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

Encoding UTF-8

biocViews Alignment, MultipleSequenceAlignment

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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**odseq-package**

**Outlier detection in multiple sequence alignments**

**Description**

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**Details**

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- **odmix**  Gaussian mixture modelling of distances in a multiple sequence alignment.
- **odseq**  Outlier detection in a multiple sequence alignment
- **odseq-package**  Outlier detection in multiple sequence alignments
- **odseq_unaligned**  Outlier detection provided a distance/similarity matrix of sequences.
- **seqs**  PFAM plus random data.

**Author(s)**

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odmix

References


See Also

odseq odseq_unaligned

Examples

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

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)

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


See Also

odseq_unaligned
Examples

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

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

```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

Returns 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")
```

seqs  
---
PFAM plus random data.

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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