Package 'odseq'

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Type Package

Title Outlier detection in multiple sequence alignments

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Description Performs outlier detection of sequences in a multiple sequence alignment using bootstrap of predefined distance metrics. Outlier sequences can make downstream analyses unreliable or make the alignments less accurate while they are being constructed. This package implements the OD-seq algorithm proposed by Jehl et al (doi 10.1186/s12859-015-0702-1) for aligned sequences and a variant using string kernels for unaligned sequences.

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VignetteBuilder knitr

Suggests knitr(>= 1.11)

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Imports msa (>= 1.2.1), kebabs (>= 1.4.1), mclust (>= 5.1)

NeedsCompilation no

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odseq-package *Outlier detection in multiple sequence alignments*

Description

Performs outlier detection of sequences in a multiple sequence alignment using bootstrap of predefined distance metrics. Outlier sequences can make downstream analyses unreliable or make the alignments less accurate while they are being constructed. This package implements the OD-seq algorithm proposed by Jehl et al (doi 10.1186/s12859-015-0702-1) for aligned sequences and a variant using string kernels for unaligned sequences.

Details

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Author(s)

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References

[1] OD-seq: outlier detection in multiple sequence alignments. *Peter Jehl, Fabian Sievers and Desmond G. Higgins*. BMC Bioinformatics. 2015.

See Also

odseq odseq_unaligned

Examples

```
library(msa)
data(seqs)
al <- msa(seqs)
odseq(al, distance_metric = "affine", B = 1000, threshold = 0.025)
```

odmix *Gaussian mixture modelling of distances in a multiple sequence alignment.*

Description

This function performs clustering of biological sequences via fitting a Gaussian mixture model of the distances defined by the odseq algorithm

Usage

```
odmix(msa_object, distance_metric, groups)
```

Arguments

msa_object	An object of formal class MsaAAMultipleAlignment, as provided by the **msa** package.
distance_metric	A string indicating the type of distance metric to be computed. Either 'linear' and 'affine' is supported at the moment.
groups	Number of groups to fit in the mixture model. If a numeric vector of size n, n models will be fitted and a list of BIC values will be given to choose a single model.

Value

A list containing the following items:

prob	A numeric matrix of size n x groups where the probability of belonging to a group is provided for each sequence.
class	The class assigned according to prob. Returns a numeric vector.
BIC	BIC values for the models proposed in groups

Author(s)

José Jiménez <jose@jimenezluna.com>

See Also

odseq_unaligned odseq

Examples

```
library(msa)
data(seqs)
al <- msa(seqs)
odmix(al, distance_metric = "affine", groups = 2)
```

odseq *Outlier detection in a multiple sequence alignment*

Description

This function will first compute a distance metric among every sequence in the multiple alignment. Then it will bootstrap an average score of these distance to provide information on the distribution of scores, which is used to distinguish outlier sequences with a certain threshold

Usage

```
odseq(msa_object, distance_metric = "linear", B = 100, threshold = 0.025)
```

Arguments

`msa_object`	An object of formal class `MsaAAMultipleAlignment`, as provided by the **msa** package.
`distance_metric`	A string indicating the type of distance metric to be computed. Either `'linear'` and `'affine'` is supported at the moment.
`B`	Integer indicating the number of bootstrap replicates to be run. The higher the more robust the detection should be.
`threshold`	Float indicating the probability to be left at the right of the bootstrap scores distribution when computing outliers. This parameter may need some tuning depending on each specific problem

Value

Returns a logical vector, where `TRUE` indicates an outlier.

Author(s)

José Jiménez <jose@jimenezluna.com>

References

[1] OD-seq: outlier detection in multiple sequence alignments. *Peter Jehl, Fabian Sievers and Desmond G. Higgins*. BMC Bioinformatics. 2015.

See Also

`odseq_unaligned`

Examples

```
library(msa)
data(seqs)
al <- msa(seqs)
odseq(al, distance_metric = "affine", B = 1000, threshold = 0.025)
```

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odseq_unaligned *Outlier detection provided a distance/similarity matrix of sequences.*

Description

Provided a similarity matrix (like the ones provided using string kernels in **kebabs**). It will then compute a score for each sequence and perform bootstrap to provide information on the distribution of the scores, which is used to distinguish outlier sequences.

Usage

```
odseq_unaligned(distance_matrix, B = 100, threshold = 0.025, type = "similarity")
```

Arguments

distance_matrix	A numeric matrix representing either similarity or distance among unaligned sequences. Package **kebabs** may be useful for this task.
B	Integer indicating the number of bootstrap replicates to be run. The higher the more robust the detection should be.
threshold	Float indicating the probability to be left at the right of the bootstrap scores distribution when computing outliers. This parameter may need some tuning depending on each specific problem
type	A string indicating the type of distance metric used. Either `'similarity'` or `'distance'`.

Value

Returns a logical vector, where `TRUE` indicates an outlier.

Author(s)

José Jiménez <jose@jimenezluna.com>

References

[1] OD-seq: outlier detection in multiple sequence alignments. *Peter Jehl, Fabian Sievers and Desmond G. Higgins*. BMC Bioinformatics. 2015.

See Also

odseq

Examples

```
library(kebabs)
data(seqs)
sp <- spectrumKernel(k = 3)
mat <- getKernelMatrix(sp, seqs)
odseq_unaligned(mat, B = 1000, threshold = 0.025, type = "similarity")
```

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seqs *PFAM plus random data.*

Description

Sequences from a certain PFAM family plus 100 random sequences.

Usage

```
data("seqs")
```

Value

An object of class `AAStringSet`.

Examples

```
data(seqs)
```

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