Package ‘DCLEAR’

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Title Distance Based Cell Lineage Reconstruction

Author Il-Youp Kwak [aut, cre],
Wuming Gong [aut]

Maintainer Il-Youp Kwak <`ikwak2@cau.ac.kr`>

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VignetteBuilder knitr

LinkingTo Rcpp, RcppArmadillo

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Suggests knitr, rmarkdown, markdown

Description R codes for distance based cell lineage reconstruction. Our methods won both subchallenges 2 and 3 of the Allen Institute Cell Lineage Reconstruction DREAM Challenge in 2020. References: Gong et al. (2021) <doi:10.1016/j.cels.2021.05.008>, Gong et al. (2022) <doi:10.1186/s12859-022-04633-x>.

URL `https://github.com/ikwak2/DCLEAR`

NeedsCompilation yes

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R topics documented:

`add_deletion` *add_deletion*

Description

Add deletion

Usage

```
add_deletion(x, tree, mutation_site, config)
```

Arguments

`x`	a character matrix
`tree`	a matrix representing the lineage tree
`mutation_site`	a binary matrix for mutation site
`config`	a lineage_tree_config object

Value

a character matrix with deletions

`add_dropout` *add_dropout*

Description

Add dropout events

Usage

```
add_dropout(x, config)
```

Arguments

`x`	a character matrix
`config`	a lineage_tree_config object

Value

a character matrix with dropout events

`as_igraph` *Generic function for as_igraph*

Description

Generic function for as_igraph

Usage

```
as_igraph(x, ...)
```

Arguments

`x`	a phylo object
`...`	additional parameters

`as_igraph,data.frame-method`

as_igraph

Description

Convert an phylo object to an igraph object, while keeping the weight (in contrast to igraph::as.igraph)

Usage

```
## S4 method for signature 'data.frame'
as_igraph(x, config)
```

Arguments

`x`	a phylo object
`config`	a ‘lineage_tree_config‘ object

Value

an igraph object

`as_igraph,phylo-method`

as_igraph

Description

Convert an phylo object to an igraph object, while keeping the weight (in contrast to igraph::as.igraph)

Usage

```
## S4 method for signature 'phylo'
as_igraph(x)
```

Arguments

`x`	a phylo object

Value

an igraph object

`as_lineage_tree` *Generic function for as_lineage_tree*

Description

Generic function for as_lineage_tree

Usage

```
as_lineage_tree(x, y, config, ...)
```

Arguments

`x`	a phyDat object
`y`	a phylo object
`config`	a lineage_tree_config object
`...`	additional parameters

`as_lineage_tree,phyDat,phylo,lineage_tree_config-method` *as_lineage_tree*

Description

Convert a phylo object and a phyDat object to a lineage_tree object

Usage

```
## S4 method for signature 'phyDat,phylo,lineage_tree_config'
as_lineage_tree(x, y, config, ...)
```

Arguments

`x`	a phyDat object
`y`	a phylo object
`config`	a lineage_tree_config object
`...`	additional parameters

Value

a lineage_tree object

`as_phylo` *Generic function for as_phylo*

Description

Generic function for as_phylo

Usage

```
as_phylo(x, ...)
```

Arguments

`x`	a graph object
`...`	additional parameters

`as_phylo,igraph-method` *as_phylo*

Description

Convert an igraph object to a phylo object

Usage

```
## S4 method for signature 'igraph'
as_phylo(x)
```

Arguments

`x`	an igraph object

Value

a phylo object or a igraph object

`DCLEAR` *DCLEAR: A package for DCLEAR: Distance based Cell LinEAge Reconstruction*

Description

Distance based methods for inferring lineage treess from single cell data

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`dist_kmer_replacement_inference` *Core function of computing kmer replacement distance*

Description

Compute the sequence distance matrix using inferred kmer replacement matrix

Usage

```
dist_kmer_replacement_inference(x, kmer_summary, k = 2)
```

Arguments

`x`	input data in phyDat format
`kmer_summary`	a kmer_summary object
`k`	k-mers (default k=2)

Value

a dist object

Author(s)

Wuming Gong (gongx030@umn.edu)

`dist_replacement` *Generic function for dist_replacement*

Description

Generic function for dist_replacement

Usage

```
dist_replacement(x, kmer_summary, k, ...)
```

Arguments

`x`	a sequence object
`kmer_summary`	a kmer_summary object
`k`	k-mer length
`...`	additional parameters

`dist_replacement,phyDat,kmer_summary,integer-method`

Compute the kmer replacement distance

Description

Compute the kmer replacement distance between sequences

Usage

```
## S4 method for signature 'phyDat,kmer_summary,integer'
dist_replacement(x, kmer_summary, k = 2, ...)
```

Arguments

`x`	input data in phyDat format
`kmer_summary`	a kmer_summary object
`k`	k-mer length
`...`	other arguments passed to substr_kmer

Value

a dist object

Author(s)

Wuming Gong (gongx030@umn.edu)

`dist_replacement,phyDat,missing,integer-method`

Compute the kmer replacement distance

Description

Compute the kmer replacement distance between sequences

Usage

```
## S4 method for signature 'phyDat,missing,integer'
dist_replacement(x, kmer_summary, k = 2L, ...)
```

Arguments

`x`	input data in phyDat format
`kmer_summary`	a kmer_summary object
`k`	k-mer length
`...`	other arguments passed to substr_kmer

Value

a dist object

Author(s)

Wuming Gong (gongx030@umn.edu)

`dist_weighted_hamming` *Generic function for dist_weighted_hamming*

Description

Generic function for dist_weighted_hamming

Usage

```
dist_weighted_hamming(x, wVec, ...)
```

Arguments

`x`	a sequence object
`wVec`	weight vector
`...`	additional parameters

`dist_weighted_hamming,phyDat,numeric-method` *dist_weighted_hamming*

Description

implementation of weighted hamming algorithm

Usage

```
## S4 method for signature 'phyDat,numeric'
dist_weighted_hamming(x, wVec, dropout = FALSE)
```

Arguments

`x`	Sequence object of 'phyDat' type.
`wVec`	Weight vector for the calculation of weighted hamming distance
`dropout`	Different weighting strategy is taken to consider interval dropout with dropout = 'TRUE'. Default is, dropout = 'FALSE'.

Value

Calculated distance matrix of input sequences. The result is a 'dist' class object.

Author(s)

Il-Youp Kwak

Examples

```
library(DCLEAR)
library(phangorn)
library(ape)

set.seed(1)
mu_d1 = c( 30, 20, 10, 5, 5, 1, 0.01, 0.001)
mu_d1 = mu_d1/sum(mu_d1)
simn = 10 # number of cell samples
m = 10  ## number of targets
sD = sim_seqdata(sim_n = simn, m = m, mu_d = 0.03,
      d = 12, n_s = length(mu_d1), outcome_prob = mu_d1, p_d = 0.005 )
## RF score with hamming distance
D_hm = dist.hamming(sD$seqs)
tree_hm = NJ(D_hm)
RF.dist(tree_hm, sD$tree, normalize = TRUE)

## RF score with weighted hamming
InfoW = -log(mu_d1)
InfoW[1:2] = 1
InfoW[3:7] = 4.5
D_wh = dist_weighted_hamming(sD$seqs, InfoW, dropout = FALSE)
tree_wh = NJ(D_wh)
RF.dist(tree_wh, sD$tree, normalize = TRUE)

## RF score with weighted hamming, cosidering dropout situation
nfoW = -log(mu_d1)
InfoW[1] = 1
InfoW[2] = 12
InfoW[3:7] = 3
D_wh2 = dist_weighted_hamming(sD$seqs, InfoW, dropout = TRUE)
tree_wh2= NJ(D_wh2)
RF.dist(tree_wh2, sD$tree, normalize = TRUE)
```

`downsample` *Generic function for downsample*

Description

Generic function for downsample

Usage

```
downsample(x, ...)
```

Arguments

`x`	a data object
`...`	additional parameters

`downsample,igraph-method`
downsample

Description

Sample a lineage tree

Usage

```
## S4 method for signature 'igraph'
downsample(x, n = 10L, ...)
```

Arguments

`x`	a igraph object
`n`	number of leaves (tips) in the down-sampled tree
`...`	additional parameters

Value

a phylo object

`downsample,lineage_tree-method` *downsample*

Description

Sample a lineage tree

Usage

```
## S4 method for signature 'lineage_tree'
downsample(x, n = 10L, ...)
```

Arguments

`x`	a lineage_tree object
`n`	number of leaves (tips) in the down-sampled tree
`...`	additional parameters

Value

a lineage_tree object

`get_distance_prior` *get_distance_prior*

Description

prior distribution of distance

Usage

```
get_distance_prior(x)
```

Arguments

`x`	a kmer_summary object

Value

a probabilistic vector of the distribution of nodal distances

Author(s)

Wuming Gong (gongx030@umn.edu)

`get_leaves` *Generic function for get_leaves*

Description

Generic function for get_leaves

Usage

```
get_leaves(x, ...)
```

Arguments

`x`	a lineage_tree object
`...`	additional parameters

`get_leaves,lineage_tree-method` *get_leaves*

Description

Get the leaf sequences

Usage

```
## S4 method for signature 'lineage_tree'
get_leaves(x, ...)
```

Arguments

`x`	a lineage_tree object
`...`	additional parameters

Value

a phyDat object

`get_node_names` *get_node_names*

Description

Convenient function for get node names

Usage

```
get_node_names(x)
```

Arguments

`x`	node id

Value

node names

Author(s)

Wuming Gong (gongx030@umn.edu)

`get_replacement_probability` *get_replacement_probability*

Description

Compute p(A,B|d), the conditional probability of seeing a replacement of from kmer A to B or vice versa

Usage

```
get_replacement_probability(x)
```

Arguments

`x`	a kmer_summary object

Value

an 3D probabilistic array (kmers by kmers by distances)

Author(s)

Wuming Gong (gongx030@umn.edu)

`get_sequence` *get_sequence*

Description

Get sequencees

Usage

```
get_sequence(x, tree, outcome, config)
```

Arguments

`x`	a character matrix
`tree`	a matrix representing the lineage tree
`outcome`	a character matrix
`config`	a lineage_tree_config object

Value

a character matrix

`get_transition_probability` *get_transition_probability*

Description

Compute p(A,X|B,Y,d), the conditional probability of seeing a replacement from A to B given the previous replacement B from Y at nodal distance d

Usage

```
get_transition_probability(x)
```

Arguments

`x`	a kmer_summary object

Value

an 3D probabilistic array (kmers by kmers by distances)

Author(s)

Wuming Gong (gongx030@umn.edu)

`lineages` *Lineage data*

Description

Lineage data

Usage

```
data(lineages)
```

Format

An object of class `list` of length 100.

Examples

```
data(lineages)
```

`positional_mutation_prob` *positional_mutation_prob*

Description

Convenient function for get node names

Usage

```
positional_mutation_prob(x, config)
```

Arguments

`x`	a phyDat object
`config`	a lineage_tree_config object

Value

a positional mutation probability matrix

`process_sequence` *Generic function for process_sequence*

Description

Generic function for process_sequence

Usage

```
process_sequence(x, ...)
```

Arguments

`x`	a sequence object
`...`	additional parameters

`process_sequence,phyDat-method` *Process sequences*

Description

Process sequences

Usage

```
## S4 method for signature 'phyDat'
process_sequence(
  x,
  division = 16L,
  dropout_character = "*",
  default_character = "0",
  deletion_character = "-"
)
```

Arguments

`x`	input data in phyDat format
`division`	cell division
`dropout_character`	Dropout character (default: '*')
`default_character`	Default character (default: '0')
`deletion_character`	Deletion character (default: '-')

Value

a 'lineage_tree_config' object

Author(s)

Wuming Gong (gongx030@umn.edu)

`prune` *Generic function for prune*

Description

Generic function for prune

Usage

```
prune(x, ...)
```

Arguments

`x`	a lineage_tree object
`...`	additional parameters

`prune,igraph-method` *prune*

Description

Trim a full lineage tree into phylogenetic tree

Usage

```
## S4 method for signature 'igraph'
prune(x, weighted = TRUE, ...)
```

Arguments

`x`	an igraph object
`weighted`	whether or not keep the edge weight (default: TRUE)
`...`	additional parameters

Value

an igraph object

`prune,lineage_tree-method` *prune*

Description

Trim a full lineage tree into phylogenetic tree

Usage

```
## S4 method for signature 'lineage_tree'
prune(x, ...)
```

Arguments

`x`	a lineage_tree object
`...`	additional parameters passed to as_phylo()

Value

a lineage_tree object

`random_tree` *random_tree*

Description

Simulate a random lineage tree

Usage

```
random_tree(n_samples, division = 16L)
```

Arguments

`n_samples`	number of samples to simulate
`division`	number of cell division

Value

a data frame

Author(s)

Wuming Gong (gongx030@umn.edu)

`rbind,phyDat-method` *rbind*

Description

Concatenate multiple phyDat objects

Usage

```
## S4 method for signature 'phyDat'
rbind(..., deparse.level = 1)
```

Arguments

`...`	a list of phyDat objects
`deparse.level`	see definition in generic rbind

Value

a phyDat object

`sample_mutation_outcome` *sample_mutation_outcome*

Description

Sample mutation outcome

Usage

```
sample_mutation_outcome(x, mp = NULL, config)
```

Arguments

`x`	an igraph object
`mp`	a mutation site matrix
`config`	a lineage_tree_config object

Value

a outcome matrix

`sample_mutation_site` *sample_mutation_site*

Description

Sample mutation site

Usage

```
sample_mutation_site(tree, config)
```

Arguments

`tree`	a data frame
`config`	a lineage_tree_config object

Value

a mutation site matrix

`sample_outcome_prob` *sample_outcome_prob*

Description

Sampling outcome probability based on a gamma distribution

Usage

```
sample_outcome_prob(config, num_states = 20L, shape = 0.1, scale = 2)
```

Arguments

`config`	a lineage_tree_config object
`num_states`	number of states used in simulation.
`shape`	shape parameter in gamma distribution
`scale`	scale parameter in gamma distribution

Value

a probability vector for each alphabet

Author(s)

Wuming Gong (gongx030@umn.edu)

`score_simulation` *score_simulation*

Description

Compare two sets of sequences

Usage

```
score_simulation(x, y, config)
```

Arguments

`x`	a character matrix
`y`	a character matrix
`config`	a lineage_tree_config object

Value

numeric scores

`simulate` *Generic function for simulate*

Description

Generic function for simulate

Usage

```
simulate(config, x, ...)
```

Arguments

`config`	a lineage_tree_config object
`x`	a sequence object
`...`	additional parameters

`simulate,lineage_tree_config,missing-method` *simulate*

Description

Simulate a cell lineage tree Adoped from https://github.com/elifesciences-publications/CRISPR_recorders_sims/blob/master/

Usage

```
## S4 method for signature 'lineage_tree_config,missing'
simulate(config, x, n_samples = 200, ...)
```

Arguments

`config`	simulation configuration; a lineage_tree_config object
`x`	missing
`n_samples`	number of samples to simulate
`...`	additional parameters

Value

a lineage_tree object

Author(s)

Wuming Gong (gongx030@umn.edu)

`simulate,lineage_tree_config,phyDat-method` *simulate*

Description

Simulate a cell lineage tree based on a set of sequences

Usage

```
## S4 method for signature 'lineage_tree_config,phyDat'
simulate(config, x, n_samples = 200L, k = 50, greedy = TRUE, ...)
```

Arguments

`config`	simulation configuration; a lineage_tree_config object
`x`	a sequence object
`n_samples`	number of samples to simulate
`k`	Number of trials
`greedy`	Whether ot not use a greedy search
`...`	additional parameters

Value

a lineage_tree object

Author(s)

Wuming Gong (gongx030@umn.edu)

`simulate_core` *simulate_core*

Description

Simulate a cell lineage tree Adoped from https://github.com/elifesciences-publications/CRISPR_recorders_sims/blob/master/

Usage

```
simulate_core(config, tree, mutation_site, outcome)
```

Arguments

`config`	simulation configuration; a lineage_tree_config object
`tree`	a matrix representing the lineage tree
`mutation_site`	a binary matrix indicating the mutation sites
`outcome`	a character matrix

Value

a ‘lineage_tree‘ object

`sim_seqdata` *sim_seqdata*

Description

Generate singe cell barcode data set with tree shaped lineage information

Usage

```
sim_seqdata(
  sim_n = 200,
  m = 200,
  mu_d = 0.03,
  d = 15,
  n_s = 23,
  outcome_prob = NULL,
  p_d = 0.003
)
```

Arguments

`sim_n`	Number of cell samples to simulate.
`m`	Number of targets.
`mu_d`	Mutation rate. (a scalar or a vector)
`d`	Number of cell divisions.
`n_s`	Number of possible outcome states
`outcome_prob`	Outcome probability vector (default is NULL)
`p_d`	Dropout probability

Value

The result is a list containing two objects, 'seqs' and 'tree'. The 'seqs' is 'phyDat' object of 'sim_n' number of simulated barcodes corresponding to each cell, and The 'tree' is a 'phylo' object, a ground truth tree structure for the simulated data.

Author(s)

Il-Youp Kwak

Examples

```
library(DCLEAR)
library(phangorn)
library(ape)
```

```
set.seed(1)
mu_d1 = c( 30, 20, 10, 5, 5, 1, 0.01, 0.001)
mu_d1 = mu_d1/sum(mu_d1)
simn = 10 # number of cell samples
m = 10  ## number of targets
sD = sim_seqdata(sim_n = simn, m = m, mu_d = 0.03,
        d = 12, n_s = length(mu_d1), outcome_prob = mu_d1, p_d = 0.005 )
## RF score with hamming distance
D_hm = dist.hamming(sD$seqs)
tree_hm = NJ(D_hm)
RF.dist(tree_hm, sD$tree, normalize = TRUE)

## RF score with weighted hamming
InfoW = -log(mu_d1)
InfoW[1:2] = 1
InfoW[3:7] = 4.5
D_wh = dist_weighted_hamming(sD$seqs, InfoW, dropout=FALSE)
tree_wh = NJ(D_wh)
RF.dist(tree_wh, sD$tree, normalize = TRUE)

## RF score with weighted hamming, cosidering dropout situation
nfoW = -log(mu_d1)
InfoW[1] = 1
InfoW[2] = 12
InfoW[3:7] = 3
D_wh2 = dist_weighted_hamming(sD$seqs, InfoW, dropout = TRUE)
tree_wh2= NJ(D_wh2)
RF.dist(tree_wh2, sD$tree, normalize = TRUE)
```

`substr_kmer` *Generic function for substr_kmer*

Description

Generic function for substr_kmer

Usage

```
substr_kmer(x, ...)
```

Arguments

`x`	a kmer object
`...`	additional parameters

`substr_kmer,kmer_summary-method` *Subseting a kmer_summary object*

Description

Summarize the short k-mer summary from the long k-mer summary

Usage

```
## S4 method for signature 'kmer_summary'
substr_kmer(x, k = 2)
```

Arguments

`x`	a kmer_summary object
`k`	k-mer length(default: 2)

Value

a new kmer_summary object

Author(s)

Wuming Gong (gongx030@umn.edu)

`subtract` *Generic function for subtract*

Description

Generic function for subtract

Usage

```
subtract(x, y, ...)
```

Arguments

`x`	a lineage_tree object
`y`	a lineage_tree object
`...`	additional parameters

`subtract,lineage_tree,lineage_tree-method` *subtract*

Description

Subtract a subtree from a large tree

Usage

```
## S4 method for signature 'lineage_tree,lineage_tree'
subtract(x, y, ...)
```

Arguments

`x`	a lineage_tree object
`y`	a lineage_tree object
`...`	additional parameters

Value

a lineage_tree object

`subtree` *Generic function for subtree*

Description

Generic function for subtree

Usage

```
subtree(x, ...)
```

Arguments

`x`	a lineage_tree object
`...`	additional parameters

`subtree,lineage_tree-method` *subtree*

Description

Extract a subtree with specific leaves

Usage

```
## S4 method for signature 'lineage_tree'
subtree(x, leaves = NULL, ...)
```

Arguments

`x`	a lineage_tree object
`leaves`	leaves of the extracted tree
`...`	additional parameters

Value

a lineage_tree object

`subtree,phylo-method` *subtree*

Description

Extract a subtree with specific leaves

Usage

```
## S4 method for signature 'phylo'
subtree(x, leaves = NULL, ...)
```

Arguments

`x`	a phylo object
`leaves`	leaves of the extracted tree
`...`	additional parameters

Value

a pylo object

`summarize_kmer` *Generic function for summarize_kmer*

Description

Generic function for summarize_kmer

Usage

```
summarize_kmer(x, ...)
```

Arguments

`x`	a sequence object
`...`	additional parameters

`summarize_kmer,phyDat-method`
summarize_kmer

Description

Summarize kmer distributions with input sequences

Usage

```
## S4 method for signature 'phyDat'
summarize_kmer(
  x,
  division = 16L,
  k = 2,
  reps = 20L,
  n_samples = 200L,
  n_nodes = 100L,
  n_targets
)
```

Arguments

`x`	input data as a phyDat object
`division`	number of cell division
`k`	k-mer (default = 2)
`reps`	number of simulated trees
`n_samples`	number of samples to simulate

`n_nodes`	number of nodes to sample (including both leaves and internval nodes)
`n_targets`	sequence length. If this argument is missing, the length of the input sequences will be used.

Value

a kmer_summary object

Author(s)

Wuming Gong (gongx030@umn.edu)

`summarize_kmer_core` *summarize_kmer_core*

Description

Summarize kmer distributions (core function)

Usage

```
summarize_kmer_core(
  k = 2,
  reps = 20L,
  n_samples = 200L,
  n_nodes = 100L,
  config = NULL
)
```

Arguments

`k`	k-mer (default = 2)
`reps`	number of simulated trees
`n_samples`	number of samples to simulate
`n_nodes`	number of nodes to sample (including both leaves and internval nodes)
`config`	lineage tree configuration (a lineage_tree_config object)

Value

a kmer_summary object

Author(s)

Wuming Gong (gongx030@umn.edu)

WH *WH*

Description

implementation of weighted hamming algorithm

Usage

```
WH(x, InfoW, dropout = FALSE)
```

Arguments

`x`	Sequence object of 'phyDat' type.
`InfoW`	Weight vector for the calculation of weighted hamming distance
`dropout`	Different weighting strategy is taken to consider interval dropout with dropout = 'TRUE'. Default is, dropout = 'FALSE'.

Value

Calculated distance matrix of input sequences. The result is a 'dist' class object.

Author(s)

Il-Youp Kwak

Examples

```
set.seed(1)
library(phangorn)
mu_d1 = c( 30, 20, 10, 5, 5, 1, 0.01, 0.001)
mu_d1 = mu_d1/sum(mu_d1)
simn = 10 # number of cell samples
m = 10  ## number of targets
sD = sim_seqdata(sim_n = simn, m = m, mu_d = 0.03,
        d = 12, n_s = length(mu_d1), outcome_prob = mu_d1, p_d = 0.005 )

## RF score with hamming distance
D_h = dist.hamming(sD$seqs)
tree_h= NJ(D_h)
RF.dist(tree_h, sD$tree, normalize = TRUE)

## RF score with weighted hamming
InfoW = -log(mu_d1)
InfoW[1:2] = 1
InfoW[3:7] = 4.5

D_wh = WH(sD$seqs, InfoW)
```

```
tree_wh= NJ(D_wh)
RF.dist(tree_wh, sD$tree, normalize = TRUE)

## RF score with weighted hamming, cosidering dropout situation
nfoW = -log(mu_d1)
InfoW[1] = 1
InfoW[2] = 12
InfoW[3:7] = 3

D_wh2 = WH(sD$seqs, InfoW, dropout=TRUE)
tree_wh2= NJ(D_wh2)
RF.dist(tree_wh2, sD$tree, normalize = TRUE)
```

`WH_train` *Train weights for WH*

Description

Train weights for WH and output weight vector

Usage

```
WH_train(X, loc0 = 2, locDropout = 1, locMissing = FALSE)
```

Arguments

`X`	a list of k number of input data, X[[1]] ... X[[k]]. The ith data have sequence information as phyDat format in X[[i]][[1]], and tree information in X[[i]][[2]] as phylo format.
`loc0`	weight location of initial state
`locDropout`	weight location of dropout state
`locMissing`	weight location of missing state, FALSE if there is no missing values

Value

a weight vector

Author(s)

Il-Youp Kwak (ikwak2@cau.ac.kr)

`WH_train_fit` *Train weights for WH, and output distance object*

Description

Train weights for WH using the given data, and fit the distance matrix for a input sequence.

Usage

```
WH_train_fit(x, X)
```

Arguments

`x`	input data in phyDat format
`X`	a list of k number of input data, X[[1]] ... X[[k]]. The ith data have sequence information as phyDat format in X[[i]][[1]], and tree information in X[[i]][[2]] as phylo format.

Value

a dist object

Author(s)

Il-Youp Kwak (ikwak2@cau.ac.kr)

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