Package 'COUSCOus'

February 28, 2016

Type Package

Title A Residue-Residue Contact Detecting Method

Version 1.0.0

Date 2016-02-17

Author Reda Rawi [aut,cre], Matyas A. Sustik [aut], Ben Calderhead [aut]

Maintainer Reda Rawi <rrawi@qf.org.qa>

Description Contact prediction using shrinked covariance (COUSCOus). COUSCOus is a residue-residue contact detecting method approaching the contact inference using the glassofast implementation of Matyas and Sustik (2012, The University of Texas at Austin UTCS Technical Report 2012:1-3. TR-12-29.) that solves the L_1 regularised Gaussian maximum likelihood estimation of the inverse of a covariance matrix. Prior to the inverse covariance matrix estimation we utilise a covariance matrix shrinkage approach, the empirical Bayes covariance estimator, which has been shown by Haff (1980) <DOI:10.1214/aos/1176345010> to be the best estimator in a Bayesian framework, especially dominating estimators of the form aS, such as the smoothed covariance estimator applied in a related contact inference technique PSICOV.

Repository CRAN

License GPL (>= 3)

Imports bio3d (>= 2.2-2), matrixcalc (>= 1.0-3), utils (>= 3.2.2)

Depends R (>= 3.2.2)

NeedsCompilation yes

Date/Publication 2016-02-28 16:26:52

R topics documented:

COUSCOus   *Contact prediction using shrinked covariance.*

Description

COUSCOus is a residue-residue contact detecting method.

Usage

```
COUSCOus(fasta.file, verbose = TRUE)
```

Arguments

fasta.file   Protein sequence alignment file name in FASTA format.

verbose   Print tracing information. The default value is TRUE.

Details

Contact prediction using shrinked covariance (COUSCOus). COUSCOus is a residue-residue contact detecting method approaching the contact inference using the glassofast implementation of Matyas and Sustik (2012, The University of Texas at Austin UTCS Technical Report 2012:1-3. TR-12-29.) that solves the L_1 regularised Gaussian maximum likelihood estimation of the inverse of a covariance matrix. Prior to the inverse covariance matrix estimation we utilise a covariance matrix shrinkage approach, the empirical Bayes covariance estimator, which has been shown by Haff (1980) <DOI:10.1214/aos/1176345010> to be the best estimator in a Bayesian framework, especially dominating estimators of the form aS, such as the smoothed covariance estimator applied in a related contact inference technique PSICOV.

Value

A data frame with 3 columns (i, j, pCorr) containing all possible pairs of residues along with their COUSCOus correlation value.

Author(s)

Reda Rawi, Matyas A. Sustik, Ben Calderhead
Maintainer: Reda Rawi <rrawi@qf.org.qa>

Examples

```
# Alignment file
file.fasta <- system.file( "examples/1oaiA0.fa", package = "COUSCOus" )

# Run COUSCOus
df.predictions <- COUSCOus( file.fasta )
```

COUSCOus-internal	*Internal COUSCOus functions*

Description

Internal COUSCOus functions

Details

These are not intended for usage. Please refer to COUSCOus()

Author(s)

Reda Rawi
Maintainers: Reda Rawi <redarawi@gmx.de>

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