

Package ‘odseq’

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Type Package

Title Outlier detection in multiple sequence alignments

Version 1.6.0

Date 2015-12-20

Author José Jiménez

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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**

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:

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Depends:          R (>= 3.2.3)
Imports:          msa (>= 1.2.1), kebabs (>= 1.4.1), mclust (>= 5.1)
NeedsCompilation: no
```

Index of help topics:

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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)

José Jiménez

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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 | <i>Gaussian mixture modelling of distances in a multiple sequence alignment.</i> |
|-------|--|

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 <code>MsaAAMultipleAlignment</code> , 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

| | |
|------------------------------|---|
| <code>msa_object</code> | An object of formal class <code>MsaAAMultipleAlignment</code> , as provided by the msa package. |
| <code>distance_metric</code> | A string indicating the type of distance metric to be computed. Either 'linear' and 'affine' is supported at the moment. |
| <code>B</code> | Integer indicating the number of bootstrap replicates to be run. The higher the more robust the detection should be. |
| <code>threshold</code> | 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)
```

| | |
|-----------------|--|
| odseq_unaligned | <i>Outlier detection provided a distance/similarity matrix of sequences.</i> |
|-----------------|--|

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")
```

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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