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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LazyData True

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VignetteBuilder knitr

Suggests knitr(>= 1.11)

Depends R (>= 3.2.3)

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

NeedsCompilation no

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**R topics documented:**

- odseq-package
- odmix
- odseq
- odseq_unaligned
- seqs

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**Description**

Performs outlier detection of sequences in a multiple sequence alignment using bootstrap of pre-defined 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**

The DESCRIPTION file: This package was not yet installed at build time.

Index: This package was not yet installed at build time.

**Author(s)**

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**References**


**See Also**

- odseq
- odseq_unaligned

**Examples**

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

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See Also

`odseq_unaligned odseq`

Examples

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


See Also

odseq_unaligned
Examples

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

Description

Outlier detection provided a distance/similarity matrix of sequences.

Usage

```r
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

A logical vector, where TRUE indicates an outlier.

Author(s)

José Jiménez <jose@jimenezluna.com>

References


See Also

odseq
Examples

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

Description

Sequences from a certain PFAM family plus 100 random sequences.

Usage

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

Value

An object of class AAStringSet.

Examples

```r
data(seqs)
```
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