# Package 'mSigHdp'

June 26, 2020

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## **Description**

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

# Usage

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

#### **Arguments**

input.catalog Input spectra catalog as a matrix or in ICAMS format. seedNumber An integer that is used to generate separate random seeds for the call to dp\_activate, and before the call of hdp\_burnin. Suggested initial value of the number of signatures, passed to dp\_activate as K.guess 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. burnin Pass to hdp\_burnin burnin. cpiter Pass to hdp\_burnin cpiter. burnin.verbosity Pass to hdp\_burnin verbosity.

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

Dirichlet processes are the same.

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

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

distributions for all Dirichlet processes are the same.

#### Value

A list with 2 elements:

hdplist A list representation of an hdpState-class object.

**likelihood** A numeric vector with the likelihood at each iteration.

AnalyzeAndPlotretval Evaluate and plot retval from CombinePosteriorChains

#### **Description**

Evaluate and plot retval from CombinePosteriorChains

#### Usage

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

#### **Arguments**

retval the output from function CombinePosteriorChains

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

if out.dir already exits.

ground.truth.sig

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

verbose If TRUE then message progress information.

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

diagnostic.plot

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

CleanChlist CleanChlist

ChainsDiagnosticPlot Diagnostic plot for a hdpSampleMulti object

# Description

Diagnostic plot for a hdpSampleMulti object

# Usage

ChainsDiagnosticPlot(retval, out.dir, verbose)

#### **Arguments**

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
out.dir	generated.  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 tryerror. 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.

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#### CombinePosteriorChains

Extract components and exposures from multiple posterior sample chains

#### **Description**

Extract components and exposures from multiple posterior sample chains

#### Usage

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

#### **Arguments**

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

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

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

all input spectra as one tumor type.

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

"SA.Syn.Ovary-AdenoCA"

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 hdp\_extract\_components.

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

hdp\_extract\_components.

#### Value

Invisibly, a list with the following elements:

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

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

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

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

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#### 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

Generate prindex 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.

 ${\tt MultipleSetupAndPosterior}$ 

Activate hierarchical Dirichlet processes and run posterior sampling in parallel.

#### **Description**

Activate hierarchical Dirichlet processes and run posterior sampling in parallel.

#### Usage

```
MultipleSetupAndPosterior(
  input.catalog,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  post.burnin = 4000,
  post.n = 50,
```

```
post.space = 50,
post.cpiter = 3,
post.verbosity = 0,
CPU.cores = 1,
num.child.process = 4,
gamma.alpha = 1,
gamma.beta = 1
```

#### **Arguments**

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

seedNumber A random seeds passed to dp\_activate.

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

initcc.

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").

 $\label{eq:continuous} \mbox{ If TRUE then message progress information.}$ 

post.burnin Pass to hdp\_posterior burnin.

post.n Pass to hdp\_posterior n.

post.space Pass to hdp\_posterior space.

post.cpiter Pass to hdp\_posterior cpiter.

post.verbosity Pass to hdp\_posterior verbosity.

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

num.child.process

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

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

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

Dirichlet processes are the same.

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

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

distributions for all Dirichlet processes are the same.

#### Value

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

ParallelPosteriorafterBurnin

ParallelPosteriorafterBurnin

Generate an HDP Gibbs sampling chain from a spectra catalog.

# Description

Generate an HDP Gibbs sampling chain from a spectra catalog.

# Usage

```
ParallelPosteriorafterBurnin(
  retval,
  seedNumber = 1,
  verbose = TRUE,
  post.burnin = 4000,
  post.n = 50,
  post.space = 50,
  post.cpiter = 3,
  post.verbosity = 0,
  num.child.process = 2,
  CPU.cores = 2
)
```

# Arguments

retval	$A\ list\ object\ containing\ hdplist\ after\ burn-in\ iteration\ and\ likelihood\ from\ Burnin\ Iteration.$			
seedNumber	Pass to hdp_posterior			
verbose	If TRUE then message progress information.			
post.burnin	Pass to hdp_posterior burnin. This can be set to a small number			
post.n	Pass to hdp_posterior n.			
post.space	Pass to hdp_posterior space.			
post.cpiter	Pass to hdp_posterior cpiter.			
post.verbosity	Pass to hdp_posterior verbosity.			
num.child.process				
	Number of posterior sampling chains; can set to 1 for testing.			
CPU.cores	Number of CPUs to use; there is no point in making this larger than num.child.process.			

#### Value

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

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PrepInit	Initialize hdp object Allocate process index for hdp initialization. Prepare for hdp_init

#### **Description**

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

#### Usage

```
PrepInit(
  multi.types,
  input.catalog,
  verbose,
  K.guess,
  gamma.alpha = 1,
  gamma.beta = 1
)
```

#### **Arguments**

multi.types

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

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

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

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

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

verbose If TRUE then message progress information.

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

initcc.

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

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

Dirichlet processes are the same.

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

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

distributions for all Dirichlet processes are the same.

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

# Description

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

# Usage

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

## **Arguments**

input.catalog	Input spectra catalog as a matrix or in ICAMS format.
seedNumber	A random seeds passed to dp_activate.
K.guess	Suggested initial value of the number of signatures, passed to dp_activate as initcc.
multi.types	A logical scalar or a character vector. If FALSE, The HDP analysis will regard all input spectra as one tumor type.
	If TRUE, the HDP analysis will infer tumor types based on the string before "::" in their names. e.g. tumor type for "SA.Syn.Ovary-AdenoCA::S.500" would be "SA.Syn.Ovary-AdenoCA"
	If multi.types is a character vector, then it should be of the same length as the number of columns in input.catalog, and each value is the name of the tumor type of the corresponding column in input.catalog.
	e.g. c("SA.Syn.Ovary-AdenoCA","SA.Syn.Kidney-RCC").
verbose	If TRUE then message progress information.

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Pass to hdp\_posterior burnin.

Pass to hdp\_posterior n. post.n Pass to hdp\_posterior space. post.space Pass to hdp\_posterior cpiter. post.cpiter post.verbosity Pass to hdp\_posterior verbosity. CPU.cores Number of CPUs to use; there is no point in making this larger than num.child.process. num.child.process Number of posterior sampling chains; can set to 1 for testing. 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. min.sample A "component" (i.e. signature) must have at least this many samples; passed to hdp\_extract\_components. ground.truth.sig Optional. Either a string with the path to file with ground truth signatures or and ICAMS catalog with the ground truth signatures. These are the signatures used to

ground.truth.exp

post.burnin

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

sures. If NULL skip checks that need this information.

overwrite If TRUE overwrite out.dir if it 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 gamma distribution from which the Dirichlet process con-

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

Dirichlet processes are the same.

construct the ground truth spectra.

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

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

distributions for all Dirichlet processes are the same.

#### Value

Invisibly, a list with the following elements:

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

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

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

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 ${\sf SetupAndActivate}$ 

Generate an HDP Gibbs sampling chain from a spectra catalog.

#### **Description**

Generate an HDP Gibbs sampling chain from a spectra catalog.

#### Usage

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

#### **Arguments**

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

seedNumber A random seeds passed to dp\_activate.

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

initcc.

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

all input spectra as one tumor type.

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

"SA.Syn.Ovary-AdenoCA"

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

type of the corresponding column in input.catalog.

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

verbose If TRUE then message progress information.

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

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

Dirichlet processes are the same.

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

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

distributions for all Dirichlet processes are the same.

# Value

Invisibly, an hdpState-class object as returned from dp\_activate.

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SetupAndPosterior

Generate an HDP Gibbs sampling chain from a spectra catalog.

#### **Description**

Generate an HDP Gibbs sampling chain from a spectra catalog.

#### **Usage**

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

#### **Arguments**

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

seedNumber A random seeds passed to dp\_activate.

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

initcc.

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

all input spectra as one tumor type.

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

"SA.Syn.Ovary-AdenoCA"

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

type of the corresponding column in input.catalog.

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

verbose If TRUE then message progress information.

post.burnin Pass to hdp\_posterior burnin.

post.n Pass to hdp\_posterior n.

post.space Pass to hdp\_posterior space.

post.cpiter Pass to hdp\_posterior cpiter.

post.verbosity Pass to hdp\_posterior verbosity.

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

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

Dirichlet processes are the same.

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gamma.beta

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

# Value

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

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