Package ‘beer’

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Type Package

Title Bayesian Enrichment Estimation in R

Version 1.8.0

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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Encoding UTF-8

LazyData false

Depends R (>= 4.2.0), PhIPData (>= 1.1.1), rjags

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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").

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See Also

Useful links:
- [https://github.com/athchen/beer/](https://github.com/athchen/beer/)
- Report bugs at [https://github.com/athchen/beer/issues](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

```r
.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()
)
```
Arguments

object  PhIPData object
prior.params  named list of prior parameters
beads.args  named list of parameters supplied to estimating beads-only prior parameters (\(a_0, b_0\))
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 \([\text{base::tempdir}]\) 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  \([\text{BiocParallel::BiocParallelParam}]\) passed to BiocParallel functions.

Value

vector of process IDs or a PhIPData object

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.prevalence  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

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  Function to check that the counts matrix only contains integers

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
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

.edgeRBeadsQLF

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

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

Description

Given a PhIPData object, beads-only shape parameters are estimated by first deriving the peptide-specific edgeR dispersion estimate $\phi_{edgeR}$. $\phi_{edgeR}$ corresponds to the squared coefficient of variation for the proportion of reads pulled for a given peptide. Using $\phi_{edgeR}$ 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

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>object</td>
<td>a PhIPData object.</td>
</tr>
<tr>
<td>threshold.cpm</td>
<td>CPM threshold to be considered present in a sample.</td>
</tr>
<tr>
<td>threshold.prevalence</td>
<td>proportion of beads-only samples that surpass threshold.cpm.</td>
</tr>
<tr>
<td>lower</td>
<td>minimum value of the beta shape parameters.</td>
</tr>
<tr>
<td>upper</td>
<td>maximum value of the beta shape parameters.</td>
</tr>
</tbody>
</table>

Value

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

See Also

[.edgeRBeads()] for estimating $\phi_{edgeR}$
Description

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

Usage

`.getABMLE`

`.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

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
    )

Arguments
    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

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

Description

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

Usage

```r
.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")
```

**Arguments**
- **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 fold-change*

**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  
**Clean up inputs for identifying super-enriched peptides**

**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

---

**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(), ...)
```

### Arguments

- **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 Details section below for additional information.

### 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"))

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

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,

- 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**

```r
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())
```

**Description**

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

**Usage**

```r
brewOne(
  object, sample, prior.params, n.chains = 1, n.adapt = 1000, n.iter = 10000, thin = 1, 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 results to an RDS in either a temp directory or the specified directory.

Examples

```r
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
))
```

Description

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

Usage

```r
edgeROne(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**

```r
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
)
```

---

**Description**

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

**Usage**

```r
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**

```r
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
)
```
Value

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

Examples

```r
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
)
```

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 $\phi^{edgeR}$. $\phi^{edgeR}$ corresponds to the squared coefficient of variation for the proportion of reads pulled for a given peptide. Using $\phi^{edgeR}$ 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:

• 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

```r
## 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**

```r
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**

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

## 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.

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)

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", ...)
guessEnriched

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 fold-changes.

**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

```r
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)
```
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)

Arguments

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.

Details

Briefly initial values are defined as follows:

1. \( \theta_{\text{guess}}[i, j] = \frac{Y[i, j]}{n[j]} \), or the the MLE for \( \theta \).
2. \( Z_{\text{guess}}[i, j] = 1 \) if \( j \) is a serum sample, and the observed read count is \( >2x \) the expected read count assuming \( c[j] = 1 \).
3. \( \pi_{\text{guess}}[j] \) is the mean of column \( j \) in \( Z_{\text{guess}} \).
4. \( c_{\text{guess}}[j] \) 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. \( \phi_{\text{guess}}[i, j] \) 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()
)

Arguments

object PhIPData object
threshold.cpm CPM threshold to be considered present in a sample
threshold.prevalence 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
beadsRR logical value specifying whether each beads-only sample should be compared
to all other beads-only samples.
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

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
summarizeRun

Summarize MCMC chain and return point estimates for BEER parameters

Examples

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

## 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")
```

Description

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

Usage

```r
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 = "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 peptides
- `burn.in` number of iterations to be burned
summarizeRunOne

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 \(c, \pi, \phi, \text{and } Z\). As super-enriched peptides are tossed out before MCMC sampling, super-enriched peptides return \(\text{NA}\) for the \(\phi\) 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 peptides
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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