAndPosterior

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 clusters. Usually, the number of clusters is two times of the number of extracted signatures. Passed to dp_activate as inited.

multi.types

A logical scalar or a character vector. If FALSE, The HDP analysis will regard all input spectra as one tumor type. HDP structure as one parent node for all tumors

If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "Ovary-AdenoCA::S.500" would be "Ovary-AdenoCA" HDP structure as a grandparent node for whole data and one parent node for each tumor type

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.

If not FALSE, HDP will give a parent node for each tumor type and a grandparent node for the whole dataset.

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

verbose

If TRUE then message progress information.

burnin

Pass to hdp_burnin burnin. The number of burn-in iterations

post.n

Pass to hdp_posterior_sample n. The number of posterior samples to col-

post.space

Pass to hdp_posterior_sample space. The number of iterations be-

tween collected samples.

cpiter

Pass to hdp_burnin cpiter. The number of iterations of concentration parameter sampling to perform after each iteration.

post.verbosity

Pass to hdp_posterior_sample verbosity. Verbosity of debugging statements. No need to change unless for development purpose

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.

We recommend gamma.alpha = 1 and gamma.beta = 20 for single-base-substitution signatures extraction; gamma.alpha = 1 and gamma.beta = 50 for doublet-basesubstitution/INDEL signature extraction

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 parameter, β_0) of the gamma distribution priors for the Dirichlet process concentration parameters (γ_0) for G_0 .

test.ground.truth.sig 27

```
checkpoint.1.chain
```

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

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. A total number of 10,000 iterations is recommended for most analysis. However, number of iterations can be adjusted based on the size of dataset. According to our experience, 20,000 iterations are needed when analyzing all PCAWG7 genomes (2,780 samples). The burnin can be continued from a checkpoint file with ExtendBurnin.

burnin.checkpoint

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

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.

post.cpiter

Pass to hdp_posterior_sample and hdp_burnin cpiter. The number of iterations of concentration parameter sampling to perform after each iteration

Value

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

```
test.ground.truth.sig \\ \textit{test.ground.truth.sig}
```

Description

Ground truth signature for testing.

Ground truth exposure for testing.

Usage

```
test.ground.truth.sig
test.ground.truth.exposure
```

Format

An ICAMS catalog (each column is a COSMICv3 signature, each row is a mutation type, e.g. ACT > AGT).

An exposure matrix (each row is a COSMICv3 signature used to generate test. spectra, each column is a sample).

28 test.spectra

test.spectra

test.spectra

Description

Synthetic SBS96 spectra for testing.

Usage

test.spectra

Format

An ICAMS catalog (each column is a sample, each row is a mutation type, e.g. ACT > AGT).

Index

```
* datasets
                                           PlotSamplesHighSigExp, 17
   test.ground.truth.sig, 27
                                           PrepInit, 18
                                           PriorSetupAndActivate, 19
   test.spectra, 28
                                           RunHdpxParallel, 13, 20
AnalyzeAndPlotretval, 2
                                           SetupAndActivate, 24
ChainBurnin, 3
                                           SetupAndPosterior, 25
chains, 4, 8, 16
ChainsDiagnosticPlot, 4
                                           test.ground.truth.exposure
CleanChlist, 4
                                                   (test.ground.truth.sig), 27
CombineChainsAndExtractSigs, 5, 8
                                           test.ground.truth.sig, 27
CombinePosteriorChains, 6
                                           test.spectra, 28
comp\_dp\_counts, 6, 23
ComponentDiagnosticPlotting, 8
dp_activate, 3, 12, 14, 18, 20, 21, 24-26
ExtendBurnin, 3, 9, 12, 16, 22, 27
extract_ccc_cdc_from_hdp, 17
extract_components_from_clusters,
       6, 17, 22
final_hdpState, 4, 8, 16
GenerateAverageCluster,9
Generateppindex, 10
GeneratePriorppindex, 10
hdp_burnin, 3, 9, 12, 15, 21, 22, 26, 27
hdp_extract_components, 7, 15
hdp_init, 18
hdp_merge_and_extract_components,
       7, 8, 15, 16
hdp_posterior, 9, 27
hdp_posterior_sample, 12, 14, 15, 22,
       26, 27
hdpState-class, 3, 9
ICAMS, 2, 5, 7, 8, 10-12, 14, 15, 17, 18,
       20-22, 24, 26-28
interpret_components, 6, 22, 23
MultipleSetupAndPosterior, 5, 11
OldRunHdpParallel, 13
```