Package 'hdpx'

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Title Hierarchical Dirichlet process for categorical count data, expanded

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biocViews

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Language en-US

Description Model categorical count data with hierarchical Dirichlet process 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 a HDP 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,
      Rcpp,
      RcppArmadillo,
      flexclust,
      parallelDist,
      clue
Suggests testthat,
      RColorBrewer,
      knitr,
      rmarkdown,
      BiocStyle,
      devtools
Collate 'aaa-classes-input.R'
      'aaa-classes-output.R'
      'aaa-generics-input.R'
      'aaa-generics-output.R'
      'cull_posterior_samples.R'
      'diagnostic_in_extraction.R'
      'dp_activate.R'
      'dp_freeze.R'
      'extract_ccc_from_hdp.R'
      'extract_components.R'
      'globals.R'
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      'hdp_addconparam.R'
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      'hdp_burnin.R'
      'hdp_getstate.R'
      'hdp_init.R'
      'hdp_multi_chain.R'
      'hdp_posterior.R'
      'hdp_posterior_sample.R'
      'hdp_prior_init.R'
      'hdp_quick_init.R'
      'hdp setdata.R'
      'interpret_components.R'
      'iterate.R'
      'new_diagnostic_plot_functions.R'
      'plot_chain.R'
      'plot_components.R'
      'RcppExports.R'
      'TestScaffold.R'
```

'utilities.R'
'utilities_nr3.R'
'xmake.s.R'
'zzz.R'

LinkingTo Rcpp,RcppArmadillo

RoxygenNote 7.1.2

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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.

comp_cos_merge 5

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
```

```
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

Usage

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

Arguments

```
An object in hdp_merge_and_extract_components.

ncat Number of categories. An internal object from hdp_merge_and_extract_components.

nsamp Number of posterior samples. An internal object from hdp_merge_and_extract_component

nch Number of posterior chains. An internal object from hdp_merge_and_extract_components.

ccc clust_categ_counts from hdp_merge_and_extract_components.

cdc clust_dp_counts from hdp_merge_and_extract_components.

diagnostic.folder

A directory where details for hdp.0 are plotted.
```

Value

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

See Also

```
hdp_merge_and_extract_components
```

8 dp_activate

nodes			
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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 $1 - 10^{5}$, 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
```

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 9

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
```

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)
```

extract_components 11

Arguments

signature The signature for which we want to get the intervals.

CCC_0 A list XXXXXXXcontaining clust_categ_counts matrix from hdp.

cos.merge cosine similarity cutoff

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(x, hc.cutoff = 0.1)
```

Arguments

x An hdpSampleChain-class or \ codehdpSampleMulti-class object

hc.cutoff the height to cut hierarchical clustering tree

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.

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 exampl, a tumor), or an 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

12 hdpConparam-class

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: 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

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, ...)
```

Arguments

```
x Object of class hdpConparam... unused
```

Methods (by generic)

• as.list: convert to list class

hdpDP-class 13

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, ...)
## S4 method for signature 'hdpDP'
numdata(x, ...)
```

Arguments

x Object of class hdpDP... unused

Methods (by generic)

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

Slots

datace 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, ...)
## 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_dp_distn(x)
```

Arguments

x Object of class hdpSampleChain

... unused

Methods (by generic)

- as.list: Convert to list class
- sampling_seed: Get random seed used by hdp_posterior
- hdp_settings: Get settings of posterior sampling chain
- final_hdpState: Get hdpState object from the end of the posterior sampling chain
- lik: Get likelihood of data given model over all iterations
- numcluster: Get the number of clusters for each posterior sample
- cp values: Get matrix of concentration parameter values for each posterior sample
- clust_categ_counts: Get category vs cluster counts for each posterior sample
- clust_dp_counts: Get dp node vs cluster counts for each posterior sample
- numcomp: Get number of extracted components for hdpSampleChain
- prop.ex: Get proportion of dataset explained (on average) for hdpSampleChain
- comp_cos_merge: Get cos.merge setting for hdpSampleChain
- comp_categ_counts: Get sample vs category counts for each component
- comp_dp_counts: Get sample vs component counts for each DP
- comp_cateq_distn: Get mean distribution over data categories for each component
- comp_dp_distn: 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 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.

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

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

## 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)
```

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```
## 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: Convert to list class
- chains: Get list of hdpSampleChain objects
- numcomp: Get number of extracted components for hdpSampleMulti
- prop.ex: Get proportion of dataset explained (on average) for hdpSampleMulti
- comp_cos_merge: Get cos.merge setting for hdpSampleMulti
- comp_categ_counts: Get sample vs category counts for each component
- comp_dp_counts: Get sample vs component counts for each DP
- comp_categ_distn: Get mean distribution over data categories for each component
- comp_dp_distn: 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.

18 hdpState-class

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, \dots)
## S4 method for signature 'hdpState'
numdp(x, ...)
## S4 method for signature 'hdpState'
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, ...)
```

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Arguments

x Object of class hdpState

... unused

Methods (by generic)

• as.list: Convert to list class

• numdp: Get number of DPs

• numconparam: Get number of concentration parameters

• base: Get base distribution

• conparam: Get list of concentration parameters

• dp: Get list of DP nodes

• dpstate: Get state of every DP

• ppindex: Get parent process index of every DP

• cpindex: Get concentration parameter index of every DP

• numcateg: Get number of data categories

• base_params: Get parameters of the base Dirichlet distribution (like psuedocounts across categories).

• activating_seed: Get seed used to initialse clustering

• pseudoDP: Get index of frozen pseudo-data DP nodes for prior info (only if initialised via hdp_prior_init)

Slots

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)

20 hdp_adddp

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 param-

eters.

alphab Rate hyperparameters for the gamma priors over the DP concentration parame-

ters.

Value

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

See Also

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

Examples

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.

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

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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

```
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)
hdp_example</pre>
```

hdp_burnin

Burnin of posterior sampling chain across activated DPs.

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.

22 hdp_init

Value

A list with the elements:

hdplist A list representation of an hdpState-class object.

likelihood A numeric vector with the likelihood at each iteration.

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.

Usage

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

Arguments

ppindex	Index (or indices) of the parental process(es) for the initial DPs. The 'top' DP should have parent process '0' (the base Dirichlet distribution).
cpindex	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.
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 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

hdp_multi_chain 23

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.

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. Components are extracted via hdp_extract_components.

24 hdp_posterior

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,hdp_extract_components,cull_posterior_samples,plot_lik,plot_numcluster,plot_data_assigned
```

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 25

```
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. Components are extracted via hdp_extract_components.

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

```
post.input
                  An S4 object from hdp_burnin.
                  The number of posterior samples to collect.
post.n
                  The number of iterations between collected samples.
post.space
                  The number of iterations of concentration parameter sampling to perform after
post.cpiter
                  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.
                  If TRUE, a checkpoint will be saved for every 10 posterior samples
checkpoint
```

Value

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

See Also

```
hdp_multi_chain,hdp_extract_components,cull_posterior_samples,plot_lik,plot_numcluster,plot_data_assigned
```

26 hdp_prior_init

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	2
	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

30 plotchain

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

plotcomp 31

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 object including output from hdp_extract_component.		
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_labels			
	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

33

(Optional) Names of the DP nodes dpnames 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) Logical - should components whose credibility intervals include 0 be included incl_nonsig (per DP)? (Default TRUE) Logical - should component zero be plotted? (Default TRUE) incl_comp0 ylab_numdata Vertical axis label for numdata plot ylab_exp Vertical exis label for exposure plot leg.title Legend title Expansion factor for bar labels (dpnames) in exposure plot cex.names cex.axis Expansion factor for vertical-axis annotation See ?par mar

plot_chain_hdpsig_exp

Plot hdp signature exposure on each chain

Description

oma

Plot hdp signature exposure on each chain

See ?par

Usage

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

Arguments

 $\texttt{hdpsample} \qquad \textbf{A hdpSampleChain or hdpSampleMulti object including output from hdp_extract_component}$

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

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. CPU.cores Number of CPUs to use in running hdp_posterior; this is used to parallelize running the posterior sampling chains, so there is no point in making this larger than num.posterior. An integer that is used to generate separate random seeds for each call to dp_activate, seedNumber and each call of hdp_posterior; please see the code on how this is done. But repeated calls with same value of seedNumber and other inputs should produce the same results. K.guess Suggested initial value of the number of signatures, passed to dp_activate as initcc. A logical scalar or a character vector. If FALSE, hdp will regard all input spectra multi.types 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 If TRUE then message progress information. verbose num.posterior Number of posterior sampling chains; can set to 1 for testing. 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. 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. checkpoint.aft.post If non-NULL, a file path to checkpoint the list of values returned from the calls

Value

The list of sample changes returned by hdp_posterior.

to hdp_posterior as a .Rdata file.

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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