Package 'penm'

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Title Build and Perturb Elastic Network Models

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Description Functions to calculate ENM models, mutate ENMs by perturbing them, perform single-site mutional scans to calculate average mutation-response matrices, and perform double-site mutational scans to calculate compensation matrices.

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penm-package *penm: Build and Perturb Elastic Network Models*

Description

Functions to calculate ENM models, mutate ENMs by perturbing them, perform single-site mutional scans to calculate average mutation-response matrices, and perform double-site mutational scans to calculate compensation matrices.

Details

The penm package includes functions to calculate various Elastic Network Models for proteins, perform normal mode analysis, and using lfenm, obtain mutant proteins and the corresponding mutant ENMs. In addition, it has functions to scan the various average-responses w.r.t. single-site mutations and double-site mutations.

admrs *Calculate a double-mutational-scan matrix analytically*

Description

Returns a compensation matrix: element (i,j) measures the degree of compensation of structural deformations produced by pairs of mutations at sites i and j. It uses analytical methods (closed formulas). Two measures are implemented: "mean_max" (default), the structural compensation maximized over mutations at j and averaged over mutations at i; "max_max" is the structural compensation maximized over mutations at i and j.

Usage

```
admrs(wt, mut_dl_sigma, mut_sd_min, option = "mean_max", response = "dr2")
```

Arguments

wt	is the (wild-type) protein to mutate (an object obtained using set_enm)
mut_dl_sigma	is the standard deviation of a normal distribution from which edge-length perturbations are picked (LFENM model).
mut_sd_min	is integer sequence-distance cutoff, only edges with sdij >= mut_sd_min are mutated
option	is either "mean_max" (default) or "max_max", depending on which compensation measure is desired.
response	is the response desired, which maybe either "dr2", "de2", or "df2"

Details

For details see doi:10.7717/peerj.11330

Value

A compensation matrix, rows are initially mutated site, j is compensation site

See Also

Other mutscan functions: `amrs()`, `sdmrs()`, `smrs()`

Examples

```
## Not run:
pdb <- bio3d::read.pdb("2acy")
wt <- set_enm(pdb, node = "ca", model = "ming_wall", d_max = 10.5, frustrated = FALSE)
dmat <- admrs(wt, mut_dl_sigma = 0.3, mut_sd_min = 1, option = "max_max", response = "dr2")

## End(Not run)
```

`amrs` *Calculate a mutation-response matrix analitically*

Description

Returns a mutation-response matrix It uses an analytical method (closed formulas). For details see doi:10.7717/peerj.11330

Usage

```
amrs(wt, mut_dl_sigma, mut_sd_min, option = "site", response = "dr2")
```

Arguments

`wt`	is the (wild-type) protein to mutate (an object obtained using `set_enm`)
`mut_dl_sigma`	is the standard deviation of a normal distribution from which edge-length perturbations are picked (LFENM model).
`mut_sd_min`	is integer sequence-distance cutoff, only edges with `sdij` >= `mut_sd_min` are mutated
`option`	is either "site" (default) or "mode"
`response`	is either "dr2" (default), "de2", or "df2"

Details

A site-by-site response matrix has elements Mij that measure the response (e.g. deformation) of site i averaged over mutations at site j. A mode-by-site response matrix has elements Mnj that measure the response (e.g. deformation) along mode n averaged over mutations at site j.

It may calculate either site-by-site or mode-by site response matrices Three type of response may be calculated, "dr2" (dr2ij and dr2nj), "de2" (de2ij and de2nj), and "df2" (df2ij and df2nj).

Value

A response matrix, columns are mutated sites, rows are responses, of a given site or normal mode.

See Also

Other mutscan functions: `admrs()`, `sdmrs()`, `smrs()`

Examples

```
## Not run:
pdb <- bio3d::read.pdb("2acy")
wt <- set_enm(pdb, node = "ca", model = "ming_wall", d_max = 10.5, frustrated = FALSE)
mrs_matrix <- amrs(wt,  mut_dl_sigma = 0.3, mut_sd_min = 1, option = "site", resonse = "dr2")

## End(Not run)
```

`sdmrs` *Calculate a double-mutational-scan matrix numerically (simulation-based)*

Description

Returns a compensation matrix: element (i,j) measures the degree of compensation of structural deformations produced by pairs of mutations at sites i and j. It uses a simulation method (calculates responses for various instances of forces, then calculates means or maxima) Two measures are implemented: "mean_max" (default), the structural compensation maximized over mutations at j and averaged over mutations at i; "max_max" is the structural compensation maximized over mutations at i and j.

Usage

```
sdmrs(
  wt,
  nmut,
  mut_dl_sigma,
  mut_sd_min,
  option = "mean_max",
  response = "dr2",
  seed = 1024
)
```

Arguments

`wt`	is the (wild-type) protein to mutate (an object obtained using `set_enm`)
`nmut`	is the number of mutations per site to simulate
`mut_dl_sigma`	is the standard deviation of a normal distribution from which edge-length perturbations are picked (LFENM model).
`mut_sd_min`	is integer sequence-distance cutoff, only edges with `sdij` >= `mut_sd_min` are mutated
`option`	is either "mean_max" (default) or "max_max", depending on which compensation measure is desired.
`response`	is the response desired, which maybe either "dr2", "de2", or "df2"
`seed`	seed for random generation of mutations

Details

For details see doi:10.7717/peerj.11330

Value

A compensation matrix, rows are initially mutated site, j is compensation site

See Also

Other mutscan functions: `admrs()`, `amrs()`, `smrs()`

Examples

```
## Not run:
pdb <- bio3d::read.pdb("2acy")
wt <- set_enm(pdb, node = "ca", model = "ming_wall", d_max = 10.5, frustrated = FALSE)
dmat <- sdmrs(wt, nmut = 10, mut_dl_sigma = 0.3, mut_sd_min = 1, option = "max_max", response = "dr2")

## End(Not run)
```

`set_enm` *Set up 'prot' object*

Description

'set_enm' set's up a 'prot' object containing information on ENM structure, parameters, and normal modes

Usage

```
set_enm(pdb, node, model, d_max, frustrated)
```

Arguments

`pdb`	pdb object obtained using bio3d::read.pdb
`node`	parameter specifying how network nodes should be built: "sc" (side chains) or "ca" (alpha carbons)
`model`	parameter specifying model type: "anm", "ming_wall", "hnm", "hnm0", "pfanm", "reach"
`d_max`	distance cutoff used to define enm contacts
`frustrated`	logical value indicating whether to include frustrations in calculation of kmat

Value

an object of class 'prot', which is a list 'lst(param, node, graph, eij, kmat, nma)'

Examples

```
## Not run:
pdb <- bio3d::read.pdb("2acy")
set_enm(pdb, node = "ca", model = "ming_wall", d_max = 10.5, frustrated = FALSE)
set_enm(pdb, node = "sc", model = "anm", d_max = 12.5, frustrated = TRUE)

## End(Not run)
```

smrs *Calculate a mutation-response matrix numerically (simulation-based)*

Description

Returns a mutation-response matrix It uses a simulation method (averages over perturbations). For details see doi:10.7717/peerj.11330

Usage

```
smrs(
  wt,
  nmut,
  mut_dl_sigma,
  mut_sd_min,
  option = "site",
  response = "dr2",
  seed = 1024
)
```

Arguments

wt	is the (wild-type) protein to mutate (an object obtained using set_enm)
nmut	is the number of mutations per site to simulate
mut_dl_sigma	is the standard deviation of a normal distribution from which edge-length perturbations are picked (LFENM model).
mut_sd_min	is integer sequence-distance cutoff, only edges with sdij >= mut_sd_min are mutated
option	is either "site" (default) or "mode"
response	is either "dr2" (default), "de2", or "df2"
seed	is a seed for random-number generation of mutations

Details

A site-by-site response matrix has elements Mij that measure the response (e.g. deformation) of site i averaged over mutations at site j. A mode-by-site response matrix has elements Mnj that measure the response (e.g. deformation) along mode n averaged over mutations at site j.

It may calculate either site-by-site or mode-by site response matrices Three type of response may be calculated, "dr2" (dr2ij and dr2nj), "de2" (de2ij and de2nj), and "df2" (df2ij and df2nj).

Value

A response matrix, columns are mutated sites, rows are responses, of a given site or normal mode.

See Also

Other mutscan functions: admrs(), amrs(), sdmrs()

Examples

```
## Not run:
pdb <- bio3d::read.pdb("2acy")
wt <- set_enm(pdb, node = "ca", model = "ming_wall", d_max = 10.5, frustrated = FALSE)
mrs_matrix <- smrs(wt, nmut = 10, mut_model = "lfenm", mut_dl_sigma = 0.3, mut_sd_min = 1, seed = 1024)

## End(Not run)
```

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