

Package ‘BioPhysConnectoR’

February 19, 2015

Version 1.6-10

Date 2013-01-09

Title BioPhysConnectoR

Author Franziska Hoffgaard <hoffgaard@bio.tu-darmstadt.de>, with contributions from Philipp Weil <weil@bio.tu-darmstadt.de> and Kay Hamacher <hamacher@bio.tu-darmstadt.de>

Maintainer Frank Keul <keul@bio.tu-darmstadt.de>

Depends R (>= 2.11.0), snow, matrixcalc

Description Utilities and functions to investigate the relation between biomolecular structures, their interactions, and the evolutionary information revealed in sequence alignments of these molecules.

License GPL-2

Repository CRAN

Date/Publication 2013-01-09 17:22:13

NeedsCompilation yes

R topics documented:

BioPhysConnectoR-package	2
aa2num	4
build.contacts	5
build.hess	6
build.interact	7
extractPDB	8
fnorm	9
get.bfacs	10
get.contact.list	11
get.entropy	12
get.freqs	13
get.mie	15
get.svd	16

invhess	17
lbpc	18
mat.norm	19
mat.read	19
mat.sort	20
mat.write	21
read.fasta	22
scpcp	23
show.code	24
sim	25
simc	26
sims	28

Index 31

BioPhysConnectoR-package

BioPhysConnectoR

Description

Functions to investigate the relation between biomolecular structures, their interactions, and the evolutionary information contained within sequence alignments of such molecules.

Details

Package: BioPhysConnectoR
 Version: 1.6-7
 Date: 2011-11-03
 Depends: R (>= 2.11.0), snow, matrixcalc
 License: GPL 2
 Packaged: 2010-23-09 13:50:31 UTC;weil
 Built: R 2.12.1; x86_64-pc-linux-gnu; 2011-11-03 16:55:01 UTC; unix

Index:

aa2num	Conversion of Amino Acids into Integer Values
BioPhysConnectoR-package	BioPhysConnectoR
build.contacts	Determine the Contact Map and Distance Matrices
build.hess	Construct the Hessian Matrix
build.interact	Compute the Interaction Matrix
build.invhess	Compute the Covariance Matrix / Inverse Hessian Matrix
extractPDB	Extract Data from a PDB-File
fnorm	Frobenius Norm of Two Matrices
get.bfacs	Determine B factors

get.contact.list	Returns a List of Contacts for a given Contact Map
get.cov	Compute the Covariance Matrix / Inverse Hessian Matrix
get.entropy	Compute the Sequence Entropy for an Alignment
get.freqs	Compute the Frequencies in an Alignment
get.mie	Mutual Information
get.svd	Singular Value Decomposition
lbpc	List the Functions of the BioPhysConnectoR Package
mat.norm	Normalisation of a Matrix
mat.read	Read Matrix Data from a File
mat.sort	Sort a Matrix According to a Specified Column
mat.write	Writes Matrix Data to a File
read.fasta	Reads aligned or un-aligned sequences from a FASTA format file
scpcp	Self-Consistent Pair Contact Probability Approximation
show.code	Output of the Amino Acid Coding Scheme
sim	Compute the Correlation Matrix and B Factors for a List of PDBs
simc	Computed Elastic Network Models for Switched-Off-List of Contacts
sims	Apply a List of Different Amino Acid Sequences

Author(s)

Franziska Hoffgaard <hoffgaard@bio.tu-darmstadt.de>, with contributions from Philipp Weil <weil@bio.tu-darmstadt.de> and Kay Hamacher <hamacher@bio.tu-darmstadt.de>

Maintainer: Franziska Hoffgaard <hoffgaard@bio.tu-darmstadt.de>

References

- Hoffgaard, Weil, Hamacher (2010) *BMC Bioinformatics* 11, 199.
 Hamacher (2006) *Journal of Chemical Theory and Computation* 2, 873–878.
 Hamacher (2008) *Gene* 422, 30–36.
 Hamacher (2009) *Eur. Biophys. J.*, in press.
 Grant, Rodrigues, ElSawy, McCammon, Caves, (2006) *Bioinformatics* 22, 2695–2696.
 Tierney, Rossini, Li (2009) *Int J Parallel Proc* 37, 78–90.
 Novomestky (2008) *matrixcalc*.
 Newman (2002) *Physical Review Letters* 89, 208701-1 – 208701- 4.
 Miyazawa, Jernigan (1996) *Journal of Molecular Biology* 256, 623–644.
 Keskin, Bahar, Badretdinov, Ptitsyn, Jernigan (1998) *Protein Science* 7, 2578–2586.
 Shannon (1948) *The Bell System Technical Journal* 27, 379–423

`aa2num`*Conversion of Amino Acids into Integer Values*

Description

A sequence containing standard amino acids is converted into a sequence of integer values. An offset for the code can be specified.

Usage

```
aa2num(seq, offset = 0, code = 0:19, verbose = FALSE)
```

Arguments

<code>seq</code>	string vector containing a sequence of standard amino acids
<code>offset</code>	offset, added to the specified code
<code>code</code>	integer vector of the values to be assigned to the amino acids
<code>verbose</code>	logical, if TRUE the specific encoding is printed

Details

The default values for the code are the integer values in the range 0 to 19. It is possible to use another numerical code for the 20 amino acids. The default coding order of the amino acids is: CYS, MET, PHE, ILE, LEU, VAL, TRP, TYR, ALA, GLY, THR, SER, ASN, GLN, ASP, GLU, HIS, ARG, LYS, PRO. Each amino acid is converted to a single element according to the code-vector. The offset `offset` is added. Both sequences with three-letter and one-letter code can be handled.

Value

Returns a sequence of integer values according to the given numerical code.

Note

The function assigns values only for the standard amino acids. This function includes source code of the **bio3d** package.

Author(s)

Franziska Hoffgaard

References

Grant, Rodrigues, ElSawy, McCammon, Caves, (2006) *Bioinformatics* 22, 2695–2696.

See Also

[show.code](#)

Examples

```
seq<-c("MET", "GLY", "PRO", "LYS", "ASN")
aa2num(seq)
```

build.contacts	<i>Determine the Contact Map and Distance Matrices</i>
----------------	--

Description

Computation of a binary matrix specifying the contacts between each two amino acids i and j in respect to their spatial distance defined by their coordinates. Distance matrices for Δx , Δy and Δz are computed as well as the matrix containing the squared distances for all amino acid pairs.

Usage

```
build.contacts(n, cuts, xyz)
```

Arguments

n	length of the amino acid sequence
cuts	squared cutoff
xyz	matrix with the x-, y- and z-coordinates of all C_α atoms of the protein

Details

If the squared distance between two C_α atoms of amino acids i and j is smaller than or equal to cuts, we assume a contact. In the contact map the value at indices $[i, j]$ and $[j, i]$ is set to 1. Otherwise, the two C_α atoms are not in contact, and the value is set to 0. Per definition an atom is not in contact with itself. The contact map is a symmetric matrix. The matrices in `$deltas` (`$dx`, `$dy` and `$dz` and `$ds`) are symmetric matrices as well. The number of contacts between distinct amino acids is stored in `$cnr`.

Value

Return value is a list with the following components:

<code>\$cm</code>	contact map
<code>\$deltas</code>	list with distance matrices for x-, y- and z-direction as well as for the squared distance between all pairs of C_α atoms
<code>\$cnr</code>	number of contacts

Author(s)

Franziska Hoffgaard

See Also[get.contact.list](#)**Examples**

```
n<-10
xyz<-matrix(rep(1:10, 3), ncol = 3)
bc<-build.contacts(n, 3, xyz)
```

`build.hess`*Construct the Hessian Matrix*

Description

The Hessian matrix is computed using the interaction matrix, the contact map, and the coordinate differences.

Usage

```
build.hess(cm, im, deltas)
```

Arguments

<code>cm</code>	contact map
<code>im</code>	interaction map
<code>deltas</code>	list of difference matrices computed with <code>build.contacts</code>

Details

For a sequence of length n a $3n \times 3n$ matrix is computed. Only if amino acids are in contact (`cm` entry equals 1) values for the Hessian matrix are computed as proposed in Hamacher (2006). If amino acids are not in contact their respective matrix entries equal 0. Values for amino acids in contact depend on coordinate differences and interaction strengths.

Value

Return value is the Hessian Matrix.

Author(s)

Franziska Hoffgaard

References

Hamacher (2006) *Journal of Chemical Theory and Computation* 2, 873–878.

See Also

[build.interact](#), [build.contacts](#)

build.interact *Compute the Interaction Matrix*

Description

Calculation of the interaction strength between all amino acids of a protein.

Usage

```
build.interact(cseq, mj1, mj2 = mj1, d, alpha = 82)
```

Arguments

cseq	(coded) amino acid sequence
mj1	matrix for intrachain interactions between amino acids
mj2	matrix for interchain interactions between amino acids
d	vector of chain lengths
alpha	strength of the peptide bond

Details

Per default only one matrix with interaction strengths between amino acids is used to compute the interaction map. But it is possible to differentiate between intrachain [Miyazawa and Jernigan (1996)] and interchain [Keskin et al. (1998)] interactions by using an additional interaction matrix. Both matrices are included in the package and can be used directly. The value of *d* specifies the lengths of the different chains in the sequence.

Per definition there is no interaction between an amino acid and itself, therefore the diagonal is set to zero. All entries that represent peptide bonds between two amino acids are set to *alpha* (only entries in the off-diagonals). The input of *cseq* can be a numeric sequences [0, 19] as well as a string vector of standard amino acid sequences in one or three-letter code.

Value

Return value is a symmetric matrix specifying the interactions between the amino acids. If *n* is the length of the sequence, the matrix dimension results in $n \times n$.

Note

Choosing one's own matrices for inter- and intrachain interactions requires some thought: this function only deals with the standard amino acids thus it requires always symmetric, 20×20 matrices.

Author(s)

Franziska Hoffgaard

References

- Miyazawa and Jernigan (1996) *Journal of Molecular Biology* 256, 623–644.
Hamacher (2006) *Journal of Chemical Theory and Computation* 2, 873–878.
Keskin, Bahar, Badretdinov, Ptitsyn and Jernigan (1998) *Protein Science* 7, 2578–2586.

See Also

[aa2num](#)

Examples

```
#Miyazawa/Jernigan matrix
mat<-as.matrix(read.table(system.file("mj1.txt", package = "BioPhysConnectoR")))

#Keskin matrix
mat2<-as.matrix(read.table(system.file("mj2.txt", package = "BioPhysConnectoR")))

cseq<-rep(1:5, 2)
d<-c(5, 5)
im<-build.interact(cseq = cseq, mj1 = mat, mj2 = mat2, d = d)
```

extractPDB

Extract Data from a PDB-File

Description

This function reads a PDB file and extracts data from it.

Usage

```
extractPDB(file.name, verbose = TRUE)
```

Arguments

file.name	name of the PDB file
verbose	logical, if TRUE prints the output from both functions <code>read.pdb()</code> and <code>atom.select()</code> .

Details

The input PDB file is read. All C_{α} atoms are extracted. For each C_{α} atom the x-, y- and z-coordinates as well as the amino acid type and the B factor are extracted. The sequence length is compared to the number of C_{α} atoms in the PDB. For each chain of the protein the length is computed.

Value

Returns a list with the following components:

pdb	list of class “pdb” as originally extracted by read.pdb() in the bio3d package
seq	sequence according to the “SEQRES” entries of the PDB file
lseq	length of the extracted sequence seq
lca	number of C_α atoms
caseq	sequence data for the C_α selection
coords	matrix of coordinates for each C_α atom, the rows are the C_α 's, the columns are x, y, z
b	B factor for each C_α
chains	integer vector with the lengths of the different chains in the protein sequence

Note

Alternate and insert records in the PDB file are ignored. When removing alternate records a message is printed. Please check the PDB file.

If the number of C_α atoms lca and the length of the extracted sequence seq differ, a message is printed. It is not advisable to use any other parts of the BioPhysConnectoR-package until you have found an appropriate solution to deal with this problem in the pdb-file.

This function includes source code of the **bio3d** package.

Author(s)

Franziska Hoffgaard

References

Grant, Rodrigues, ElSawy, McCammon, Caves, (2006) *Bioinformatics* 22, 2695–2696.

Examples

```
pdb<-extractPDB(system.file("1KZK.pdb", package = "BioPhysConnectoR"))
```

fnorm

Frobenius Norm of Two Matrices

Description

Computation of the Frobenius norm of two matrices as the sum of the squared differences between these matrices.

Usage

```
fnorm(mat1, mat2)
```

Arguments

mat1	numerical matrix
mat2	numerical matrix

Value

Return value is the Frobenius norm.

Note

Both input matrices must have the same dimensions.

Author(s)

Franziska Hoffgaard

Examples

```
a<-matrix(runif(15, 1, 7), 5, 3)
b<-matrix(rnorm(15, 1, 7), 5, 3)
fn<-fnorm(a, b)
```

get.bfacs

Determine B factors

Description

The function calculates B factors from the inverse Hessian matrix.

Usage

```
get.bfacs(covmat)
```

Arguments

covmat	inverse Hesse matrix
--------	----------------------

Details

The B factors for each C_{α} atom are computed from the diagonal of the covariance matrix by summing up the corresponding entries.

Value

Return value is a vector with the B factors for each C_α .

Author(s)

Franziska Hoffgaard

See Also

[build.invhess](#)

Examples

```
#extract the example pdb
pdb<-extractPDB(system.file("1KZK.pdb", package = "BioPhysConnectoR"))

#build the contact matrix for a given squared cutoff of 169
bc<-build.contacts(pdb$lca, 169, pdb$coords)

#for this example we use the fictitious value 12 as interaction strength
interaction.mat<-build.interact(cseq = rep(0, 198), mj1 = matrix(12, 20, 20),
d = pdb$chains)

#compute the inverse hessian matrix
cov.mat<-get.cov(cm = bc$cm, im = interaction.mat, deltas = bc$deltas)
bfac<-get.bfacs(cov.mat)
```

get.contact.list *Returns a List of Contacts for a given Contact Map*

Description

From a given contact map a list of contacts is computed.

Usage

```
get.contact.list(cm, d = NULL, single = TRUE, val = 1)
```

Arguments

cm	binary matrix which specifies which amino acid position are in contact
d	vector specifying the last amino acids of each chain
single	bool, if TRUE only indices $i < j$ are returned
val	numeric value, indices of matrix entries with this value are returned

Details

All amino acid pairs with `cm[i, j] == val` are extracted from the `cm`. Each pair is listed once $[i, j] = [j, i]$ (if `single = TRUE`) with $i < j$. If `d` is specified the contacts of the off-diagonal (peptide bonds) are left out, otherwise they will be returned as well. The values of `d` are the indices of the off-diagonal entries that do not represent a peptide bond.

Value

Return value is a list with the indices of all pairs of amino acids that fulfill the above stated condition.

Author(s)

Franziska Hoffgaard

See Also

[build.contacts](#), [simc](#)

Examples

```
mat<-matrix(c(0, 0, 1, 1, 1, 0, 0, 1, 0, 0, 1, 1, 0, 0, 1, 1, 0, 0, 0,
              0, 1, 0, 1, 0, 0), ncol = 5)
get.contact.list(mat)
```

get.entropy

Compute the Sequence Entropy for an Alignment

Description

Computes the sequence entropy of an alignment. It is possible to specify which characters to omit in the computation. The joint entropy is computed using `get.entropy2p()`.

Usage

```
get.entropy(aln, bool = FALSE, gapchar = "NOGAPCHAR",
            verbose = FALSE)
```

```
get.entropy2p(aln, bool = FALSE, gapchar = "NOGAPCHAR",
              verbose = FALSE)
```

Arguments

<code>aln</code>	alignment matrix
<code>bool</code>	logical, if TRUE gaps are ignored when computing the entropy of each column of the alignment
<code>gapchar</code>	character vector containing the unique set of characters representing gaps in the amino acid sequence
<code>verbose</code>	logical, TRUE for getting output messages

Details

The Shannon (1948) entropy for an alignment is computed as follows:

$$H(X) = - \sum_{x \in X} p(x) \cdot \log_2(p(x))$$

The joint entropy is computed for every possible column pair:

$$H(X, Y) = - \sum_{x \in X} \sum_{y \in Y} p(x, y) \cdot \log_2(p(x, y))$$

where X and Y are two columns of the alignment.

Value

Return value for `get.entropy()` is a vector containing the entropy for each column.

Return value for `get.entropy2p()` is a matrix containing the joint entropies in the lower triangle.

Author(s)

Franziska Hoffgaard

References

Shannon (1948) *The Bell System Technical Journal* 27, 379–423.

See Also

[get.mie](#)

Examples

```
a1n<-matrix(c("M", "H", "X", "P", "V", "-", "H", "X", "L", "V", "M", "L",
"X", "P", "V"), 3, byrow = TRUE)
h1<-get.entropy(a1n, bool = TRUE , gapchar = "-")
h2<-get.entropy(a1n)

h3<-get.entropy2p(a1n)
```

get.freqs

Compute the Frequencies in an Alignment

Description

One and two point frequencies of a specified column or specified columns are computed for a given alignment.

Usage

```
freq1p(aln, i = NULL)
```

```
freq2p(i, aln, j2 = NULL, lett = NULL, cluster = NULL)
```

Arguments

aln	alignment
i	reference column for the frequency computation
j2	columns to compute the two point frequency together with column i
lett	character vector containing the unique alphabet of the alignment
cluster	snow cluster object created with makeCluster()

Details

The columns j2 are the specified columns (not i) to compute the frequencies and the rows represent all possible two letter pairs according to the alphabet. The computation of freq2p() is parallelized using parLapply() from the package **snow**. If cluster is left at its default value the computation is carried out in serial.

Value

A matrix is returned for the freq2p(). For freq1p(), if no i is specified, a matrix containing the frequencies of the symbols in the alignment is returned. For a certain i a vector with the respective frequencies of the symbols is the result.

Author(s)

Franziska Hoffgaard, Philipp Weil

References

Tierney, Rossini, Li (2009) *Int J Parallel Proc* 37, 78–90.

See Also

[get.entropy](#), [get.mie](#)

Examples

```
seqa<-unlist(strsplit("PQITLWQRPLVTIKIGGQL",split=""))
seqb<-unlist(strsplit("PQITLWKRPLVTIRIGGQL",split=""))
seqc<-unlist(strsplit("PQITLWQRPLVTIKIGGQL",split=""))
aln<-matrix(c(seqa,seqb,seqc),nrow=3,byrow=TRUE)
f1<-freq1p(aln)
f1a<-freq1p(aln, 1)
f2<-freq2p(1, aln, 2:10)
## Not run:
```

```
## Cluster example
clu<-makeCluster(2)
f2<-freq2p(1, aln, 2:10, cluster=clu)
stopCluster(clu)

## End(Not run)
```

get.mie

*Mutual Information***Description**

The joint information content (mutual information) for an alignment is computed. Considering the gap problem there are four ways to compute it.

Usage

```
get.mie(aln, method = "ORMI", gapchar = NULL, nullmod = NULL, logMI = FALSE)
```

Arguments

aln	matrix of which the mutual information will be computed
method	method, that is used for the computation (see details)
gapchar	symbols of the input matrix that should be handled as gaps. These symbols are omitted in the computations (see details)
nullmod	integer specifying how many shuffle runs should be performed
logMI	boolean, if TRUE the log(MI) will be calculated, default is FALSE

Details

Methods: The mutual information (MI) is computed as follows:

$$I(X, Y) = \sum_{x \in X} \sum_{y \in Y} p(x, y) \cdot \log_2 \left(\frac{p(x, y)}{p(x) \cdot p(y)} \right)$$

$$I(X, Y) = H(X) + H(Y) - H(X, Y)$$

ORMI In the ORiginal MI gaps are treated simply as any other character.

SUMI The SUBset MI omits for each pair of columns all the rows with at least one gap character for the computation.

DEMI In the Delta Entropy MI the entropies for the columns are computed separately by leaving out any gap characters. The joint entropy also considers only rows without any gap character. DEMI follows as $H(X) + H(Y) - H(X, Y)$.

ESMI The Enhanced Sampling MI omits the gap characters and rows with gaps for the computation of the probabilities. The information content is computed via the probabilities.

The null model is computed by shuffling each column content and computing the resulting MI. Over all shuffle runs the MI values in each entry of the matrix is averaged. The averaged squared MI values and the variance is computed as well.

Value

Return value is the MI matrix per default.

If a null model should be computed the returned value is a list of matrices.

<code>\$mi</code>	MI matrix
<code>\$nullmodel</code>	MI matrix of the null model
<code>\$nullsquare</code>	matrix of the averaged MI squared values for the null model
<code>\$nullvar</code>	matrix of the variance of each MI value over the whole shuffle run for the null model

Author(s)

Franziska Hoffgaard

See Also

[get.entropy](#), [get.entropy2p](#), [freq1p](#), [freq2p](#)

Examples

```

seqa<-unlist(strsplit("PQITLWQRPLVTIKIGGQL",split=""))
seqb<-unlist(strsplit("PQITLWKRPLVTIRIGGQL",split=""))
seqc<-unlist(strsplit("PQITLWQRPLVTIKIGGQL",split=""))
a<-matrix(c(seqa,seqb,seqc),nrow=3,byrow=TRUE)
mi<-get.mie(a)
mi2<-get.mie(a, method = "SUMI", gapchar = "-")
mi_null<-get.mie(a,nullmod=100)
mi2_null<-get.mie(a, method = "SUMI", gapchar = "-",nullmod=100)

```

get.svd

Singular Value Decomposition

Description

Computation of the singular value decomposition for a matrix. Sorts the eigenvalues in ascending order by maintaining their original order in an index array.

Usage

```
get.svd(hessian.mat, linalg = TRUE)
```

Arguments

<code>hessian.mat</code>	input matrix is a Hessian matrix
<code>linalg</code>	logical, specifies whether LINPACK or LAPACK routines are used

Value

Return value is a list with the following components:

<code>\$v</code>	matrix with eigenvectors in each column
<code>\$indx</code>	index array for the sorted eigenvalues
<code>\$ev</code>	vector with the sorted eigenvalues
<code>\$u</code>	matrix with eigenvectors in each column

Note

This function uses the `svd()` function of R.

Author(s)

Franziska Hoffgaard

See Also

[mat.sort](#), [build.hess](#)

Examples

```
a<-matrix(round(runif(9, 1, 5)), 3, 3)
out<-get.svd(a)
```

invhess

Compute the Covariance Matrix / Inverse Hessian Matrix

Description

Computes the inverse Hessian matrix. The covariance matrix is computed as a pseudo-inverse derived from the eigenvalues and eigenvectors by a singular value decomposition (`get.svd()`) of the Hessian matrix. Otherwise, if neither the Hessian matrix nor the eigenvalues need to be stored, the inverse Hessian can directly be computed from the contact, interaction and distance matrices.

Usage

```
build.invhess(svd_obj, singularity = 6)

get.cov(cm, im, deltas)
```

Arguments

svd_obj	svd object computed by <code>get.svd()</code> containing the eigenvector matrices, the eigenvalues and the index vector
singularity	number of eigenvalues equal/close to zero due to symmetries
cm	contact map for a protein
im	matrix of interaction strengths between the amino acids of the protein
deltas	difference matrices (x, y, z, squared) for all pairs of C_α atoms as derived from <code>build.contacts()</code>

Details

The calculation of the matrix omits by default the first six eigenvalues, because of translational and rotational symmetry in the model. The computation depends on the eigenvalues and -vectors. The number of eigenvalues to omit in the calculation can be specified by `singularity`. If the number of eigenvalues equalling zero is unknown and should be determined, the parameter `singularity` can be set to NULL. The threshold for zero is set to 10^{-8} .

Value

Return value is the covariance matrix (also called inverse Hessian matrix).

Author(s)

Franziska Hoffgaard

References

Hamacher (2006) *Journal of Chemical Theory and Computation* 2, 873–878.

See Also

[build.hess](#), [get.svd](#)

lbpc

List the Functions of the BioPhysConnectoR Package

Description

A shortcut for `ls("package:BioPhysConnectoR")` to get an overview of the implemented functions.

Usage

`lbpc()`

Value

No return value. Prints the function names.

Author(s)

Franziska Hoffgaard

`mat.norm`*Normalization of a Matrix*

Description

A matrix is normalized by dividing each entry $[i, j]$ by the square root of the product of the diagonal entries $[i, i]$ and $[j, j]$. The input matrix should be a square matrix with positive diagonal entries.

Usage

```
mat.norm(mat)
```

Arguments

`mat` numerical matrix to be normalized

Value

The normalized matrix is returned.

Author(s)

Franziska Hoffgaard

Examples

```
a<-matrix(runif(16, 1, 15), 4, 4)
b<-mat.norm(a)
```

`mat.read`*Read Matrix Data from a File*

Description

A matrix is constructed from a specified input file.

Usage

```
mat.read(file.name, ij = FALSE, sym = FALSE)
```

Arguments

file.name	file name
ij	logical, if TRUE the format in the file is: $i \ j \ value$, otherwise each row of the file represents one row in the matrix
sym	logical, if TRUE the matrix is symmetric, only important if $ij = TRUE$

Details

There are two ways a matrix can be specified in the input file. If each line represents a row in the matrix (default), the matrix can simply be read. Otherwise it is possible to have an input file with the form: $i \ j \ value$, this means the value at position $[i, j]$ of the matrix is set to $value$. If $ij = TRUE$ and $sym = TRUE$ only one half of the matrix needs to be provided.

Value

Return value is the matrix.

Author(s)

Franziska Hoffgaard

 mat.sort

Sort a Matrix According to a Specified Column

Description

Sorts a matrix in respect to one or more specified columns by preserving its row context. If more than one columns is given the function uses the columns in the specified order for sorting.

Usage

```
mat.sort(mat, sort, decreasing = FALSE)
```

Arguments

mat	matrix to be sorted
sort	column indices
decreasing	logical, if TRUE the column is ordered decreasingly

Value

Returns the sorted matrix.

Author(s)

Franziska Hoffgaard

Examples

```

mat<-matrix(data = as.integer(runif(16, 1, 20)), nrow = 4)

#Sort the matrix in respect to the second column of mat
m<-mat.sort(mat, 2)

#Sorting mat according to more than one column
mat<-matrix(data = c(rep(3, 3), as.integer(runif(13, 1, 20))), nrow = 4)
m1<-mat.sort(mat, c(1, 2))
m2<-mat.sort(mat, c(2, 1))

```

mat.write	<i>Writes Matrix Data to a File</i>
-----------	-------------------------------------

Description

Matrix data are written to a specified output file.

Usage

```
mat.write(mat, file.name, ij = FALSE, sym = FALSE, sparse=FALSE, formatted=TRUE)
```

Arguments

mat	matrix which should be written
file.name	file name
ij	logical, if TRUE the format in the file will be: <i>i j value</i> , otherwise each row of the file represents one row in the matrix
sym	logical, if TRUE the matrix is symmetric, only important if ij = TRUE
sparse	logical, if TRUE the matrix is written in sparse format (e.g. only non-zero values are written to the file), only important if ij = TRUE
formatted	logical, if TRUE a blank line is inserted after all entries of one row, only important if ij = TRUE

Details

In general there are two ways the output file can be written. First the matrix can be written to the file as `write.table` does and second the file can be written with the form: *i j value*, this means the value at position $[i, j]$. If the latter by `ij = TRUE` is selected, three more options can be chosen. If `sym = TRUE` the output file just contains the upper triangle and the diagonal of the matrix. If `sparse = TRUE` only non-zero values are written. If `formatted = TRUE` a blank line separates the entries of different rows.

Value

No values are returned.

Author(s)

Philipp Weil

See Also[mat.read](#)

read.fasta	<i>Read FASTA formatted Sequences</i>
------------	---------------------------------------

Description

Read aligned or un-aligned sequences from a FASTA format file.

Usage

```
read.fasta(file, rm.dup = TRUE, to.upper = FALSE, to.dash=TRUE)
```

Arguments

file	input sequence file.
rm.dup	logical, if TRUE duplicate sequences (with the same names/ids) will be removed.
to.upper	logical, if TRUE residues are forced to uppercase.
to.dash	logical, if TRUE '.' gap characters are converted to '-' gap characters.

Value

A list with two components:

ali	an alignment character matrix with a row per sequence and a column per equivalent aminoacid/nucleotide.
ids	sequence names as identifiers.

Note

For a description of FASTA format see: http://www.ebi.ac.uk/help/formats_frame.html.
When reading alignment files, the dash '-' is interpreted as the gap character.

Author(s)

Barry Grant

ReferencesGrant, B.J. et al. (2006) *Bioinformatics* **22**, 2695–2696.

scpcp

*Self-Consistent Pair Contact Probability Approximation***Description**

The model of the Self-Consistent Pair Contact Probability (SCPCP) (Micheletti et al., 2001; Hamacher et al., 2006) computes equilibrium properties of structures with known native states. For a given contact map, extracted from a PDB file or artificially created, the fraction of native contacts, the free and internal energies are computed as well as the degree to which an amino acid is in its native state conformation. The maximum number of iteration and the preferred accuracy for the approximation can be specified.

Usage

```
scpcp(T, R, cm, pstart = 0.5, maxiter = 2000, chains=NULL, maxtol = 1e-11,
      file = NULL, im = NULL)
```

Arguments

T	temperature
R	distance cutoff between current and native state
cm	contact map
pstart	initial probability value
chains	vector denoting the chain lengths
maxiter	maximum number of iterations
maxtol	tolerance
file	output file name
im	interaction matrix

Details

Results of each iteration as well as the final results are written into the given output file.

Value

Returns a list with the following components

\$free	free energy
\$intern	internal energy
\$entropy	entropy
\$q	fraction of native contacts
\$bfacs	vector containing the B factors
\$pi	probability vector
\$gmat	resulting G matrix
\$iter	number of iterations
\$err	deviation of probabilities

Author(s)

Franziska Hoffgaard

References

Micheletti, Banavar, Maritan (2001) *Physical Review Letters* 87, 088102-1.
Hamacher, Trylska, McCammon (2006) *PLoS Computational Biology* 2, e10.
Hamacher (2009) *Eur. Biophys. J.*, in press.

Examples

```
## Not run:
p<-extractPDB(system.file("1KZK.pdb", package = "BioPhysConnectoR"))
cm<-build.contacts(n = p$lca, xyz = p$coords, cuts = 169)$cm
chains<-p$chains
im<-build.interact(cseq=p$cseq,d=chains,mj1=matrix(0.05,20,20),alpha=1)
res<-scpcp(cm = cm, maxtol = 10^(-10), T = 5, R = 0.8, im = im,
  maxiter = 10, pstart = 0.5, chains=chains)

## End(Not run)
```

show.code

Output of the Amino Acid Coding Scheme

Description

Displays an encoding table for the standard amino acids.

Usage

```
show.code(code = 0:19, offset = 0)
```

Arguments

code	vector of 20 integer values used for coding the standard amino acids
offset	offset added to the values of code

Details

This function shows the coding order of the standard amino acid as used in `aa2num()`. The offset is included.

Value

No values are returned.

Author(s)

Franziska Hoffgaard

See Also[aa2num](#)**Examples**`show.code()`

`sim`*Compute the Covariance Matrices and B Factors for a List of PDBs*

Description

For a given list of PDB-files the respective covariance matrices and resulting B factors are computed.

Usage

```
sim(pdb, mj1 = NULL, mj2 = NULL, mj.avg = FALSE, alpha = 82,  
    cuts = 169, path = getwd(), cluster = NULL)
```

Arguments

<code>pdbs</code>	list of PDB file names
<code>mj1</code>	matrix for the intrachain interaction strengths
<code>mj2</code>	matrix for the interchain interaction strengths
<code>mj.avg</code>	logical, if TRUE only the average value of the interaction matrix is used as value for the interaction of any two amino acids
<code>alpha</code>	strength of the peptide bond
<code>cuts</code>	squared distance cutoff
<code>path</code>	path to the output files
<code>cluster</code>	snow cluster object created with <code>makeCluster()</code>

Details

Each PDB file is extracted. All features necessary for the computation of the covariance matrix in the elastic network model are computed. Both the covariance matrix and the B factors are computed and written to a file. The computation is parallelized using `parLapply()` from the package **snow**. If `cluster` is left at its default value the computation is carried out in serial.

Value

No values are returned. The B factors and inverse Hessian matrices are written into files.

Author(s)

Franziska Hoffgaard, Philipp Weil

References

Hamacher and McCammon (2005) *Journal of Chemical Theory and Computation* 2, 873.
Tierney, Rossini, Li (2009) *Int J Parallel Proc* 37, 78–90.

See Also

[sims](#), [simc](#)

Examples

```
## Not run:
#build a list of pdb-files
pdbs<-list(system.file("1KZK.pdb", package = "BioPhysConnectoR"),
           system.file("1EBY.pdb", package = "BioPhysConnectoR"))
sim(pdbs, cuts = 169)

## Cluster example
clu<-makeCluster(2)
sim(pdbs, cuts = 169, cluster = clu)
stopCluster(clu)

## End(Not run)
```

simc

Computed Elastic Network Models for Switched-Off-List of Contacts

Description

For each entry in the contact list the contact will be broken and the resulting covariance matrix and new B factors will be computed in the elastic network model. Furthermore the Frobenius norms between the original and the new covariance matrix can be evaluated.

Usage

```
simc(pdb, mj1 = NULL, mj2 = NULL, mj.avg = FALSE, c1 = NULL,
     alpha = 82, cuts = 169, path = getwd(), inv2file = FALSE,
     bfacs = TRUE, frob = TRUE, loc = NULL, norm = FALSE,
     file = NULL, cluster = NULL)
```

Arguments

pdb	file name of the PDB
mj1	matrix for the intrachain interaction strengths
mj2	matrix for the interchain interaction strengths
mj.avg	logical, if TRUE only the average value of the matrices is used as value for the interaction of any two amino acids
c1	optional contact list to process
alpha	strength of the peptide bond
cuts	squared cutoff distance
path	path to the output files
inv2file	logical, if TRUE the inverse Hessian matrix is written to a file, otherwise it will not be stored
bfacs	logical, if TRUE, the B factors are written to a file, otherwise they will not be stored
frob	logical, if TRUE, the Frobenius norm is computed
loc	dimensions i1, j1, i2, j2 for a matrix subset of which the frobenius norm should be computed
norm	logical, if TRUE the Frobenius norm is computed for the normalized matrices
file	personalized file name prefix
cluster	snow cluster object created with makeCluster()

Details

If no contact list is given, the full contact list is extracted from the PDB-file. Each contact (except covalent contacts) in the list is broken and the corresponding covariance matrix and B factors are computed. Those can be written into files. A user-defined contact list can be specified as well. For the computation of the Frobenius norm, different regions can be specified in `loc` as matrix. Each row determines a region `[i1:j1,i2:j2]` to be used for the norm. The routine is parallelized for the list of contacts using `parLapply()` from the package **snow**. If `cluster` is left at its default value the computation is carried out in serial.

Value

No values are returned.

Author(s)

Franziska Hoffgaard, Philipp Weil

References

- Hamacher and McCammon (2005) *Journal of Chemical Theory and Computation* 2, 873.
Hamacher (2008) *Gene* 422, 30–36.
Tierney, Rossini, Li (2009) *Int J Parallel Proc* 37, 78–90.

See Also[sim](#), [sims](#)**Examples**

```
## Not run:
cl<-matrix(c(3,1,4,1,5,1,9,1,10,1,11,1,24,1,66,1,67,1,68,1),ncol=2,byrow=TRUE)
out<-simc(system.file("1KZK.pdb", package = "BioPhysConnectoR"), cuts = 169, cl=cl)

## Cluster example
makeCluster(2)->clu
out<-simc(system.file("1KZK.pdb", package = "BioPhysConnectoR"), cuts = 169, cl=cl,
          cluster=clu)
stopCluster(clu)

## End(Not run)
```

sims*Apply a List of Different Amino Acid Sequences*

Description

For a set of sequences given in an alignment and a corresponding PDB file the covariance matrix for each sequence is computed based on the given molecular structure. The latter can be directed into a file. The Frobenius norms are computed upon request.

Usage

```
sims(pdb, alignment, mj1 = NULL, mj2 = NULL, mj.avg = FALSE,
     alpha = 82, cuts = 169, path = getwd(), mimethod = "ORMI",
     gapchar = "NOGAPCHAR", inv2file = FALSE, bfacs = TRUE,
     frob = TRUE, loc = NULL, norm = FALSE, cluster = NULL)
```

Arguments

pdb	PDB file
alignment	alignment file in fasta format
mj1	matrix for the intrachain interaction strengths
mj2	matrix for the interchain interaction strengths
mj.avg	logical, if TRUE only the average value of each matrix is used as value for the interaction of any two amino acids
alpha	strength of the peptide bond
cuts	squared distance cutoff
path	path to the output files
mimethod	method for the computation of the mutual information

gapchar	character vector denoting gaps in the alignment
inv2file	logical, if TRUE, the inverse Hessian matrix is written to a file
bfacs	logical, if TRUE, the B factors are written to a file
frob	logical, if TRUE, the Frobenius norm is computed
loc	dimensions i1, j1, i2, j2 for a matrix subset of which the Frobenius norm should be computed
norm	logical, if TRUE the Frobenius norm is computed for the normalized matrices
cluster	snow cluster object created with <code>makeCluster()</code>

Details

For an alignment the sequence entropy and mutual information is computed. Furthermore for each sequence in the alignment and the structure information from the PDB file the covariance matrix and B factors can be computed and the output can be written to files. The computation is parallelized using `parLapply()` from the package **snow**. If `cluster` is left at its default value the computation is carried out in serial.

Value

Return value is a list with the following components:

<code>\$entropy</code>	sequence entropy of the alignment
<code>\$mi</code>	mutual information of the alignment

If the Frobenius norm is computed, the value(s) will be returned as well:

<code>\$res</code>	vector consisting of: row number, sequence name, Frobenius norm
--------------------	---

Note

Make sure your alignment contains the IUPAC standard amino acids only without any gap characters.
This function includes source code of the **bio3d** package.

Author(s)

Franziska Hoffgaard, Philipp Weil

References

Hamacher and McCammon (2005) *Journal of Chemical Theory and Computation* 2, 873.
Grant, Rodrigues, ElSawy, McCammon, Caves, (2006) *Bioinformatics* 22, 2695–2696.
Tierney, Rossini, Li (2009) *Int J Parallel Proc* 37, 78–90.

See Also

[get.entropy](#), [get.mie](#), [sim](#), [simc](#)

Examples

```
## Not run:
sims(system.file("1KZK.pdb",package="BioPhysConnectoR"),system.file("align.fasta",
  package="BioPhysConnectoR"))

## Cluster example
clu<-makeCluster(2)
sims(system.file("1KZK.pdb",package="BioPhysConnectoR"),system.file("align.fasta",
  package="BioPhysConnectoR",cluster = clu))
stopCluster(clu)

## End(Not run)
```

Index

*Topic **IO**

- extractPDB, 8
- mat.read, 19
- mat.write, 21
- read.fasta, 22

*Topic **package**

- BioPhysConnectoR-package, 2

*Topic **utilities**

- aa2num, 4
- build.contacts, 5
- build.hess, 6
- build.interact, 7
- fnorm, 9
- get.bfacs, 10
- get.contact.list, 11
- get.entropy, 12
- get.freqs, 13
- get.mie, 15
- get.svd, 16
- invhess, 17
- lbpc, 18
- mat.norm, 19
- mat.sort, 20
- scpcp, 23
- show.code, 24
- sim, 25
- simc, 26
- sims, 28

aa2num, 4, 8, 25

BioPhysConnectoR

(BioPhysConnectoR-package), 2

BioPhysConnectoR-package, 2

build.contacts, 5, 6, 12

build.hess, 6, 17, 18

build.interact, 6, 7

build.invhess, 11

build.invhess (invhess), 17

extractPDB, 8

fnorm, 9

freq1p, 16

freq1p (get.freqs), 13

freq2p, 16

freq2p (get.freqs), 13

get.bfacs, 10

get.contact.list, 6, 11

get.cov (invhess), 17

get.entropy, 12, 14, 16, 29

get.entropy2p, 16

get.entropy2p (get.entropy), 12

get.freqs, 13

get.mie, 13, 14, 15, 29

get.svd, 16, 18

invhess, 17

lbpc, 18

mat.norm, 19

mat.read, 19, 22

mat.sort, 17, 20

mat.write, 21

read.fasta, 22

scpcp, 23

show.code, 4, 24

sim, 25, 28, 29

simc, 12, 26, 26, 29

sims, 26, 28, 28