

Package ‘mbmixture’

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Title Microbiome Mixture Analysis

Description Evaluate whether a microbiome sample is a mixture of two samples, by fitting a model for the number of read counts as a function of single nucleotide polymorphism (SNP) allele and the genotypes of two potential source samples.
Lobo et al. (2021) <[doi:10.1093/g3journal/jkab308](https://doi.org/10.1093/g3journal/jkab308)>.

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Depends R (>= 3.1.0)

Imports stats, parallel, numDeriv

Suggests knitr, rmarkdown, testthat, devtools, roxygen2

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URL <https://github.com/kbroman/mbmixture>

BugReports <https://github.com/kbroman/mbmixture/issues>

VignetteBuilder knitr

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bootstrapNull	<i>Bootstrap to assess significance</i>
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Description

Perform a parametric bootstrap to assess whether there is significant evidence that a sample is a mixture.

Usage

```
bootstrapNull(  
  tab,  
  n_rep = 1000,  
  interval = c(0, 1),  
  tol = 0.000001,  
  check_boundary = TRUE,  
  cores = 1,  
  return_raw = TRUE  
)
```

Arguments

tab	Dataset of read counts as 3d array of size 3x3x2, genotype in first sample x genotype in second sample x allele in read.
n_rep	Number of bootstrap replicates
interval	Interval to which each parameter should be constrained
tol	Tolerance for convergence
check_boundary	If TRUE, explicitly check the boundaries of interval.
cores	Number of CPU cores to use, for parallel calculations. (If 0, use parallel::detectCores() .) Alternatively, this can be links to a set of cluster sockets, as produced by parallel::makeCluster() .
return_raw	If TRUE, return the raw results. If FALSE, just return the p-value. Unlink bootstrapSE() , here the default is TRUE.

Value

If return_raw=FALSE, a single numeric value (the p-value). If return_raw=TRUE, a vector of length n_rep with the LRT statistics from each bootstrap replicate.

See Also

[bootstrapSE\(\)](#)

Examples

```
data(mbmixdata)
# just 100 bootstrap replicates, as an illustration
bootstrapNull(mbmixdata, n_rep=100)
```

bootstrapSE	<i>Bootstrap to get standard errors</i>
-------------	---

Description

Perform a parametric bootstrap to get estimated standard errors.

Usage

```
bootstrapSE(
  tab,
  n_rep = 1000,
  interval = c(0, 1),
  tol = 0.000001,
  check_boundary = FALSE,
  cores = 1,
  return_raw = FALSE
)
```

Arguments

tab	Dataset of read counts as 3d array of size 3x3x2, genotype in first sample x genotype in second sample x allele in read.
n_rep	Number of bootstrap replicates
interval	Interval to which each parameter should be constrained
tol	Tolerance for convergence
check_boundary	If TRUE, explicitly check the boundaries of interval.
cores	Number of CPU cores to use, for parallel calculations. (If 0, use parallel::detectCores() .) Alternatively, this can be links to a set of cluster sockets, as produced by parallel::makeCluster() .
return_raw	If TRUE, return the raw results. If FALSE, just return the estimated standard errors.

Value

If return_raw=FALSE, a vector of two standard errors. If return_raw=TRUE, an matrix of size n_rep x 2 with the detailed bootstrap results.

See Also

[bootstrapNull\(\)](#)

Examples

```
data(mbmixdata)
# just 100 bootstrap replicates, as an illustration
bootstrapSE(mbmixdata, n_rep=100)
```

mbmixdata

Example dataset for mbmixture package

Description

Example dataset for mbmixture package.

Usage

```
data(mbmixdata)
```

Format

Dataset of read counts as 3d array of size 3x3x2, genotype in first sample x genotype in second sample x allele in read.

Examples

```
data(mbmixdata)
mle_pe(mbmixdata)
```

mbmix_loglik	<i>log likelihood function for microbiome mixture</i>
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Description

Calculate log likelihood function for microbiome sample mixture model at particular values of p and e .

Usage

```
mbmix_loglik(tab, p, e = 0)
```

Arguments

tab	Dataset of read counts as 3d array of size $3 \times 3 \times 2$, genotype in first sample x genotype in second sample x allele in read.
p	Contaminant probability (proportion of mixture coming from the second sample).
e	Sequencing error rate.

Value

The log likelihood evaluated at p and e .

Examples

```
data(mbmixdata)
mbmix_loglik(mbmixdata, p=0.74, e=0.002)
```

mle_e	<i>MLE of e for fixed p</i>
-------	---

Description

Calculate the MLE of the sequencing error rate e for a fixed value of the contaminant probability p .

Usage

```
mle_e(
  tab,
  p = 0.05,
  interval = c(0, 1),
  tol = 0.000001,
  check_boundary = FALSE
)
```

Arguments

tab	Dataset of read counts as 3d array of size 3x3x2, genotype in first sample x genotype in second sample x allele in read.
p	Assumed value for the contaminant probability
interval	Interval to which each parameter should be constrained
tol	Tolerance for convergence
check_boundary	If TRUE, explicitly check the boundaries of interval.

Value

A single numeric value, the MLE of e , with the log likelihood as an attribute.

Examples

```
data(mbmixdata)
mle_e(mbmixdata, p=0.74)
```

mle_p	<i>MLE of p for fixed e</i>
-------	---

Description

Calculate the MLE of the contaminant probability p for a fixed value of the sequencing error rate e .

Usage

```
mle_p(
  tab,
  e = 0.002,
  interval = c(0, 1),
  tol = 0.000001,
  check_boundary = FALSE
)
```

Arguments

tab	Dataset of read counts as 3d array of size 3x3x2, genotype in first sample x genotype in second sample x allele in read.
e	Assumed value for the sequencing error rate
interval	Interval to which each parameter should be constrained
tol	Tolerance for convergence
check_boundary	If TRUE, explicitly check the boundaries of interval.

Value

A single numeric value, the MLE of p , with the log likelihood as an attribute.

Examples

```
data(mbmixdata)
mle_p(mbmixdata, e=0.002)
```

mle_pe	<i>Find MLEs for microbiome mixture</i>
--------	---

Description

Find joint MLEs of p and e for microbiome mixture model

Usage

```
mle_pe(
  tab,
  interval = c(0, 1),
  tol = 0.000001,
  check_boundary = FALSE,
  SE = FALSE
)
```

Arguments

tab	Dataset of read counts as 3d array of size 3x3x2, genotype in first sample x genotype in second sample x allele in read.
interval	Interval to which each parameter should be constrained
tol	Tolerance for convergence
check_boundary	If TRUE, explicitly check the boundaries of interval.
SE	If TRUE, get estimated standard errors.

Value

A vector containing the estimates of p and e along with the evaluated log likelihood and likelihood ratio test statistics for the hypotheses $p=0$ and $p=1$.

Examples

```
data(mbmixdata)
mle_pe(mbmixdata)
```

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