Package 'beer'

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Type Package

Title Bayesian Enrichment Estimation in R

Version 1.13.0

Description BEER implements a Bayesian model for analyzing

phage-immunoprecipitation sequencing (PhIP-seq) data. Given a PhIPData object, BEER returns posterior probabilities of enriched antibody responses, point estimates for the relative fold-change in comparison to negative control samples, and more. Additionally, BEER provides a convenient implementation for using edgeR to identify enriched antibody responses.

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beer-package

beer: an R package for quantifying antibody reactivities for PhIP-Seq data

Description

The core functions of beer are **brew** and **runEdgeR**. To learn more about beer, see the vignette using browseVignettes(package = "beer").

.beadsRRBeer

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See Also

Useful links:

- https://github.com/athchen/beer/
- Report bugs at https://github.com/athchen/beer/issues

. beadsRRBeer Function to run the beads-only round robin using BEER

Description

Each sample is run in comparison to all other beads-only samples to approximate the false positive rate of detecting enrichments.

Usage

```
.beadsRRBeer(
    object,
    prior.params = list(method = "edgeR", a_pi = 2, b_pi = 300, a_phi = 1.25, b_phi =
        0.1, a_c = 80, b_c = 20, fc = 1),
    beads.args = list(lower = 1),
    jags.params = list(n.chains = 1, n.adapt = 1000, n.iter = 10000, thin = 1, na.rm =
    TRUE, burn.in = 0, post.thin = 1, seed = as.numeric(format(Sys.Date(), "%Y%m%d"))),
    sample.dir = NULL,
    assay.names = c(phi = NULL, phi_Z = "logfc", Z = "prob", c = "sampleInfo", pi =
        "sampleInfo"),
    summarize = TRUE,
    BPPARAM = bpparam()
)
```

object	PhIPData object
prior.params	named list of prior parameters
beads.args	named list of parameters supplied to estimating beads-only prior parameters (a_0, b_0)
jags.params	named list of parameters for running MCMC using JAGS
sample.dir	path to temporarily store RDS files for each sample run, if NULL then [base::tempdir] is used to temporarily store MCMC output and cleaned afterwards.
assay.names	named vector indicating where MCMC results should be stored in the PhIPData object
summarize	logical indicating whether to return a PhIPData object.
BPPARAM	[BiocParallel::BiocParallelParam] passed to BiocParallel functions.

Value

vector of process IDs or a PhIPData object

.beadsRREdgeR

Function to run the beads-only round robin using edgeR

Description

Each sample is run in comparison to all other beads-only samples to approximate the false positive rate of detecting enrichments.

Usage

```
.beadsRREdgeR(
    object,
    threshold.cpm = 0,
    threshold.prevalence = 0,
    assay.names = c(logfc = "logfc", prob = "prob"),
    de.method = "exactTest",
    BPPARAM = BiocParallel::bpparam()
)
```

Arguments

object	A PhIPData object of only beads-only samples.
threshold.cpm	CPM threshold to be considered present in a sample
threshold.preva	alence proportion of beads-only samples that surpass threshold.cpm.
assay.names	named vector specifying the assay names for the log2(fold-change) and exact test p-values. If the vector is not names, the first and second entries are used as defaults.
de.method	character describing which edgeR test for differential expression should be used. Must be one of 'exactTest' or 'glmQLFTest'.
BPPARAM	[BiocParallel::BiocParallelParam] passed to BiocParallel functions.

Value

vector of process IDs

.brewSamples

Description

Encapsulated function to run each sample against all beads-only samples. The code is wrapped in this smaller function to (1) modularize the code and (2) make sure the cli output colors don't change.

Usage

```
.brewSamples(
   object,
   sample.id,
   beads.id,
   se.matrix,
   prior.params,
   beads.prior,
   beads.args,
   jags.params,
   tmp.dir,
   BPPARAM
)
```

Arguments

object	PhIPData object
sample.id	vector of sample IDs to iterate over
beads.id	vector of IDs corresponding to beads-only samples
se.matrix	matrix indicating which peptides are clearly enriched
prior.params	list of prior parameters
beads.prior	data frame of beads-only prior parameters
beads.args	named list of parameters supplied to estimating beads-only prior parameters (a_0, b_0)
jags.params	list of JAGS parameters
tmp.dir	directory to store JAGS samples
BPPARAM	[BiocParallel::BiocParallelParam] passed to BiocParallel functions.

Value

vector of process id's for internal checking of whether functions were parallelized correctly.

.checkCounts

Description

Function to check that the counts matrix only contains integers

Usage

```
.checkCounts(object)
```

Arguments

object PhIPData object

Value

nothing if all counts are integers, and error otherwise

.checkOverwrite Function to check whether an assay will be overwritten

Description

If the an assay is not specified (e.g. with NA), then .checkOverwrite() will return FALSE (rather than NA).

Usage

.checkOverwrite(object, assay.names)

Arguments

object	PhIPData object
assay.names	character vector of assay names

Value

logical vector indicating whether data in an assay will be overwritten

. edgeRBeads Estimate edgeR dispersion parameters from the beads-only data using qCML

Description

Wrapper function to estimate edgeR dispersion parameters from beads-only samples. Peptides can be pre-filtered based on a minimum read count per million (cpm) and the proportion of beads-only samples that surpass the cpm threshold.

Usage

```
.edgeRBeads(object, threshold.cpm = 0, threshold.prevalence = 0)
```

Arguments

objectPhIPData object (can have actual serum samples)threshold.cpmCPM threshold to be considered present in a samplethreshold.prevalenceproportion of beads-only samples that surpass threshold.cpm.

Value

a DGEList object with common, trended, and tagwise dispersion estimates

.edgeRBeadsQLF	Estimate edgeR dispersion parameters from the beads-only samples using Cox-Reid profile adjusted likelihood method for estimating dispersions.
	persions.

Description

Wrapper function to estimate edgeR dispersion parameters from beads-only samples. Peptides can be pre-filtered based on a minimum read count per million (cpm) and the proportion of beads-only samples that surpass the cpm threshold.

Usage

```
.edgeRBeadsQLF(object, threshold.cpm = 0, threshold.prevalence = 0)
```

Arguments

object	PhIPData object (can have actual serum samples)	
threshold.cpm	CPM threshold to be considered present in a sample	
threshold.prevalence		
	proportion of beads-only samples that surpass threshold.cpm.	

Value

a DGEList object with common, trended, and tagwise dispersion estimates

```
.getABEdgeR
```

Description

Given a PhIPData object, beads-only shape parameters are estimated by first deriving the peptidespecific edgeR dispersion estimate ϕ^{edgeR} . ϕ^{edgeR} corresponds to the squared coefficient of variation for the proportion of reads pulled for a given peptide. Using ϕ^{edgeR} to derive an estimate of the variance for the proportion of reads pulled by a single peptide, the mean and variance are converted to shape parameters of a beta distribution.

Usage

```
.getABEdgeR(
  object,
  threshold.cpm = 0,
  threshold.prevalence = 0,
  lower = 1,
  upper = Inf
)
```

Arguments

object	a PhIPData object.	
threshold.cpm	CPM threshold to be considered present in a sample.	
threshold.prevalence		
	proportion of beads-only samples that surpass threshold.cpm.	
lower	minimum value of the beta shape parameters.	
upper	maximum value of the beta shape parameters.	

Value

dataframe with rows corresponding to peptides and columns corresponding to estimated shape parameters of the beta distribution.

See Also

[.edgeRBeads()] for estimating ϕ^{edgeR}

.getABMLE	Wrapper function to derive MLE estimates of a, b from beads-only
	samples

Description

Wrapper function to derive MLE estimates of a, b from beads-only samples

.getABMLEProp

Usage

```
.getABMLE(
  object,
  prop.offset = 1e-08,
  optim.method = "default",
  lower = 1,
  upper = Inf
)
```

Arguments

object	a PhIPData object
prop.offset	offset to use when the proportion of reads is 0.
optim.method	optimization method passed to [stats::optim].
lower	lower bound for the shape parameters.
upper	upper bound for the shape parameters.

Value

a data frame of MLE estimates of a, b

See Also

[stats::optim] for available optimization methods

.getABMLEProp	Helper function to derive MLE estimates of a, b from a vector of pro-
	portions

Description

Helper function to derive MLE estimates of a, b from a vector of proportions

Usage

```
.getABMLEProp(
  prop,
  prop.offset = 1e-08,
  optim.method = "default",
  lower = 1,
  upper = Inf
)
```

prop	vector of proportions.
prop.offset	offset to use when the proportion of reads is 0.
optim.method	optimization method passed to [stats::optim].
lower	lower bound for the shape parameters.
upper	upper bound for the shape parameters.

Value

a data frame of MLE estimates of a, b

See Also

[stats::optim] for available optimization methods

.getABMOM	Wrapper function to derive MOM estimates of a, b from beads-only
	samples

Description

Wrapper function to derive MOM estimates of a, b from beads-only samples

Usage

```
.getABMOM(
  object,
  offsets = c(mean = 1e-08, var = 1e-08),
  lower = 1,
  upper = Inf,
  ...
)
```

Arguments

object	a PhIPData object.
offsets	vector defining the offset to use when the mean and/or variance are zero.
lower	lower bound for the shape parameters.
upper	upper bound for the shape parameters.
	parameters passed to [base::mean] and [stats::var].

Value

a data frame with MOM estimates of a, b

.getABMOMProp Helper function to derive MOM estimates of a, b from a vector of proportions

Description

Helper function to derive MOM estimates of a, b from a vector of proportions

Usage

```
.getABMOMProp(
  prop,
  offsets = c(mean = 1e-08, var = 1e-08),
  lower = 1,
  upper = Inf,
  ...
)
```

Arguments

prop	vector of proportions.
offsets	vector defining the offset to use when the mean and/or variance are zero.
lower	lower bound for the shape parameters.
upper	upper bound for the shape parameters.
	parameters passed to [base::mean] and [stats::var].

Value

a data frame with MOM estimates of a, b

.guessEnrichedEdgeR Guess super-enriched peptides based on edgeR fold-change estimates

Description

Guess super-enriched peptides based on edgeR fold-change estimates

Usage

```
.guessEnrichedEdgeR(object, threshold = 15, fc.name = "logfc")
```

object	PhIPData object.
threshold	minimum estimated fc for a peptide to be considered super-enriched.
fc.name	assay name corresponding to the assay that stores the edgeR estimated log2 fold-changes.

Value

logical matrix of the with the same dimensions as object indicating which peptides are considered super-enriched.

.guessEnrichedMLE Guess enriched peptides based on MLE estimates of the true foldchange

Description

Guess enriched peptides based on MLE estimates of the true fold-change

Usage

```
.guessEnrichedMLE(object, beads.prior, threshold = 15)
```

Arguments

object	PhIPData object.
beads.prior	data.frame of prior parameters for beads-only samples.
threshold	minimum estimated fc for a peptide to be considered super-enriched.

Value

logical matrix of the with the same dimensions as object indicating which peptides are considered super-enriched.

.tidyAssayNames Clean-up specified assay names

Description

Tidy inputs related to 'assay.names'. Supplies default values for missing parameters and ensures that all required parameters are present.

Usage

```
.tidyAssayNames(assay.names)
```

Arguments

assay.names named list specifying where to store each assay.

Value

tidied list of assay.names

.tidyInputsJAGS Clean inputs for JAGS parameters

Description

Tidy inputs related to 'jags.params'. Supplies default values for missing parameters and ensures that all required parameters are present.

Usage

.tidyInputsJAGS(jags.params)

Arguments

jags.params named list of JAGS parameters

Value

tidied list of JAGS parameters.

.tidyInputsPrior Clean up inputs for prior estimation

Description

Tidy inputs related to 'prior.parameters'. Supplies default values for missing parameters and ensures that all required parameters are present.

Usage

.tidyInputsPrior(prior.params, object, beads.args)

Arguments

prior.params	named list of prior parameters
object	PhIPData object
beads.args	parameters used to estimate a_0, b_0

Value

tidied list of prior parameters.

.tidyInputsSE

Description

Tidy inputs related to 'se.params'. Supplies default values for missing parameters and ensures that all required parameters are present.

Usage

.tidyInputsSE(se.params, beads.prior)

Arguments

se.params	named list of parameters for super-enriched estimation
beads.prior	data.frame with beads-only parameters

Value

tidied list of parameters for identifying super-enriched peptides.

beadsRR

Beads-only round robin

Description

To approximate the false positive rate of each approach, each beads-only sample is run individually against all other samples. For BEER, this means that the sample to be compared is encoded as an actual sample, and prior parameters for beads-only samples are re-estimated. Thus, the beads-only round robin also serves to assess how similar the beads-only samples are to one another.

Usage

```
beadsRR(object, method, BPPARAM = BiocParallel::bpparam(), ...)
```

object	PhIPData object
method	one of 'beer' or 'edgeR' specifying which method to use.
BPPARAM	[BiocParallel::BiocParallelParam] passed to BiocParallel functions.
	parameters passed to the method specific functions. See the <i>Details</i> section below for additional information.

brew

Details

If method == 'beer', then valid parameters include prior.params, beads.args, jags.params, sample.dir, assay.names, and summarize. A description of the first four parameters can be found in brew. summarize is a logical value indicating whether a PhIPData object with the summarized results should be returned. When running beadsRR, summarize typically does not need to be changed.

When method == 'edgeR', threshold.cpm, threshold.prevalence, and assay.names are valid additional parameters that can be supplied to beadsRR. See edgeR for additional details on each of these parameters.

Value

a PhIPData object

See Also

brew for BEER parameters, edgeR for edgeR parameters, and [BiocParallel::BiocParallelParam] for parallelization.

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))</pre>
```

```
beadsRR(sim_data, method = "beer")
beadsRR(sim_data, method = "edgeR")
beadsRR(sim_data, method = "edgeR", de.method = "glmQLFTest")
```

brew

Bayesian Enrichment Estimation in R (BEER)

Description

Run BEER to estimate posterior probabilities of enrichment, sample-specific attenuation constants, relative fold-changes in comparison to beads-only samples, and proportion of peptides enriched per sample as described in Chen et. al. See *Details* for more information on input parameters.

Usage

```
brew(
    object,
    prior.params = list(method = "edgeR", a_pi = 2, b_pi = 300, a_phi = 1.25, b_phi =
        0.1, a_c = 80, b_c = 20, fc = 1),
    beads.args = list(lower = 1),
    se.params = list(method = "mle"),
    jags.params = list(n.chains = 1, n.adapt = 1000, n.iter = 10000, thin = 1, na.rm =
    TRUE, burn.in = 0, post.thin = 1, seed = as.numeric(format(Sys.Date(), "%Y%m%d"))),
    sample.dir = NULL,
    assay.names = c(phi = NULL, phi_Z = "logfc", Z = "prob", c = "sampleInfo", pi =
            "sampleInfo"),
    beadsRR = FALSE,
    BPPARAM = bpparam()
)
```

Arguments

object	PhIPData object
prior.params	named list of prior parameters
beads.args	named list of parameters supplied to estimating beads-only prior parameters (a_0, b_0)
se.params	named list of parameters specific to identifying clearly enriched peptides
jags.params	named list of parameters for running MCMC using JAGS
sample.dir	path to temporarily store RDS files for each sample run, if NULL then [base::tempdir] is used to temporarily store MCMC output and cleaned afterwards.
assay.names	named vector indicating where MCMC results should be stored in the PhIPData object
beadsRR	logical value specifying whether each beads-only sample should be compared to all other beads-only samples.
BPPARAM	[BiocParallel::BiocParallelParam] passed to BiocParallel functions.

Details

prior.params. List of prior parameters. Parameters include,

- method: method used to estimate beads-only prior parameters a_0, b_0. Valid methods include 'custom' or any of the methods specified in getAB. If method = 'custom' is specified, a_0 and b_0 must be included in the list of prior parameters. 'edgeR' is used as the default method for estimating a_0, b_0.
- a_pi, b_pi: prior shape parameters for the proportion of peptides enriched in a sample. Defaults to 2 and 300, respectively.
- a_phi, b_phi: prior shape parameters of the gamma distribution that describe the valid range of enriched-fold changes. The shift is specified by fc. The default values of a_phi and b_phi are 1.25 and 0.1, respectively.
- a_c, b_c: prior shape parameters for the attenuation constant. Default values for a_c and b_c are 80 and 20.
- fc: minimum fold change for an enriched-peptide. fc describes the shift in the gamma distribution.

beads.args. Named list of parameters supplied to getAB. The estimation method used is specified in prior.params, but other valid parameters include lower and upper bounds for elicited parameters. As JAGS recommends that a, b > 1 for the beta distribution, beads.args defaults to list(lower = 1).

se.params. Named list of parameters supplied to guessEnriched. By default list(method = 'mle') is used to identify clearly enriched peptides.

jags.params. Named list of parameters for MCMC sampling. By default, BEER only runs one chain with 1,000 adaptation iteration and 10,000 sampling iterations. If unspecified, BEER uses the current date as the seed.

sample.dir. Path specifying where to store the intermediate results. If NULL, then results are stored in the default temporary directory. Otherwise, the MCMC samples for running BEER on each sample is stored as a single RDS file in the specified directory.

assay.names. Named list specifying where to store the point estimates. If NULL, estimates are not added to the PhIPData object. Valid exported estimates include,

brewOne

- phi: fold-change estimate after marginalizing over the posterior probability of enrichment. By default point estimates are not exported.
- phi_Z: fold-change estimate presuming the peptide is enriched. By default phi_Z estimates are stored in 'logfc' assay.
- Z: posterior probability of enrichment. Estimates are stored in the 'prob' assay by default.
- c: attenuation constant estimates. Stored in 'sampleInfo' by default.
- pi: point estimates for the proportion of peptides enriched in a sample. Stored in 'sampleInfo' by default.

Value

A PhIPData object with BEER results stored in the locations specified by assay. names.

See Also

[BiocParallel::BiocParallelParam] for subclasses, beadsRR for running each beads-only sample against all remaining samples, getAB for more information about valid parameters for estimating beads-only prior parameters, guessEnriched for more information about how clearly enriched peptides are identified, and [rjags::jags.model] for MCMC sampling parameters.

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))
## Default back-end evaluation
brew(sim_data)
## Serial
brew(sim_data, BPPARAM = BiocParallel::SerialParam())
## Snow
brew(sim_data, BPPARAM = BiocParallel::SnowParam())</pre>
```

brew0ne

Run BEER for one sample

Description

This function is not really for external use. It's exported for parallelization purposes. For more detailed descriptions see brew.

Usage

```
brewOne(
   object,
   sample,
   prior.params,
   n.chains = 1,
   n.adapt = 1000,
   n.iter = 10000,
   thin = 1,
```

edgeROne

```
na.rm = TRUE,
...,
seed = as.numeric(format(Sys.Date(), "%Y%m%d"))
)
```

Arguments

object	PhIPData object
sample	sample name
prior.params	vector of prior parameters
n.chains	number of chains to run
n.adapt	number of iterations to use as burn-in.
n.iter	number of iterations for the MCMC chain to run (after n.adapt)
thin	thinning parameter
na.rm	what to do with NA values (for JAGS)
	extra parameters for JAGS
seed	number/string for reproducibility purposes.

Value

nothing, saves the the results to an RDS in either a temp directory or the specified directory.

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))
beads_prior <- getAB(subsetBeads(sim_data), "edgeR")
brewOne(sim_data, "9", list(
    a_0 = beads_prior[["a_0"]],
    b_0 = beads_prior[["b_0"]],
    a_pi = 2, b_pi = 300,
    a_phi = 1.25, b_phi = 0.1,
    a_c = 80, b_c = 20,
    fc = 1
))</pre>
```

edgeROne	Run edgeR for one sample	e against all the beads-only samples.	

Description

This function is not really for external use. It's exported for parallelization purposes. For more detailed descriptions see runEdgeR.

Usage

edgeROne(object, sample, beads, common.disp, tagwise.disp, trended.disp)

edgeROneQLF

Arguments

object	PhIPData object
sample	sample name of the sample to compare against beads-only samples
beads	sample names for beads-only samples
common.disp	edgeR estimated common dispersion parameter
tagwise.disp	edgeR estimated tagwise dispersion parameter
trended.disp	edgeR estimated trended dispersion parameter

Value

list with sample name, log2 fc estimate, and log10 p-value

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))
beads_disp <- beer:::.edgeRBeads(sim_data)
edgeROne(
    sim_data, "9", colnames(sim_data)[sim_data$group == "beads"],
    beads_disp$common.dispersion, beads_disp$tagwise.disp,
    beads_disp$trended.disp
)</pre>
```

edgeROneQLF	Run edgeR for one sample against all the beads-only samples using
	edgeR's QLF Test for differential expression.

Description

This function is not really for external use. It's exported for parallelization purposes. For more detailed descriptions see runEdgeR.

Usage

```
edgeROneQLF(object, sample, beads, common.disp, tagwise.disp, trended.disp)
```

Arguments

object	PhIPData object
sample	sample name of the sample to compare against beads-only samples
beads	sample names for beads-only samples
common.disp	edgeR estimated common dispersion parameter
tagwise.disp	edgeR estimated tagwise dispersion parameter
trended.disp	edgeR estimated trended dispersion parameter

Value

list with sample name, log2 fc estimate, and log10 p-value

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))
beads_disp <- beer:::.edgeRBeadsQLF(sim_data)
edgeROneQLF(
    sim_data, "9", colnames(sim_data)[sim_data$group == "beads"],
    beads_disp$common.dispersion, beads_disp$tagwise.disp,
    beads_disp$trended.disp
)</pre>
```

```
getAB
```

Estimate beads-only shape parameters

Description

Beta shape parameters are estimated using the proportion of reads-pulled per peptide across the beads-only samples. Currently, only three estimation methods are supported: edgeR, method of moments (MOM), maximum likelihood (MLE). Note that edgeR can only be used on PhIPData objects while MOM and MLE methods can also be applied to vectors of values between 0 and 1. Parameters that can be passed to each method are listed in the details.

Usage

getAB(object, method = "mom", ...)

Arguments

object	a PhIPData object or a vector
method	one of c("edgeR", "mle", "mom") designating which method to use to estimate beads-only prior parameters. MOM is the default method used to estimate shape parameters.
	parameters passed to specific estimating functions. See details for more information

Details

edgeR derived estimates rely on edgeR's peptide-specific dispersion estimates, denoted ϕ^{edgeR} . ϕ^{edgeR} corresponds to the squared coefficient of variation for the proportion of reads pulled for a given peptide. Using ϕ^{edgeR} to derive an estimate of the variance for the proportion of reads pulled by a single peptide, the mean and variance are transformed into shape parameters satisfying the lower and upper bounds. When method = "edgeR", the following additional parameters can be specified.

- threshold.cpm: CPM threshold to be considered present in a sample.
- threshold.prevalence: proportion of beads-only samples that surpass threshold.cpm.
- lower: minimum value of the beta shape parameters.
- upper: maximum value of the beta shape parameters.

Method of Moments (MOM) estimates are derived by transforming the sample mean and variance to shape parameters of the beta distribution. For method = "mom", the following parameters can be adjusted:

getBF

- offsets: vector defining the offset to use when the mean and/or variance are zero.
- lower: lower bound for the shape parameters.
- upper: upper bound for the shape parameters.
- ...: parameters passed to [base::mean] and [stats::var].

Maximum Likelihood (MLE) estimates rely on [stats::optim] to derive shape parameters that maximize the likelihood of observed data. By default the L-BFGS-B optimization method is used. Parameters for MLE estimates include:

- prop.offset: offset to use when the proportion of reads is 0.
- optim.method: optimization method passed to [stats::optim].
- lower: lower bound for the shape parameters.
- upper: upper bound for the shape parameters.

Value

a data frame of beta shape parameters where each row corresponds to a peptide.

Examples

```
## PhIPData object
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))
getAB(sim_data, method = "edgeR")
getAB(sim_data, method = "mle")
getAB(sim_data, method = "mom")
## Vector of proportions
prop <- rbeta(100, 2, 8)
getAB(prop, method = "mle")
getAB(prop, method = "mom")
```

getBF

Calculate Bayes Factors

Description

Calculate Bayes Factors

Usage

```
getBF(
   object,
   assay.postprob = "prob",
   assay.name = "bayes_factors",
   prior.params = list(a_pi = 2, b_pi = 300)
)
```

Arguments

object	PhIPData object
assay.postprob	string indicating the assay where posterior probabilities are stored.
assay.name	name indicating where the results should be stored in the PhIPData object
prior.params	prior parameters for the probability of enrichment (a_pi, b_pi)

Value

PhIPData object with the results stored in the location specified by assay.name.

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))</pre>
```

```
## Calculate Bayes Factors
getBF(sim_data, "prob", "bayes_factor")
```

getExpected

Calculate expected read counts or proportion of reads

Description

Calculate expected read counts or proportion of reads

Usage

```
getExpected(
   object,
   type = c("rc", "prop"),
   assay.names = c("expected_rc", "expected_prop")
)
```

Arguments

object	PhIPData object
type	any of 'rc' or 'prop' indicating whether the function should return the expected read counts or expected proportion of reads, respectively
assay.names	name(s) indicating where the results should be stored in the PhIPData object

Value

PhIPData object with the results stored in the location specified by assay.name.

guessEnriched

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))
## Calculate expected read counts
getExpected(sim_data, "rc", "expected_rc")
## Calculate expected proportion of reads
getExpected(sim_data, "prop", "expected_prop")
## Calculate both
getExpected(sim_data)</pre>
```

guessEnriched

Identifying clearly enriched peptides

Description

As clearly enriched peptides will always have a 100% posterior probability of enrichment, BEER removes these peptides a priori to running the model. Clearly enriched peptides can be identified using edgeR estimated fold-changes or maximum likelihood estimates based on the specified prior parameters. Additional parameters for each method can be found in the details below.

Usage

```
guessEnriched(object, method = "mle", ...)
```

Arguments

object	a PhIPData object
method	one of "mle" or "edgeR", specifying which method to use to identify clearly enriched peptides
	additional parameters dependent on the method used. See details for more information

Details

edgeR. Identification of clearly enriched peptides relies on edgeR fold-change estimates, so edgeR must be run on the PhIPData object beforehand. Additional parameters for identifying clearly enriched peptides based on edgeR estimated fold-changes are listed below:

- object: a PhIPData object.
- threshold: minimum estimated fc for a peptide to be considered super-enriched. The default value is 15.
- fc.name: assay name corresponding to the assay that stores the edgeR estimated log2 foldchanges.

MLE. As the number of reads tends to be quite large, the estimates for the proportion of reads pulled are generally accurate. Clearly enriched peptides are identified by first comparing the observed read count to the expected read count based on the beads-only prior parameters. Peptides with observed read counts larger than 5 times the expected read counts are temporarily labeled as

enriched, and attenuation constants are estimated by regressing the observed read counts on the expected read counts for all non-enriched peptides. Using this attenuation constant, peptides with fold-changes above some predefined threshold after adjusting for the attenuation constant are considered enriched. Parameters for identifying clearly enriched peptides using the MLE approach are listed below.

- object: a PhIPData object.
- threshold: minimum estimated fc for a peptide to be considered super-enriched.
- beads.prior: data.frame of prior parameters for beads-only samples.

Value

a logical matrix of the with the same dimensions as object indicating which peptides are considered super-enriched.

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))
edgeR_out <- runEdgeR(sim_data)
guessEnriched(edgeR_out, method = "edgeR", threshold = 15, fc.name = "logfc")
guessEnriched(edgeR_out,
    method = "mle",
    beads.prior = getAB(edgeR_out, method = "edgeR"),
    threshold = 15
)</pre>
```

guessInits

Derive initial estimates of unknown model parameters

Description

To reduce converge time and to reduce the likelihood of the slice sampler getting stuck, we use maximum likelihood to derive initial estimates for unknown model parameters.

Usage

```
guessInits(object, beads.prior)
```

object	a PhIPData object
beads.prior	a data frame with two columns (named a_0, b_0) containing estimated shape parameters from beads-only samples.

runEdgeR

Details

Briefly initial values are defined as follows:

- 1. theta_guess[i, j] = Y[i, j]/n[j], or the MLE for theta.
- 2. Z_guess[i, j] = 1 if j is a serum sample, and the observed read count is >2x the expected read count assuming c[j] = 1.
- 3. pi_guess[j] is the mean of column *j* in Z_guess.
- 4. c_guess[j] is the estimated slope from regressing the observed read counts against the expected read counts (without adjusting for the attenuation constant) for non-enriched peptides only.
- 5. phi_guess[i,j] is the ratio of the observed read counts to the expected read counts multiplied by the attenuation constant.

Value

a list of estimated initial values.

See Also

Methods in [Chen et. al 2022](https://www.biorxiv.org/content/10.1101/2022.01.19.476926v1)

runEdgeR

Run edgeR on PhIP-Seq data

Description

Run edgeR on PhIP-Seq data

Usage

```
runEdgeR(
   object,
   threshold.cpm = 0,
   threshold.prevalence = 0,
   assay.names = c(logfc = "logfc", prob = "prob"),
   beadsRR = FALSE,
   de.method = "exactTest",
   BPPARAM = BiocParallel::bpparam()
)
```

object	PhIPData object	
threshold.cpm	CPM threshold to be considered present in a sample	
threshold.preva	lence	
	proportion of beads-only samples that surpass threshold.cpm.	
assay.names	named vector specifying the assay names for the log2(fold-change) and exact test p-values. If the vector is not names, the first and second entries are used as defaults	

summarizeRun

	logical value specifying whether each beads-only sample should be compared to all other beads-only samples.
	character describing which edgeR test for differential expression should be used. Must be one of 'exactTest' or 'glmQLFTest'
BPPARAM	[BiocParallel::BiocParallelParam] passed to BiocParallel functions.

Value

PhIPData object with log2 estimated fold-changes and p-values for enrichment stored in the assays specified by 'assay.names'.

See Also

[BiocParallel::BiocParallelParam], beadsRR

Examples

```
sim_data <- readRDS(system.file("extdata", "sim_data.rds", package = "beer"))</pre>
```

Default back-end evaluation
runEdgeR(sim_data)

```
## Serial
runEdgeR(sim_data, BPPARAM = BiocParallel::SerialParam())
```

Snow
runEdgeR(sim_data, BPPARAM = BiocParallel::SnowParam())

```
## With glmQLFTest
runEdgeR(sim_data, de.method = "glmQLFTest")
```

summarizeRun	Summarize MCMC chain and return point estimates for BEER param-
	eters

Description

Posterior means are used as point estimates for c, π, ϕ , and Z. As super-enriched peptides are tossed out before MCMC sampling, super-enriched peptides return NA for the ϕ and Z point estimates. Indices corresponding to a particular peptide in the MCMC sampler are mapped back to the original peptide names.

Usage

```
summarizeRun(
   object,
   jags.files,
   se.matrix,
   burn.in = 0,
   post.thin = 1,
   assay.names = c(phi = NULL, phi_Z = "logfc", Z = "prob", c = "sampleInfo", pi =
```

summarizeRunOne

```
"sampleInfo"),
BPPARAM = BiocParallel::bpparam()
)
```

Arguments

object	a PhIPData object
jags.files	list of files containing MCMC sampling results
se.matrix	logical matrix indicating which peptides were identified as super-enriched pep- tides
burn.in	number of iterations to be burned
post.thin	thinning parameter
assay.names	named vector of specifying where to store point estimates
BPPARAM	[BiocParallel::BiocParallelParam] passed to BiocParallel functions.

Value

PhIPData object with point estimates stored in the assays specified by 'assay.names'.

summarizeRunOne	Derive point estimates for c, pi, phi, and Z for a particular sample
-----------------	--

Description

Posterior means are used as point estimates for c, π, ϕ , and Z. As super-enriched peptides are tossed out before MCMC sampling, super-enriched peptides return NA for the ϕ and Z point estimates. Indices corresponding to a particular peptide in the MCMC sampler are mapped back to the original peptide names.

Usage

```
summarizeRunOne(object, file, se.matrix, burn.in = 0, post.thin = 1)
```

Arguments

object	a PhIPData object
file	path to rds file
se.matrix	logical matrix indicating which peptides were identified as super-enriched pep- tides
burn.in	number of iterations to be burned
post.thin	thinning parameter

Value

list of point estimates for c, pi, phi and Z

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