# Package 'hdpx'

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Title Hierarchical Dirichlet process for categorical count data, expanded

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biocViews

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**Description** Model categorical count data with hierarchical Dirichlet process (HDP) mixture models. If you want to do mutational signature discovery, you probably want to use package mSigHdp, which calls this package. This package is only supported on Linux systems. Includes functions to initialise an HDP model with a custom tree structure, perform Gibbs sampling of the posterior distribution, and analyse the output. The underlying mathematical theory is described by Teh et al. (Hierarchical Dirichlet Processes, Journal of the American Statistical Association, 2006, 101:476). This R package is based on code forked from Nicola Roberts, https://github.com/nicolaroberts/hdp. Roberts adapted the R code from open source MATLAB code and incorporated C code from Yee Whye Teh (MATLAB and C code available at http://www.stats.ox.ac.uk/~teh/research/npbayes/npbayes-r21.tgz). Subsequent changes by Rozen and Liu are mostly confined to the R code. These include (1) corrections to garbage collection in the interface to the C code and (2) a new function for computing unsigned Stirling numbers of the first kind (3) a complete re-working of the process by which "raw clusters" sampled in posterior chains are combined into ``components" (sets of mutations generated by one mutational process) (4) new functions for plotting to visualize and evaluate components extracted by the new procedures. There are also revised suggestions for burnin procedures and for setting hyperparameters for the concentration parameters; see https://github.com/steverozen/mSigHdp.

License file LICENSE

URL https://github.com/steverozen/hdpx

BugReports https://github.com/steverozen/hdpx/issues

```
Imports lsa,
      cluster,
      methods,
      coda,
      dendextend,
      Matrix,
      ggplot2,
      ICAMS,
      reshape2,
      stats,
      beeswarm,
      parallelDist
Suggests testthat,
      RColorBrewer,
      knitr,
      rmarkdown,
      BiocStyle,
      devtools
Collate 'aaa-classes-input.R'
      'aaa-classes-output.R'
      'aaa-generics-input.R'
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      'cull_posterior_samples.R'
      'diagnostic_in_extraction.R'
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      'extract_ccc_from_hdp.R'
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# LinkingTo Rcpp,RcppArmadillo

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4 comp\_categ\_distn

# Description

Get sample vs category counts for each component

### Usage

```
comp_categ_counts(x)
```

### **Arguments**

Х

hdpSampleChain or hdpSampleMulti

#### Value

List of matrices (one for each component) counting the sample-category data assignment across all DP nodes. Number of rows is the number of posterior samples, and number of columns is the number of data categories.

comp\_categ\_distn

Get mean distribution over data categories for each component

# Description

Get mean distribution over data categories for each component

### Usage

```
comp_categ_distn(x)
```

# **Arguments**

Х

hdpSampleChain or hdpSampleMulti

### Value

List with elements "mean" and "cred.int", containing matrices with the mean (and lower/upper 95% credibility interval) distribution over data categories for each component. Number of rows is the number of components, and number of columns is the number of data categories. Rows sum to 1.

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comp\_cos\_merge

Get cos.merge setting

# Description

Get cos.merge setting

# Usage

```
comp_cos_merge(x)
```

### **Arguments**

Х

 $hdpSampleChain\ or\ hdpSampleMulti$ 

#### Value

number of components

comp\_dp\_counts

Get sample vs component counts for each DP

# Description

Get sample vs component counts for each DP

# Usage

```
comp_dp_counts(x)
```

# Arguments

Х

 $hdpSampleChain\ or\ hdpSampleMulti$ 

### Value

List of matrices (one for each DP) counting sample-component assignment (aggregating across data categories). Number of rows is the number of posterior samples, and number of columns is the number of components.

comp\_dp\_distn

Get mean distribution over components for each DP

#### **Description**

Get mean distribution over components for each DP

### Usage

```
comp_dp_distn(x)
```

#### **Arguments**

Х

hdpSampleChain or hdpSampleMulti

#### Value

List with elements "mean" and "cred.int", containing matrices with the mean (and lower/upper 95% credibility interval) distribution over components for each DP. Number of rows is the number of DPs, and number of columns is the number of components. Rows sum to 1.

```
cull_posterior_samples
```

Cull early posterior samples from a hdpSampleChain object

# Description

Extend the 'burn-in' period and reduce the number of posterior samples taken from a sampling chain by culling the first ncull posterior samples. If components have been previously calculated for this sampling chain, they will be removed and must be recalculated.

### Usage

```
cull_posterior_samples(chain, ncull)
```

### **Arguments**

chain A hdpSampleChain object

ncull The number of posterior samples to cull

#### Value

A hdpSampleChain object with the designated 'burn-in' period extended, and the number of posterior samples reduced by ncull

### See Also

```
plot_lik, plot_numcluster, plot_data_assigned
```

```
default_merge_raw_cluster_args
```

Default arguments for combining "raw clusters" into "aggregated raw clusters".

### **Description**

Default arguments for combining "raw clusters" into "aggregated raw clusters".

### Usage

```
default_merge_raw_cluster_args()
```

#### Value

A list with the following elements:

```
* identical.cutoff
* nearly.identical.cutoff
* clustering.cutoff
* discard.singletons
```

```
diagnostic_in_extraction
```

Diagnostic plotting inside of hdp\_merge\_and\_extract\_components function. This function generates details of the raw clusters in hdp.0

# Description

Diagnostic plotting inside of hdp\_merge\_and\_extract\_components function. This function generates details of the raw clusters in hdp.0  $\,$ 

```
diagnostic_in_extraction(
  clust_hdp0_ccc,
  ncat,
  nsamp,
  nch,
  ccc,
  cdc,
  diagnostic.folder
)
```

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### **Arguments**

clust\_hdp0\_ccc

This function is deprecated.

ncat Number of categories.

nsamp Number of posterior samples.
nch Number of posterior chains.

 $\begin{array}{ccc} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$ 

diagnostic.folder

A directory where details for hdp.0 are plotted.

#### Value

The plots of presence of a raw cluster in each chain.

dp\_activate Activate DP nodes

### Description

Specify the number of starting clusters, and activate the DP nodes to be included in the posterior sampling process (hdp\_posterior). When initialised, the DP nodes are 'held out' (not available for posterior sampling).

## Usage

```
dp_activate(hdp, dpindex, initcc, seed = sample(1:10^7, 1))
```

# Arguments

hdp A hdpState object

dpindex Indices of the DPs to activate (include all parent DPs)

initcc Number of data clusters to start with (every data item is randomly assigned to a

cluster to start with)

seed The (integer) seed that can be set to reproduce output. Default is a random seed

from  $1 - 10^7$ , reported in the output.

#### **Details**

Note that this step can be slow and memory-intensive for very large datasets.

# Value

A hdpState object with activated DPs and an initial random cluster allocation for each data item. See hdpState-class

#### See Also

```
hdp_init, hdp_addconparam, hdp_adddp, hdp_setdata, hdp_posterior
```

dp\_freeze 9

#### **Examples**

```
my_hdp <- hdp_init(ppindex=0, cpindex=1, hh=rep(1, 6), alphaa=rep(1, 3), alphab=rep(2, 3)
my_hdp <- hdp_adddp(my_hdp, 2, 1, 2)
my_hdp <- hdp_adddp(my_hdp, 10, c(rep(2, 5), rep(3, 5)), 3)
my_hdp <- hdp_setdata(my_hdp, 4:13, example_data_hdp)
# active all DPs and start with two data clusters
my_hdp <- dp_activate(my_hdp, 1:13, 2)</pre>
```

dp freeze

Freeze DP nodes

#### **Description**

Freezes previously active DP nodes. A frozen DP node is not included in posterior sampling, but its statistics *are* considered in the sampling of other active DPs. This is useful for conditioning on a previous dataset. First, set up a HDP for one dataset, run the posterior sampling chain, and then freeze all old nodes (except the top DP). Add new DP nodes with new data and run a second posterior sampling chain over the new nodes (*given* the information in the frozen nodes).

### Usage

```
dp_freeze(hdp, dpindex)
```

# **Arguments**

hdp A hdpState object

dpindex Indices of the DPs to freeze

### Value

A hdpState object with the specified DP nodes frozen. See hdpState-class

#### See Also

hdp\_init, hdp\_addconparam, hdp\_adddp, hdp\_setdata, dp\_activate, hdp\_posterior

```
example_data_hdp Fake categorical count data
```

### **Description**

Fake categorical count data with 10 samples and 6 categories. Generated from two underlying categorical data distributions with a different average mixture ratio in the first five samples from the last five samples.

# Usage

```
example_data_hdp
```

#### **Format**

A numeric count matrix with 10 rows and 6 columns

```
example_data_hdp_prior
```

Fake categorical count data with priors

### **Description**

Fake categorical count data with 100 samples and 10 categories. Generated from four underlying categorical data distributions. Two of the underlying components are available as known prios in example\_known\_priors.

### Usage

```
example_data_hdp_prior
```

#### **Format**

A numeric count matrix with 100 rows and 10 columns

```
example_known_priors
```

Example known priors

### **Description**

Two example prior components for the example data example\_data\_hdp\_prior. 10 rows (one per data category) and 2 columns (one per prior component, each sums to 1).

#### **Usage**

```
example_known_priors
```

### **Format**

A numeric matrix with 10 rows and 2 columns.

```
extract_ccc_from_hdp
```

Find the ccc and cdc that matched to a spectrum in ccc\_0 and cdc\_0 this function is to summarize the credint and mean of cccs and cdcs and for further diagnostic plotting.

# Description

Find the ccc and cdc that matched to a spectrum in ccc\_0 and cdc\_0 this function is to summarize the credint and mean of cccs and cdcs and for further diagnostic plotting.

```
extract_ccc_from_hdp(signature, ccc_0, cos.merge = 0.9)
```

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#### **Arguments**

signature	A numerical vector representing the signature for which want to find information in $\ccolon 0$ .
ccc_0	"CCCs" from sample chains. A list of lists of numerical matrices. At the top level, one list for each Gibbs sample chain. Each element of a top-level list is a numerical matrix, with columns for raw clusters and rows being mutation types. The number of rows in these matrices should be the length of signature.
cos.merge	The minimum cosine similarity for declaring a match between signature and a column of one of the matrices in in ccc_0. This should probably be the same as the cuttoff for separating clusters of mutations after divisive clustering extract_components.

#### Value

Invisibly, a list with at least the elements

```
-ccc_mean
-ccc_credint
```

extract\_components Combine "raw clusters" of mutations in "components" (clusters of mutations generated by one mutational process).

# Description

Combine "raw clusters" of mutations in "components" (clusters of mutations generated by one mutational process).

# Usage

```
extract_components(
   sample.chains,
   merge.raw.cluster.args = default_merge_raw_cluster_args()
)
```

#### **Arguments**

### Value

A list with the elements

components Aggregated clusters as a data frame. Rows represent the categories (i.e. for mutational signature analysis, the mutation type, e.g. ACT -> AGT). Columns are aggregated clusters, i.e. clusters after all "raw clusters" across all Gibbs samples have been combined according to the divisive clustering. Each cell contains number of items (for mutational signature analysis, the number of mutations) of a particular category in a particular aggregated cluster.

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**components.post.samples** A data frame with two columns: one is the index of column in components and the other is the number of posterior samples that contributed to that aggregated cluster (column in components).

**components.cdc** A numerical matrix. Each row is a Dirichlet process (DP). This can either be a leaf DP, which for mutational signatures corresponds to a biological sample (for example, a tumor), or a parent or ancestor DP. Each column corresponds to the cluster in the corresponding column n components

each.chain.noise.clusters Deprecated.

each.chain.noise.cdc Deprecated.

multi.chains An hdpSampleChain-class or hdpSampleMulti-class object updated with component information.

**nsamp** The total number of posterior samples across all Gibbs sampling chains.

#### See Also

```
hdp_posterior,hdp_multi_chain,plot_comp_size,plot_comp_distn,plot_dp_comp_exposur
```

hdpBase-class

hdpBase class for the base distribution

### **Description**

hdpBase class for the base distribution

### Usage

```
## S4 method for signature 'hdpBase'
as.list(x, ...)
```

# Arguments

x Object of class hdpBase

... unused

### Methods (by generic)

• as.list(hdpBase): convert to list class

#### **Slots**

hh parameters for base Dirichlet distribution (pseudocounts)

classqq overall count matrix for data items of each category (rows) in each cluster (columns) numclass number of clusters

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hdpConparam-class hdpConparam class for the DP concentration parameter/s

### **Description**

hdpConparam class for the DP concentration parameter/s

# Usage

```
## S4 method for signature 'hdpConparam'
as.list(x, \dots)
```

#### **Arguments**

- Object of class hdpConparam Х unused . . .
- Methods (by generic)

• as.list(hdpConparam): convert to list class

### **Slots**

```
alphaa shape parameter for the gamma prior over alpha
alphab rate parameter for the gamma prior over alpha
numdp number of DP nodes sharing this concentration parameter
alpha concentration parameter value
totalnd number of data items in each DP with this concentration parameter
totalnt number of tables in each DP with this concentration parameter
```

hdpDP-class

hdpDP class for a DP node

# **Description**

note that the 'items' in parent nodes are the tables of their children

### Usage

```
## S4 method for signature 'hdpDP'
as.list(x, \dots)
## S4 method for signature 'hdpDP'
numdata(x, ...)
```

### **Arguments**

- Object of class hdpDP x
- unused . . .

### Methods (by generic)

- as.list(hdpDP): convert to list class
- numdata (hdpDP): Get number of data items at this DP.

#### **Slots**

```
datacc cluster index for each data item
classed number of items assigned to each cluster in this DP
classed number of tables assigned to each cluster in this DP
beta weight on each cluster in this DP (including empty cluster at end)
alpha concentration parameter for this DP
numdata number of data items registered to this DP node
datass value of each data item
```

hdpSampleChain-class

hdpSampleChain class for posterior samples off one MCMC chain

### **Description**

hdpSampleChain class for posterior samples off one MCMC chain

```
## S4 method for signature 'hdpSampleChain'
as.list(x, \dots)
## S4 method for signature 'hdpSampleChain'
sampling\_seed(x, ...)
## S4 method for signature 'hdpSampleChain'
hdp_settings(x, ...)
## S4 method for signature 'hdpSampleChain'
final_hdpState(x, ...)
## S4 method for signature 'hdpSampleChain'
lik(x, ...)
## S4 method for signature 'hdpSampleChain'
numcluster(x, ...)
## S4 method for signature 'hdpSampleChain'
cp_values(x, ...)
## S4 method for signature 'hdpSampleChain'
clust_categ_counts(x, ...)
```

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```
## S4 method for signature 'hdpSampleChain'
clust_dp_counts(x, ...)

## S4 method for signature 'hdpSampleChain'
numcomp(x)

## S4 method for signature 'hdpSampleChain'
prop.ex(x)

## S4 method for signature 'hdpSampleChain'
comp_cos_merge(x)

## S4 method for signature 'hdpSampleChain'
comp_categ_counts(x)

## S4 method for signature 'hdpSampleChain'
comp_dp_counts(x)

## S4 method for signature 'hdpSampleChain'
comp_categ_distn(x)

## S4 method for signature 'hdpSampleChain'
comp_categ_distn(x)
```

#### **Arguments**

. . .

x Object of class hdpSampleChain

unused

# Methods (by generic)

- as.list(hdpSampleChain): Convert to list class
- sampling\_seed(hdpSampleChain): Get random seed used by hdp\_posterior
- hdp\_settings (hdpSampleChain): Get settings of posterior sampling chain
- final\_hdpState (hdpSampleChain): Get hdpState object from the end of the posterior sampling chain
- lik (hdpSampleChain): Get likelihood of data given model over all iterations
- numcluster (hdpSampleChain): Get the number of clusters for each posterior sample
- cp\_values (hdpSampleChain): Get matrix of concentration parameter values for each posterior sample
- clust\_categ\_counts (hdpSampleChain): Get category vs cluster counts for each posterior sample
- clust\_dp\_counts (hdpSampleChain): Get dp node vs cluster counts for each posterior sample
- numcomp (hdpSampleChain): Get number of extracted components for hdpSampleChain
- prop.ex (hdpSampleChain): Get proportion of dataset explained (on average) for hdp-SampleChain
- comp\_cos\_merge (hdpSampleChain): Get cos.merge setting for hdpSampleChain

• comp\_categ\_counts (hdpSampleChain): Get sample vs category counts for each component

- comp\_dp\_counts (hdpSampleChain): Get sample vs component counts for each DP
- comp\_categ\_distn(hdpSampleChain): Get mean distribution over data categories for each component
- comp\_dp\_distn (hdpSampleChain): Get mean distribution over components for each DP

#### **Slots**

seed Random seed used by hdp\_posterior

settings Settings of the posterior sampling chain: burnin, n (number of samples collected), space (iters between samples), cpiter (con param moves between iters)

hdp hdpState object after the final iteration

lik Likelihood of data given model at each iteration

numcluster Number of raw data clusters in each posterior sample

- cp\_values Matrix of concentration parameter values (one column for each parameter) in each posterior sample (rows).
- clust\_categ\_counts List of matrices (one from each posterior sample) counting the categorycluster data assignment across all DP nodes. Number of rows is the number of categories (constant), and number of columns is the number of clusters in that posterior sample (variable).
- clust\_dp\_counts List of matrices (one from each posterior sample) counting within-DP cluster assignment (aggregating across data categories). Number of rows is the number of DPs (constant), and number of columns is the number of clusters in that posterior sample (variable).

numcomp Number of global components

prop.ex (Average) proportion of dataset explained by the extracted components

- comp\_cos\_merge cos.merge setting used by hdp\_extract\_components; deprecated
- comp\_categ\_counts List of matrices (one for each component) counting the sample-category data assignment across all DP nodes. Number of rows is the number of posterior samples, and number of columns is the number of data categories.
- comp\_dp\_counts List of matrices (one for each DP) counting sample-component assignment (aggregating across data categories). Number of rows is the number of posterior samples, and number of columns is the number of components.
- comp\_categ\_distn List with elements mean and cred.int, containing matrices with the mean (and lower/upper 95% credibility interval) distribution over data categories for each component. Number of rows is the number of components, and number of columns is the number of data categories. Rows sum to 1.
- comp\_dp\_distn List with elements "mean" and "cred.int", containing matrices with the mean (and lower/upper 95% credibility interval) distribution over components for each DP. Number of rows is the number of DPs, and number of columns is the number of components. Rows sum to 1.

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```
hdpSampleMulti-class
```

hdpSampleMulti class for multiple independent hdpSampleChain objects for the same HDP

### **Description**

hdpSampleMulti class for multiple independent hdpSampleChain objects for the same HDP

#### Usage

```
## S4 method for signature 'hdpSampleMulti'
as.list(x, \dots)
## S4 method for signature 'hdpSampleMulti'
chains(x, ...)
## S4 method for signature 'hdpSampleMulti'
numcomp(x)
## S4 method for signature 'hdpSampleMulti'
prop.ex(x)
## S4 method for signature 'hdpSampleMulti'
comp_cos_merge(x)
## S4 method for signature 'hdpSampleMulti'
comp_categ_counts(x)
## S4 method for signature 'hdpSampleMulti'
comp_dp_counts(x)
## S4 method for signature 'hdpSampleMulti'
comp_categ_distn(x)
## S4 method for signature 'hdpSampleMulti'
comp_dp_distn(x)
```

#### **Arguments**

```
X Object of class hdpSampleMulti... unused
```

#### **Methods (by generic)**

- as.list(hdpSampleMulti): Convert to list class
- chains (hdpSampleMulti): Get list of hdpSampleChain objects
- numcomp (hdpSampleMulti): Get number of extracted components for hdpSampleMulti
- prop.ex(hdpSampleMulti): Get proportion of dataset explained (on average) for hdp-SampleMulti

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- comp\_cos\_merge (hdpSampleMulti): Get cos.merge setting for hdpSampleMulti
- comp\_categ\_counts (hdpSampleMulti): Get sample vs category counts for each component
- comp\_dp\_counts (hdpSampleMulti): Get sample vs component counts for each DP
- comp\_categ\_distn(hdpSampleMulti): Get mean distribution over data categories for each component
- comp\_dp\_distn (hdpSampleMulti): Get mean distribution over components for each DP

#### **Slots**

- chains List of hdpSampleChain objects storing multiple independent runs of the posterior sampling chain for the same data and HDP struct
- numcomp Number of global components extracted by hdp\_extract\_components (not including component 0)
- prop.ex (Average) proportion of dataset explained by the extracted components
- comp\_cos\_merge cos.merge setting used by hdp\_extract\_components
- comp\_categ\_counts List of matrices (one for each component) counting the sample-category data assignment across all DP nodes. Number of rows is the number of posterior samples, and number of columns is the number of data categories.
- comp\_dp\_counts List of matrices (one for each DP) counting sample-component assignment (aggregating across data categories). Number of rows is the number of posterior samples, and number of columns is the number of components.
- comp\_categ\_distn List with elements "mean" and "cred.int", containing matrices with the mean (and lower/upper 95% credibility interval) distribution over data categories for each component. Number of rows is the number of components, and number of columns is the number of data categories. Rows sum to 1.
- comp\_dp\_distn List with elements "mean" and "cred.int", containing matrices with the mean (and lower/upper 95% credibility interval) distribution over components for each DP. Number of rows is the number of DPs, and number of columns is the number of components. Rows sum to 1.

hdpState-class

hdpState class for a Hierarchical Dirichlet Process in one state

# Description

hdpState class for a Hierarchical Dirichlet Process in one state

```
## S4 method for signature 'hdpState'
as.list(x, ...)
## S4 method for signature 'hdpState'
numdp(x, ...)
## S4 method for signature 'hdpState'
```

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```
numconparam(x, ...)
## S4 method for signature 'hdpState'
base(x, ...)
## S4 method for signature 'hdpState'
conparam(x, ...)
## S4 method for signature 'hdpState'
dp(x, ...)
## S4 method for signature 'hdpState'
dpstate(x, ...)
## S4 method for signature 'hdpState'
ppindex(x, ...)
## S4 method for signature 'hdpState'
cpindex(x, ...)
## S4 method for signature 'hdpState'
numcateg(x, ...)
## S4 method for signature 'hdpState'
base_params(x, ...)
## S4 method for signature 'hdpState'
activating_seed(x, ...)
## S4 method for signature 'hdpState'
pseudoDP(x, ...)
```

#### **Arguments**

x Object of class hdpState

... unused

# Methods (by generic)

- as.list(hdpState): Convert to list class
- numdp (hdpState): Get number of DPs
- numconparam (hdpState): Get number of concentration parameters
- base (hdpState): Get base distribution
- conparam (hdpState): Get list of concentration parameters
- dp (hdpState): Get list of DP nodes
- dpstate(hdpState): Get state of every DP
- ppindex (hdpState): Get parent process index of every DP
- cpindex (hdpState): Get concentration parameter index of every DP
- numcateg (hdpState): Get number of data categories

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• base\_params (hdpState): Get parameters of the base Dirichlet distribution (like psue-docounts across categories).

- activating\_seed (hdpState): Get seed used to initialse clustering
- pseudoDP (hdpState): Get index of frozen pseudo-data DP nodes for prior info (only if initialised via hdp\_prior\_init)

#### **Slots**

```
numdp number of DP nodes in the hierarchical Dirichlet Process

numconparam number of concentration parameters

base base distribution (hdpBase object)

conparam concentration parameters (list of hdpConparam objects)

dp DP nodes (list of hdpDP objects)

dpstate state of DP nodes for posterior sampling process: active (2), frozen (1), or heldout (0)

ppindex parent node index for each DP

cpindex concentration parameter index for each DP

ttindex DP index of those sharing a concentration parameter

initce number of initial clusters

seed_activate random seed used to initiate cluster membership

pseudoDP (Optional) index of pseudodata nodes (only if initialised via hdp_prior_init)
```

hdp\_addconparam

Add concentration parameters to a hdpState object

#### Description

Add concentration parameters to a hdpState object by specifying the shape and rate parameters of the gamma prior/s. DPs using these new concentration parameters can be added with hdp\_adddp. Data is assigned via hdp\_setdata. When initialised, the DP nodes are 'heldout' (not available for posterior sampling) and will need to be activated (see dp\_activate). Finally, the posterior sampling process (a Gibbs sampler) is run via hdp\_posterior.

### Usage

```
hdp_addconparam(hdp, alphaa, alphab)
```

# Arguments

hdp	A hdpState object
alphaa	Shape hyperparameters for the gamma priors over the DP concentration parameters.
alphab	Rate hyperparameters for the gamma priors over the DP concentration parameters

#### Value

A hdpState object updated with the new concentration parameters. See hdpState-class

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#### See Also

```
hdp_init, hdp_adddp, hdp_setdata, dp_activate, hdp_posterior
```

### **Examples**

```
hdp_example <- hdp_init(c(0, 1, 1), c(1, 2, 2), rep(1, 6), rep(2, 2), rep(0.5, 2)) hdp_example <- hdp_addconparam(hdp_example, rep(1, 2), rep(1, 2))
```

hdp\_adddp

Add DPs to a hdpState object

### **Description**

Add DP nodes to a hdpState object and specify each parent relationship and concentration parameter. Concentration parameters can be added to a hdpState object with hdp\_addconparam. Data is assigned via hdp\_setdata. When initialised, the DP nodes are 'heldout' (not available for posterior sampling) and will need to be activated (see dp\_activate). Finally, the posterior sampling process (a Gibbs sampler) is run via hdp\_posterior.

### Usage

```
hdp_adddp(hdp, numdp, ppindex, cpindex)
```

#### **Arguments**

hdp A hdpState object

numdp The number of DPs to add

ppindex Index (or indices) of the parental process(es) for the new DPs.

cpindex Index (or indices) of the concentration parameters for the new DPs.

#### Value

A hdpState object with the updated HDP structure. See hdpState-class

#### See Also

```
hdp_init, hdp_setdata, dp_activate, hdp_posterior
```

### **Examples**

hdp\_example

```
my_hdp <- hdp_init(ppindex=0, cpindex=1, hh=rep(1, 6), alphaa=rep(1, 3), alphab=rep(2, 3)
# add two more DPs with parent '1' and concentration parameter '2'
my_hdp <- hdp_adddp(my_hdp, 2, 1, 2)
my_hdp
hdp_example <- hdp_init(c(0, 1, 1), c(1, 2, 2), rep(1, 6), rep(2, 2), rep(0.5, 2))
# add six more DPs, three with parent '2', three with parent '3',
# and all with concentration parameter '2'
hdp_example <- hdp_adddp(hdp_example, 6, c(2, 2, 2, 3, 3, 3), 2)</pre>
```

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hdp_burnin	Burnin of posterior sampling chain across activated DPs.	
	of Feeders and Feeders	

#### **Description**

Run a Gibbs sampler over the activated nodes of a hierarchical Dirichlet process. Each iteration re-assigns the cluster allocation of every data item.

### Usage

```
hdp_burnin(hdp, burnin, cpiter = 1, verbosity = 0)
```

### **Arguments**

hdp	An hdpState-class object or a list representation of this. The list representation contains elements that correspond to slots in anhdpState-class
	object.
burnin	The number of burn-in iterations.
cpiter	The number of iterations of concentration parameter sampling to perform after each iteration.
verbosity	Verbosity of debugging statements. 0 (least verbose) – 4 (most verbose). 0

highly recommended - only change for debugging small examples.

### Value

A list with the elements:

 $\textbf{hdplist} \ \ A \ list \ representation \ of \ an \ \texttt{hdpState-class} \ object.$ 

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

hdp_init	Initialise a hdpState object	

### **Description**

Initialise a hdpState object with one or more DP nodes and their parent relationships, the parameters of the base Dirichlet distribution, and a set of hyperparameters for the gamma priors over the DP concentration parameters. Further DP nodes can be added with hdp\_adddp, and further concentration parameters can be added with hdp\_addconparam. Data is assigned via hdp\_setdata. When initialised, the DP nodes are 'heldout' (not available for posterior sampling) and will need to be activated (see dp\_activate). Finally, the posterior sampling process (a Gibbs sampler) is run via hdp\_posterior.

```
hdp_init(ppindex, cpindex, hh, alphaa, alphab)
```

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#### **Arguments**

ppind	dex	Index (or indices) of the parental process(es) for the initial DPs. The 'top' DP should have parent process '0' (the base Dirichlet distribution).
cpin	dex	Index (or indices) of the concentration parameter(s) for the initial DPs.
hh		Parameters of the base Dirichlet distribution (like psuedocounts across categories). Must be a vector with length equal to the number of data item categories.
alpha	aa	Shape hyperparameters for the gamma priors over the DP concentration parameters.
alpha	ab	Rate hyperparameters for the gamma priors over the DP concentration parameters.

#### Value

A hdpState object with the initial HDP structure. See hdpState-class

#### See Also

```
hdp_quick_init,hdp_prior_init,hdp_addconparam,hdp_adddp,hdp_setdata,dp_activate,hdp_posterior
```

#### **Examples**

```
# initialise a HDP with just one 'top' DP node off the base distribution,
# a uniform Dirichlet base distribution over six possible data categories,
# and three possible concentration parameters to be shared across the HDP tree
# (top DP using conparam number 1), each with hyperparameters (1,2).
hdp_init(ppindex=0, cpindex=1, hh=rep(1, 6), alphaa=rep(1, 3), alphab=rep(2, 3))
# initialise a HDP with one 'top' DP node off the base distribution,
# AND two children DP nodes off that parent. The two children DPs share a different
# concentration parameter (hyperparameters are (2, 0.5)).
hdp_init(ppindex=c(0, 1, 1), cpindex=c(1, 2, 2), hh=rep(1, 6), alphaa=rep(2, 2), alphab=rep(2, 2), alp
```

hdp\_multi\_chain Gather multiple independent posterior sampling chains for the same HDP

#### **Description**

Gather multiple independent posterior sampling chains for the same HDP

# Usage

```
hdp_multi_chain(chain_list)
```

### **Arguments**

chain\_list A list of hdpSampleChain objects for the same data and HDP structure, but run with different random seeds.

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#### Value

A hdpSampleMulti object

#### See Also

```
hdp_posterior
```

hdp\_posterior

Posterior sampling chain across activated DPs.

### **Description**

Run a Gibbs sampler over the activated DP nodes of a Hierarchichal Dirichlet Process. Each iteration re-assigns the cluster allocation of every data item. Run burnin iterations, and then collect n samples from the chain with space iterations between each collected sample. To plot output, see plot\_lik, plot\_numcluster, and plot\_data\_assigned. Can collect multiple independent HDP sampling chains in a hdpSampleMulti object via hdp\_multi\_chain.

# Usage

```
hdp_posterior(
  hdp,
  burnin,
  n,
  space,
  cpiter = 1,
  seed = sample(1:10^7, 1),
  verbosity = 0
)
```

# Arguments

hdp	A hdpState object
burnin	The number of burn-in iterations.
n	The number of posterior samples to collect.
space	The number of iterations between collected samples.
cpiter	The number of iterations of concentration parameter sampling to perform after each iteration.
seed	The (integer) seed that can be set to reproduce output. Default is a random seed from $1-10^{7}$ , reported in the output.
verbosity	Verbosity of debugging statements. $0$ (least verbose) $-4$ (most verbose). $0$ highly recommended - only change for debugging small examples.

### Value

A hdpSampleChain object with the salient information from each posterior sample. See hdpSampleChain-class

#### See Also

```
hdp_multi_chain,cull_posterior_samples,plot_lik,plot_numcluster,plot_data_assigne
```

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#### **Examples**

```
my_hdp <- hdp_init(ppindex=0, cpindex=1, hh=rep(1, 6), alphaa=rep(1, 3), alphab=rep(2, 3)
my_hdp <- hdp_adddp(my_hdp, 2, 1, 2)
my_hdp <- hdp_adddp(my_hdp, 10, c(rep(2, 5), rep(3, 5)), 3)
my_hdp <- hdp_setdata(my_hdp, 4:13, example_data_hdp)
my_hdp <- dp_activate(my_hdp, 1:13, 2)
my_hdp_chain <- hdp_posterior(my_hdp, 100, 100, 10)</pre>
```

hdp\_posterior\_sample

Posterior sampling chain across activated DPs.

#### **Description**

Run a Gibbs sampler over the burnin chains from hdp\_burnin. Each iteration re-assigns the cluster allocation of every data item. Run burnin iterations, and then collect n samples from the chain with space iterations between each collected sample. To plot output, see plot\_lik, plot\_numcluster, and plot\_data\_assigned. Can collect multiple independent HDP sampling chains in a hdpSampleMulti object via hdp\_multi\_chain.

### Usage

```
hdp_posterior_sample(
  post.input,
  post.n,
  post.space,
  post.cpiter = 1,
  seed = sample(1:10^7, 1),
  post.verbosity = 0,
  checkpoint = F
)
```

### **Arguments**

```
An S4 object from hdp_burnin.
post.input
post.n
                  The number of posterior samples to collect.
                  The number of iterations between collected samples.
post.space
post.cpiter
                  The number of iterations of concentration parameter sampling to perform after
                  each iteration.
                  The (integer) seed that can be set to reproduce output. Default is a random seed
seed
                  from 1 - 10^7, reported in the output.
post.verbosity
                  Verbosity of debugging statements. 0 (least verbose) – 4 (most verbose). 0
                  highly recommended - only change for debugging small examples.
checkpoint
                  If TRUE, a checkpoint will be saved for every 10 posterior samples
```

### Value

A hdpSampleChain object with the salient information from each posterior sample. See hdpSampleChain-class

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#### See Also

hdp\_multi\_chain, cull\_posterior\_samples, plot\_lik, plot\_numcluster, plot\_data\_assigne

hdp\_prior\_init

*Initialise a HDP structure incorporating prior knowledge* 

### **Description**

Initialise a hdpState object incorporating prior knowlegde of some components (categorical data distributions). The structure has one top parent DP node with no associated data ('active' and available for posterior sampling), and one child DP node per prior component ('frozen' and held out from posterior sampling).

#### Usage

```
hdp_prior_init(prior_distn, prior_pseudoc, hh, alphaa, alphab)
```

### **Arguments**

prior_distn	Matrix of prior distributions (columns must each sum to 1, number of rows matches number of data categories)
prior_pseudo	С
	Vector of pseudocounts contributed by each prior distribution
hh	Parameters of the base Dirichlet distribution. Must be a vector with length equal to the number of data item categories.
alphaa	Shape hyperparameters for the gamma priors over the DP concentration parameters.
alphab	Rate hyperparameters for the gamma priors over the DP concentration parameters.

#### Value

A hdpState object with one frozen node per prior component. See hdpState-class

### See Also

```
hdp_init
```

# Examples

hdp\_quick\_init 27

hdp_quick_init	Initialise a simple, default HDP structure
----------------	--

### **Description**

Initialise a hdpState object with a basic default structure of one top parent DP node with no associated data, and one child DP node per row of data. Every DP node shares the same concentration parameter, and will automatically be 'activated' (made available for posterior samplig). The base distribution is a uniform Dirichlet with psuedocount 1 in each data category. Can immediately run hdp\_posterior to collect posterior samples. To define a custom HDP structure, see hdp\_init and hdp\_prior\_init.

### Usage

```
hdp_quick_init(data, initcc = 2, alphaa = 1, alphab = 1)
```

### **Arguments**

data	$\boldsymbol{A}$ data.frame or matrix of counts with one row for every sample and one column for every data category.
initcc	Number of initial data clusters (every data item is randomly assigned to a cluster to start with).
alphaa	Shape hyperparameter for the gamma prior over the concentration parameter.
alphab	Rate hyperparameter for the gamma prior over the concentration parameter.

#### Value

A hdpState object with a basic default structure. See hdpState-class

### See Also

```
hdp_init,hdp_posterior,hdp_prior_init
```

### **Examples**

```
my_quick_hdp <- hdp_quick_init(example_data_hdp)
my_quick_hdp_chain <- hdp_posterior(my_quick_hdp, 100, 50, 10, 5)</pre>
```

hdp\_setdata

Assign data to DP nodes in a hdpState object

### **Description**

Assign data to 'heldout' (state is 0) DP nodes in a hdpState object. 'Heldout' DPs are not available for posterior sampling, and will need to be activated (see dp\_activate). The posterior sampling process (a Gibbs sampler) is run via hdp\_posterior.

```
hdp_setdata(hdp, dpindex, data)
```

### **Arguments**

hdp A hdpState object

dpindex Indices of the DPs to assign data to (in same order as rows of data)

data A data.frame or matrix of counts with one row for every sample (same

order as dpindex) and one column for every data category.

#### Value

A hdpState object updated with the new data. See hdpState-class

#### See Also

```
hdp_init, hdp_adddp, dp_activate, hdp_posterior
```

### **Examples**

```
example_data_hdp
my_hdp <- hdp_init(ppindex=0, cpindex=1, hh=rep(1, 6), alphaa=rep(1, 3), alphab=rep(2, 3)
my_hdp <- hdp_adddp(my_hdp, 2, 1, 2)
my_hdp <- hdp_adddp(my_hdp, 10, c(rep(2, 5), rep(3, 5)), 3)
my_hdp <- hdp_setdata(my_hdp, 4:13, example_data_hdp)
dp(my_hdp)</pre>
```

interpret\_components

Separate high and low confidence components (aggregated clusters) and exposures

# Description

Separate high and low confidence components (aggregated clusters) and exposures

#### Usage

```
interpret_components(
  multi.chains.retval,
  high.confidence.prop = 0.9,
  verbose = FALSE
)
```

# Arguments

```
multi.chains.retval
```

A list that contains all the elements returned by extract\_components.

high.confidence.prop

Components found in >= high.confidence.prop proportion of posterior samples are high confidence components.

verbose if TRUE, generate progress messages.

numcomp 29

#### Value

In the information that follows, a "component" is the union of multiple raw clusters of mutations (in the case of mutational signature analysis). Invisibly, a list with the following elements:

high\_confidence\_components A data frame containing the components found in >= high.confidence.prop of posterior samples. Each column is a component; in the case of mutational signatures the rows are mutation types.

- **high\_confidence\_components\_post\_number** A data frame in which the first column contains the index of a column in high\_confidence\_components and the second column contains the number of posterior samples that contributed to that component.
- high\_confidence\_components\_cdc A matrix in which each row corresponds to one of the Dirichlet processes, and each column corresponds to one component in high\_confidence\_components. In the case of mutational signature analysis, most of the columns correspond to an input biological sample (e.g. individual tumor).
- low\_confidence\_components Analogous to high\_confidence\_compents except for components with constituent raw clusters found in < high.confidence.prop posterior samples.

low\_confidence\_components\_post\_number Analogous to high\_confidence\_components\_post\_number.
low\_confidence\_components\_cdc Analogous to high\_confidence\_components\_cdc.

numcomp

Get number of extracted components

# Description

Get number of extracted components

# Usage

numcomp(x)

# **Arguments**

х

hdpSampleChain or hdpSampleMulti

### Value

number of components

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plotchain

Diagnostic plots for HDP posterior sampling chain

### **Description**

Diagnostic plots for HDP posterior sampling chain

### Usage

```
plot_lik(
  chain,
  start = 1,
  end = length(lik(chain)),
  col_lik = "blue",
  col_burn = "red",
  xlab = "Iteration",
  ylab = "Likelihood",
)
plot_numcluster(
  chain,
  col = "blue",
xlab = "Sample",
  ylab = "Number of raw clusters",
  . . .
)
plot_data_assigned(
  chain,
  legend = TRUE,
  col_early = "hotpink",
  col_late = "skyblue3",
  dat\_prop = 0.995,
  xlab = "Number of raw clusters",
  ylab = "Cumulative prop. of data assigned",
)
```

# Arguments

chain	A hdpSampleChain object
start	The starting iteration to plot from (default 1)
end	The final iteration to plot to (default is end of chain)
col_lik	Plot colour of likelihood (default blue)
col_burn	Plot colour of burnin (default red)
xlab	Horizontal axis label
ylab	Vertical axis label
	Other arguments to plot

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col	Plot colour for numcluster (default blue)
legend	Logical - should a legend be included? (default TRUE)
col_early	Color ramp side for early posterior samples
col_late	Color ramp side for late posterior samples
dat_prop	Extend horiztonal axis to dat_prop proportion of data assigned

plotcomp

Plot extracted components

# **Description**

Plot extracted components

Plot hdp signature exposure in each sample

```
plot_comp_size(
 hdpsample,
  legend = TRUE,
 col_a = "hotpink",
 col_b = "skyblue3",
  xlab = "Component",
 ylab = "Number of data items",
  . . .
)
plot_comp_distn(
 hdpsample,
  comp = NULL,
  cat_names = NULL,
  grouping = NULL,
  col = "grey70",
  col_nonsig = NULL,
  show_group_labels = FALSE,
  cred_int = TRUE,
  weights = NULL,
  plot_title = NULL,
  group_label_height = 1.05,
  cex.cat = 0.7,
)
plot_dp_comp_exposure(
 hdpsample,
  input.catalog,
  ex.signature,
  col_comp,
  dpnames = NULL,
  main_text = NULL,
```

32 plotcomp

```
incl_numdata_plot = TRUE,
incl_nonsig = TRUE,
incl_comp0 = 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

hdpsample	A hdpSampleChain or hdpSampleMulti.	
legend	Logical - should a legend be included? (default TRUE)	
col_a	$Color\ ramp\ side\ for\ early\ posterior\ samples\ (if\ hdpSampleChain)\ or\ first\ chain\ (if\ hdpSampleMulti)$	
col_b	$Color\ ramp\ side\ for\ late\ posterior\ samples\ (if\ hdpSampleChain)\ or\ last\ chain\ (if\ hdpSampleMulti)$	
xlab	Horizontal axis label	
ylab	Vertical axis label	
	Other arguments to plot	
comp	$(Optional)\ Number(s)\ of\ the\ component(s)\ to\ plot\ (from\ 0\ to\ the\ max\ component\ number).$ The default is to plot all components.	
cat_names	(Optional) Data category names to label the horizontal axis	
grouping	(Optional) A factor indicating data category groups.	
col	Either a single colour for all data categories, or a vector of colours for each group (in the same order as the levels of the grouping factor)	
col_nonsig	(Optional) Colour for any data category whose $95\%$ credibility interval overlaps with zero (if set, overrides col argument)	
show_group_la	abels	
	Logical - should group labels be added to the top horizontal axis? (default FALSE) (only works if categories alreayd come in orders)	
cred_int	Logical - should 95% credibility intervals be plotted? (default TRUE)	
weights	(Optional) Weights over the data categories to adjust their relative contribution (multiplicative)	
plot_title	(Optional) Character vector of custom plot titles (one for each component plotted)	
group_label_height		
	Multiplicative factor from top of plot for group label placement	
cex.cat	Expansion factor for the (optional) cat_names	
input.catalog		
	input catalog for samples	
ex.signature	extracted signature from hdp	
col_comp	Colours of each component, from 0 to the max number	

plot\_chain\_hdpsig\_exp

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dpnames (Optional) Names of the DP nodes

main\_text (Optional) Text at top of plot

incl\_numdata\_plot

Logical - should an upper barplot indicating the number of data items per DP be

included? (Default TRUE)

incl\_nonsig Logical - should components whose credibility intervals include 0 be included

(per DP)? (Default TRUE)

incl\_comp0 Logical - should component zero be plotted? (Default TRUE)

ylab\_numdata Vertical axis label for numdata plot

ylab\_exp Vertical exis label for exposure plot

leg.title Legend title

cex.names Expansion factor for bar labels (dpnames) in exposure plot

cex.axis Expansion factor for vertical-axis annotation

mar See ?par oma See ?par

plot\_chain\_hdpsig\_exp

Plot hdp signature exposure on each chain

### **Description**

Plot hdp signature exposure on each chain

# Usage

```
plot_chain_hdpsig_exp(hdpsample, chains, legend = TRUE)
```

# Arguments

 $\verb|hdpsample| A hdpSample Chain or hdpSample Multi object.$ 

 ${\tt chains} \qquad \qquad A \ hdp Sample Chain \ or \ hdp Sample Multi \ object \ in \ the \ list \ representation$ 

legend Logical - should a legend be included? (default TRUE)

```
plot_component_posterior_samples
```

Plot the distribution of raw clusters highly similar as the component in posterior chains

### **Description**

Plot the distribution of raw clusters highly similar as the component in posterior chains

### Usage

```
plot_component_posterior_samples(components, retval)
```

### **Arguments**

components A matrix that containing components with each row corresponding a category

and each column corresponding a component

retval An object return from extract\_ccc\_from\_hdp

```
plot_component_with_credint
```

Plot signatures and their 95% credible intervals

### **Description**

Plot signatures and their 95% credible intervals

# Usage

```
plot_component_with_credint(
  retval,
  cat_names = NULL,
  col = "grey70",
  cred_int = TRUE,
  weights = NULL,
  group_label_height = 1.05,
  cex.cat = 0.7
)
```

# Arguments

retval	an object return from extract_ccc_from_hdp.
cat_names	names displayed on x-axis, e.g. SBS96 mutation classes
col	Either a single colour for all data categories, or a vector of colours for each group (in the same order as the levels of the grouping factor)
cred_int	Logical - should 95% credibility intervals be plotted? (default TRUE)
weights	(Optional) Weights over the data categories to adjust their relative contribution (multiplicative)

prop.ex 35

```
group_label_height

Multiplicative factor from top of plot for group label placement

cex.cat Expansion factor for the (optional) cat_names
```

prop.ex

Get proportion of dataset explained (on average)

# Description

Get proportion of dataset explained (on average)

### Usage

```
prop.ex(x)
```

#### **Arguments**

Х

hdpSampleChain or hdpSampleMulti

### Value

number of components

TestScaffold1

Debugging scaffold for c code in hdpx/hdp

### **Description**

Debugging scaffold for c code in hdpx/hdp

```
TestScaffold1(
  input.catalog,
  CPU.cores = 1,
  seedNumber = 1,
  K.guess,
  multi.types = FALSE,
  verbose = TRUE,
  num.posterior = 4,
  post.burnin = 4000,
  post.n = 50,
  post.space = 50,
  post.cpiter = 3,
  post.verbosity = 0,
  cos.merge = 0.9,
  min.sample = 1,
  checkpoint.aft.post = NULL
)
```

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#### **Arguments**

input.catalog Input spectra catalog as a matrix or in ICAMS format. Number of CPUs to use in running hdp\_posterior; this is used to parallelize CPU.cores running the posterior sampling chains, so there is no point in making this larger than num.posterior. seedNumber An integer that is used to generate separate random seeds for each call to dp\_activate, and each call of hdp\_posterior; please see the code on how this is done. But repeated calls with same value of seedNumber and other inputs should produce the same results. 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, hdp will regard all input spectra as one tumor type. If TRUE, hdp will infer tumor types based on the string before "::" in their names. e.g. tumor type for "SA.Syn.Ovary-AdenoCA::S.500" would be "SA.Syn.Ovary-AdenoCA" If multi.types is a character vector, then it should be of the same length as the number of columns in input.catalog, and each value is the name of the tumor type of the corresponding column in input.catalog, e.g. c ("SA.Syn.Ovary-AdenoC verbose If TRUE then message progress information. num.posterior Number of posterior sampling chains; can set to 1 for testing. Pass to hdp\_posterior burnin. post.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. cos.merge The cosine similarity threshold for merging raw clusters from the posterior sampling chains into "components" i.e. signatures. min.sample A "component" (i.e. signature) must have at least this many samples. checkpoint.aft.post If non-NULL, a file path to checkpoint the list of values returned from the calls to hdp\_posterior as a .Rdata file.

#### Value

The list of sample changes returned by hdp\_posterior.

xmake.s 37

xmake.s Return a function to calculate the unsigned Stirling numbers of the first kind.

### **Description**

Return a function to calculate the unsigned Stirling numbers of the first kind.

### Usage

```
xmake.s()
```

#### Value

A function to calculate a vector of unsigned Stirling numbers, s(n, k), k = 1...n, each divided by the maximum Stirling number in the series. The returned function is a closure with state that includes a list of all the unsigned Stirling number series  $\leq$  the argument, n,

i.e. [s(1,1)], [s(2,1),s(2,2)], ..., [s(n,1),...,s(n,n)]. Memory usage could be substantial, but the stored state does not include the many trailing zeros in the vectors. For this to work within the hdp (https://github.com/nicolaroberts/hdp) package the function returned \*must\* be called stir.closure.

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