Package 'admixturegraph'

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Type Package

Title Admixture Graph Manipulation and Fitting

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Description Implements tools for building and visualising admixture graphs and for extracting equations from them. These equations can be compared to fstatistics obtained from data to test the consistency of a graph against data -for example by comparing the sign of f_4-statistics with the signs predicted by the graph -- and graph parameters (edge lengths and admixture proportions) can be fitted to observed statistics.

License GPL-2

Depends R (>= 3.2.2)

Imports doParallel, dplyr, foreach, ggplot2, graphics, MASS, methods, neldermead, parallel, pracma, stats, utils, grDevices

Suggests knitr, rmarkdown, testthat

URL https://github.com/mailund/admixture_graph

BugReports https://github.com/mailund/admixture_graph/issues

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R topics documented:

admixturegraph-package	4
add_an_admixture	5
add_an_admixture2	7
add_a_leaf	8
add_graph_f4	9
add_graph_f4_sign	10
admixture_edge	10
admixture_proportions	11
admix_props	11
agraph	12
agraph children	13
agraph parents	13
agraph weights	14
all graphs	14
all paths	15
all path overlaps	15
bears	16
build edge optimisation matrix	16
burn in	17
calculate concentration	17
canonise expression	18
canonise graph	18
coef.agraph fit	19
cost function	19
_ edge	20
edge optimisation function	21
eight leaves trees	22
evaluate f4	23
examine edge optimisation matrix	23
extract admixture proportion parameters	24
extract graph parameters	25
extract trees	25
f2	26
f3	26
f4	27
f4stats	27
fast fit	28
fast plot	30
filter on leaves	31
fitted.agraph fit	31
fit graph	32
fit graph list	34
fit permutations and graphs	35
five leaves graphs	36
format path	37
four_leaves_graphs	38

get_graph_f4_sign	. 39
graphs_2_0	. 39
graphs_3_0	. 40
graphs_3_1	. 40
graphs_4_0	. 41
graphs_4_1	. 41
graphs_4_2	. 42
graphs_5_0	. 42
graphs_5_1	. 43
graphs_5_2	. 43
graphs_6_0	. 44
graphs_6_1	. 44
graphs_6_2	. 45
graphs 7 0	. 45
graphs 7 1	. 46
graphs 8 0	. 46
graph environment	. 47
graph to vector	. 47
is descendant of	48
is negative	. 48
is positive	49
is unknown	49
is zero	49
log likelihood	50
log sum of logs	. 51
make an outgroup	51
make mcmc model	52
make permutations	53
model haves factor n	54
model_likelihood	55
model_likelihood_n	55
mvnonneg	56
no admixture events	57
no_admixture_events agraph	57
no_admixture_events agraph fit	58
no_admixture_events agraph_it list	58
no poor fits	. 50 59
no poor fits agraph fit	. 59
no_poor_fits agraph_fit_list	. 57
overlans sign	. 00
Dyent edges	. 00
parent_cuges	. 01
paul_ovenap	. 01
	. 02
plot.agraphi_iit	. 04
piol.145tats	. 03
piot_iit_1	. 03
piot_iit_2	. 00
puol_iits	. 0/

poor_fits.agraph_fit	67
poor_fits.agraph_fit_list	68
print.agraph_fit	68
project_to_population	69
remove_duplicates	69
rename_nodes	70
residuals.agraph_fit	70
run_metropolis_hasting	71
seven_leaves_graphs	72
seven_leaves_trees	73
sf2	73
sf3	74
sf4	74
six_leaves_graphs	75
split_population	76
split_population.agraph_fit	76
split_population.data.frame	77
summary.agraph_fit	77
sum_of_squared_errors	78
sum_of_squared_errors.agraph_fit	78
sum_of_squared_errors.agraph_fit_list	79
thinning	79
vector_to_graph	80
	81

Index

admixturegraph-package

admixturegraph: Visualising and analysing admixture graphs.

Description

The package provides functionality to analyse and test admixture graphs against the f statistics described in the paper Ancient Admixture in Human History, Patterson *et al.*, Genetics, Vol. 192, 1065–1093, 2012.

Details

The f statistics $-f_2$, f_3 , and f_4 – extract information about correlations between gene frequencies in different populations (or single diploid genome samples), which can be informative about patterns of gene flow between these populations in form of admixture events. If a graph is constructed as a hypothesis for the relationship between the populations, equations for the expected values of the f statistics can be extracted, as functions of edge lengths – representing genetic drift – and admixture proportions.

This package provides functions for extracting these equations and for fitting them against computed f statistics. It does not currently provide functions for computing the f statistics – for that we refer to the ADMIXTOOLS software package.

add_an_admixture Adds a new admixture event to a graph.

Description

Given an admixture graph, selects a child edge and a parent edges and adds a new edge from the parent edge to the child edge with an admixture event, if possible. Thus, the resulting graph is an extension of the input graph in the sense that erasing one of the admixture edges (the new one) we get the original admixture graph. However, we know that in practice when fitting data to admixture graphs, the best graph with k admixture events is not always an extension like that from the best graph with k - 1 admixture events. For a more relaxed way of adding a new admixture event, try add_an_admixture2.

Usage

```
add_an_admixture(graph, admixture_variable_name, labels_matter = FALSE,
    outgroup = "")
```

Arguments

graph	An admixture graph.
admixture_varia	ble_name
	A name for the new admixture proportion.
labels_matter	When FALSE (the default value), we consider two admixture graphs similar when they have the same topology but permuted admixture proportion names. When TRUE, the already existing admixture events and the edges leading to them are considered labeled.
outgroup	An optional parameter for the preferred outgroup.

Value

A list of graphs made by adding a new admixture event to the input graph. The list has no duplicate elements (what that means depends on the value of labels_matter).

See Also

all_graphs
fit_permutations_and_graphs
fit_graph_list
add_a_leaf
add_an_admixture2
make_an_outgroup

Examples

To illustrate what the parameter labels_matter does, consider the following graph:

There are 15 ways this graph can be extended to a graph with two admixture events by # adding an admixture edge, as can be seeing by having the program explicitly construct # all the cases:

```
short_list <- add_an_admixture(graph, "q")
print(length(short_list))</pre>
```

However, maybe we already have a specific historical event in mind corresponding to the # original admixture event in graph, or a fixed value for the admixture proportion p. # Then, for example, it makes a difference to us whether we consider the possibility of # another admixture event occurring before that event,

```
leaves <- c("A", "B", "C")</pre>
inner_nodes <- c("R", "x", "y", "z", "M", "N")
edges <- parent_edges(c(edge("x", "R"),</pre>
                          edge("z", "R"),
                          edge("y", "z"),
edge("A", "x"),
                          edge("B", "M"),
                          edge("C", "y"),
                          admixture_edge("N", "x", "z"),
                          admixture_edge("M", "N", "y")))
admixtures <- admixture_proportions(c(admix_props("N", "x", "z", "q"),</pre>
                                         admix_props("M", "N", "y", "p")))
example1 <- agraph(leaves, inner_nodes, edges, admixtures)</pre>
plot(example1, show_admixture_labels = TRUE, title = "example 1")
# or after that event,
leaves <- c("A", "B", "C")</pre>
inner_nodes <- c("R", "x", "y", "z", "M", "N")</pre>
edges <- parent_edges(c(edge("x", "R"),</pre>
                          edge("y", "R"),
                          edge("z", "y"),
                          edge("A", "x"),
                          edge("B", "N"),
```

add_an_admixture2 Adds a new admixture event to a graph.

Description

Given an admixture graph, selects a child edge and two parent edges, disconnects the child edge from its original parent node and connects it to the two parent edges with an admixture event, if possible. Thus, contrary to add_an_admixture, the resulting graph need not be an extension of the input graph in the sense that erasing one of the admixture edges we get the original admixture graph. In practice, we know that when fitting data to admixture graphs, the best graph with k admixture events is not always an extension like that from the best graph with k - 1 admixture events. Most likely it doesn't need to be an extension like this (the two new admixture edges can both go where ever) either.

Usage

```
add_an_admixture2(graph, admixture_variable_name, outgroup = "")
```

Arguments

graph	An admixture graph.	
admixture_variable_name		
	A name for the new admixture proportion.	
outgroup	An optional parameter for the preferred outgroup.	

Value

A list of graphs made by adding a new admixture event to the input graph. The list contains duplicate elements, and may even contain graphs with *eyes* (two inner nodes with the property that all the paths between any two leaves visits both or neither of them).

See Also

all_graphs
fit_permutations_and_graphs
fit_graph_list
add_a_leaf
add_an_admixture
make_an_outgroup

add_a_leaf *Adds a new leaf to a graph.*

Description

Given an admixture graph, selects an edge and branches off a new edge ending at a new leaf.

Usage

```
add_a_leaf(graph, leaf_name, outgroup = "")
```

Arguments

graph	An admixture graph.
leaf_name	A name for the new leaf.
outgroup	An optional parameter for the preferred outgroup, which can be the new leaf

Value

A list of graphs made by adding a new leaf to the input graph. The list has no duplicate elements.

See Also

all_graphs
fit_permutations_and_graphs
fit_graph_list
add_an_admixture
add_an_admixture2
make_an_outgroup

8

add_graph_f4

Examples

```
# Take a look at how much trees there are:
leaves <- c("1", "2")</pre>
inner_nodes <- c("R")</pre>
edges <- parent_edges(c(edge("1", "R"), edge("2", "R")))</pre>
admixtures <- NULL
Lambda <- agraph(leaves, inner_nodes, edges, admixtures)</pre>
set <- list(Lambda)</pre>
for (i in seq(1, 6)) {
  new_set <- list()</pre>
  for (tree in set) {
    new_set <- c(new_set, add_a_leaf(tree, paste(i + 2)))</pre>
  }
  set <- new_set</pre>
  cat("There are ")
  cat(length(set))
  cat(" different trees with ")
  cat(i + 2)
  cat(" labeled leaves.")
  cat("\n")
}
# In general, there are 1*3*5*...*(2n - 5) different trees with n labeled leaves
# (A001147 in the online encyclopedia of integer sequences).
# Exhaustive search through the graph space is hard!
```

add_graph_f4	Evalutes the f_4 statistics for all rows in a data frame and extends the
	data frame with the graph f_4 .

Description

The data frame, data, must contain columns W, X, Y, and Z. The function then computes the $f_4(W, X; Y, Z)$ statistics (also known as the *D* statistics) for all rows and adds these as a column, graph_f4, to the data frame.

Usage

```
add_graph_f4(data, graph, env)
```

Arguments

data	The data frame to get the labels to compute the f_4 statistics from.
graph	The admixture graph.
env	The environment to evaluate the f_4 statistics in.

Value

A data frame identical to data except with an additional column, graph_f4, containing the f_4 values as determined by the graph and the environment.

add_graph_f4_sign *Extend a data frame with f_4 statistics predicted by a graph.*

Description

Extracts the sign for the f_4 statistics predicted by the graph for all rows in a data frame and extends the data frame with the graph f_4 .

Usage

add_graph_f4_sign(data, graph)

Arguments

data	The data frame to get the labels to compute the f_4 statistics from.
graph	The admixture graph.

Details

The data frame, data, must contain columns W, X, Y, and Z. The function then computes the sign of the f4(W, X; Y, Z) statistics for all rows and adds these as a column, graph_f4_sign, to the data frame.

Value

A data frame identical to data except with an additional column, graph_f4_sign, containing the sign of the f_4 statistics as determined by the graph.

admixture_edge	Create an admixture	edge from a child	d to two parents.
----------------	---------------------	-------------------	-------------------

Description

Syntactic suggar for constructing edges in an admixture graph.

Usage

```
admixture_edge(child, parent1, parent2, prop = NA)
```

Arguments

child	The name of the child node.
parent1	The name of the parent node.
parent2	The name of the parent node.
prop	Admixture proportions from parent1 to child. If this parameter is not provided, you must explicitly specify the admixture proportion parameters in the agraph function call.

admixture_proportions Create the list of admixture proportions for an admixture graph.

Description

Syntactic suggar for constructing edges in an admixture graph.

Usage

```
admixture_proportions(admix_props)
```

Arguments

admix_props The admixture proportions.

admix_props	Specify the proportions in an admixture event.
-------------	--

Description

Syntactic suggar for constructing edges in an admixture graph.

Usage

```
admix_props(child, parent1, parent2, prop)
```

Arguments

child	The child node.
parent1	The first parent.
parent2	The second parent.
prop	The admixture proportions coming from the first parent.

Description

Create an admixture graph object, an acyclic directed graph.

Usage

```
agraph(leaves, inner_nodes, parent_edges,
    admixture_proportions = extract_admixture_proportion_parameters(parent_edges))
```

Arguments

leaves	The names of the leaves in the admixture graph. Do not use (,) or a single ${\sf R}.$	
inner_nodes	The name of the inner nodes in the admxture graph. Do not use (, $\ $) or a single R except for the root if you wish.	
parent_edges	The list of edges in the graph, created by parent_edges.	
admixture_propo	rtions	
	The list of admixture proportions; created by ${\tt admixture_proportions}$. Do not	
	use +, -, *, (,).	

Value

An admixture graph object.

See Also

```
edge
admixture_edge
admix_props
parent_edges
admixture_proportions
plot.agraph
```

Examples

```
admixture_edge("b", "ab", "bc")))
admixtures <- admixture_proportions(c(admix_props("b", "ab", "bc", "x")))
graph <- agraph(leaves, inner_nodes, edges, admixtures)</pre>
```

agraph_children Build the child incidene matrix from an parent edge list.

Description

Build the child incidene matrix from an parent edge list.

Usage

agraph_children(nodes, parent_edges)

Arguments

nodes	Nodes in the admxture graph.
parent_edges	An $n \times 2$ matrix where the first column is the child node and the second is the parent

Value

An incidence matrix for the child structure of an admixture graph.

See Also

agraph_parents

agraph_parents Build the parent incidence matrix from an edge list.

Description

Build the parent incidence matrix from an edge list.

Usage

```
agraph_parents(nodes, parent_edges)
```

Arguments

nodes	Nodes in the admxture graph.
parent_edges	An $n\times 2$ matrix where the first column is the child node and the second is the
	parent.

Value

An incidence matrix for the parent structure of an admixture graph.

See Also

agraph_children

agraph_weights Build the matrix of admixture proportions from an edge list.

Description

Build the matrix of admixture proportions from an edge list.

Usage

agraph_weights(nodes, admixture_weights, parents)

Arguments

nodes	The name of the nodes in the admxture graph.
admixture_weigh	ts
	An $n \times 3$ matrix where the first column is the child node, the second is the parent and the third is the admixture weight on that edge.
parents	The parent edge list. Used for checking graph consistency.

Value

A matrix containing the admixture weights.

all_graphs All graphs.

Description

Gives a list of all the graphs with at most a given number of admixture events. No duplicates.

Usage

```
all_graphs(populations, admixture_events)
```

Arguments

populations A vector of populations (leaf names). admixture_events

The maximum number of admixture events allowed.

all_paths

Value

A list of admixture graphs.

See Also

fit_graph_list

all_paths

Compute all paths from one leaf to another.

Description

Computes all paths from one leaf to another.

Usage

all_paths(graph, src, dst)

Arguments

graph	The admixture graph.
src	The starting leaf.
dst	The destination leaf.

Value

A list containing all the paths from src to dst.

all_path_overlaps Get the list of overlaps of all paths.

Description

Gets the list of overlaps of all paths.

Usage

```
all_path_overlaps(paths1, paths2)
```

Arguments

paths1	Paths between one pair of leaves.
paths2	Paths between another pair of leaves.

Value

A list of the overlaps of all combinations of paths from paths1 and paths2.

bears

Description

Computed f_4(W,X;Y,Z) statistics for different populations of bears.

Usage

bears

Format

A data frame with 18 rows and 6 variables:

- W The W population
- X The X population
- Y The Y population
- \mathbf{Z} The Z population
- **D** The D ($f_4(W,X;Y,Z)$) statistics
- Z.value The blocked jacknife Z values

Source

http://onlinelibrary.wiley.com/doi/10.1111/mec.13038/abstract

build_edge_optimisation_matrix

Build a matrix coding the linear system of edges once the admix variables have been fixed.

Description

The elements are characters containing numbers, admix variable names, parenthesis and arithmetical operations. (Transform into expressions with parse and then evaluate with eval). The default column names are the edge names from extract_graph_parameters, the rows have no names.

Usage

```
build_edge_optimisation_matrix(data, graph,
    parameters = extract_graph_parameters(graph))
```

burn_in

Arguments

data	The data set.
graph	The admixture graph.
parameters	In case one wants to tweak something in the graph.

Value

A list containing the full matrix (full), a version with zero columns removed (column_reduced) and parameters to pass forward (parameters).

burn_in Removes the first k rows from a trace.	
--	--

Description

Removes the first k rows from a trace.

Usage

burn_in(trace, k)

Arguments

trace	A trace from an MCMC run.
k	Number of rows to discard as burn-in.

calculate_concentration

Building a proxy concentration matrix.

Description

If we don't have the true concentration matrix of the data rows calculated, but at least have the Z scores of individual rows, (unrealistically) assuming independence and calculating the concentration matrix from those is still better than nothing (*i. e.* the identity matrix).

Usage

calculate_concentration(data, Z.value)

Arguments

data	The data containing at least the expected values of f statistics (column D) and
	possibly also products of expected values and f statistics divided by standard
	deviations of (the Z scores, column Z.value).
Z.value	Tells whether the Z scores are available or should we just use the identity matrix.

Value

The Cholesky decomposition of the inverted covariance matrix.

canonise_expression Used to recognize similar expressions and to possibly simplify them.

Description

It's best to simplify algebraic expression a little before evaluating.

Usage

```
canonise_expression(x)
```

Arguments

```
х
```

The input is assumed to be a character consisting of one or more terms. Each term starts with either + or - and after that contains one or more factors separated by \star . Each factor is either an admix variable, a number or a clause (1 - x) (mind the spaces, this is how the function f4 outputs), where x is again either an admix variable or a number. Everything is pretty much ruined if variable names are numbers or contain forbidden symbols +, -, \star , (,).

Value

A polynomial in a canonical form with no parenthesis or spaces and the monomials in lexicographical order. If everything is cancelled out then +0.

canonise_graph Canonise graph.

Description

Given a graph builds a unique logical vector depending only on the leaf names and the graph topology (not the inner node names, root position or the input order of edges or inner nodes). Can be used to detect graph isomorphism, that is, to weed out duplicates from a graph list. Only for comparison of graphs with the same leaf set!

Usage

canonise_graph(graph)

Arguments

graph An admixture graph.

coef.agraph_fit

Value

A logical vector coding the parental matrix of a canonised version of the input graph.

coef.agraph_fit *Parameters for the fitted graph.*

Description

Extracts the graph parameters for the graph fitted to data. Note that the optimal parameters are generally not unique.

Usage

S3 method for class 'agraph_fit'
coef(object, ...)

Arguments

object	The fitted object.
	Additional parameters.

See Also

```
link{summary.agraph_fit}
```

cost_function The cost function fed to Nelder-Mead.

Description

We want Nelder-Mead to run fast so the cost function operates with the column reduced edge optimisation matrix and does not give any extra information about the fit. For the details, use edge_optimisation_function instead.

Usage

```
cost_function(data, concentration, matrix, graph,
    parameters = extract_graph_parameters(graph), iteration_multiplier = 3)
```

Arguments

data	The data set.
concentration	The Cholesky decomposition of the inverted covariance matrix.
matrix	A column reduced edge optimisation matrix (typically given by the function build_edge_optimisation_matrix).
graph	The admixture graph.
parameters	In case one wants to tweak something in the graph.
iteration_multiplier	
	Given to mynonneg.

Value

Given an input vector of admix variables, returns the smallest error regarding the edge variables.

See Also

```
mynonneg
edge_optimisation_function
log_likelihood
```

edge

Create an edge from a child to a parent.

Description

Syntactic suggar for constructing edges in an admixture graph.

Usage

```
edge(child, parent)
```

Arguments

child	The name of the child node.
parent	The name of the parent node.

edge_optimisation_function

More detailed edge fitting than mere cost_function.

Description

Returning the cost, an example edge solution of an optimal fit, and linear relations describing the set of all edge solutions. Operating with the full edge optimisation matrix, not the column reduced one.

Usage

```
edge_optimisation_function(data, concentration, matrix, graph,
    parameters = extract_graph_parameters(graph), iteration_multiplier = 3)
```

Arguments

data	The data set.	
concentration	The Cholesky decomposition of the inverted covariance matrix.	
matrix	A full edge optimisation matrix (typically given by the function build_edge_optimisation_matrix).	
graph	The admixture graph.	
parameters	In case one wants to tweak something in the graph.	
iteration_multiplier		
	Given to mynonneg.	

Value

Given an input vector of admix variables, returns a list containing the minimal error (cost), the graph-f4 statistics (approximation), an example solution (edge_fit), linear relations describing all the solutions (homogeneous) and one way to choose the free (free_edges) and bounded (bounded_edges) edge variables.

See Also

mynonneg

cost_function

log_likelihood

eight_leaves_trees Eight leaves trees.

Description

Kind of obsolete since the introduction of all_graphs. A comprehensive listing of all the four unrooted trees with eight leaves. The position of the root can be moved later with the function make_an_outgroup.

Usage

eight_leaves_trees

Format

A list of functions on eight leaves. The outputs of these functions are agraph objects.

See Also

all_graphs
make_permutations
fit_permutations_and_graphs
fit_graph_list
add_a_leaf
add_an_admixture
add_an_admixture2
make_an_outgroup
Other graphs: five_leaves_graphs, four_leaves_graphs, seven_leaves_graphs, six_leaves_graphs

Examples

```
# While the usage of this function is pretty self-explanatory, let's plot all the graphs
# just for browsing.
for (i in seq(1, length(eight_leaves_trees))) {
    graph <- eight_leaves_trees[[i]](c("A", "B", "C", "D", "E", "F", "G", "H"))
    # This is how you include quotation marks in strings by the way:
    title <- paste("eight_leaves_trees[[", i,
                              "]](c(\"A\", \"B\", \"C\", \"D\", \"E\", \"F\", \"G\", \"H\"))", sep = "")
    plot(graph, color = "brown", title = title)
}</pre>
```

evaluate_f4

Description

Evaluates an f_4 statistics in a given environment.

Usage

evaluate_f4(graph, env, W, X, Y, Z)

Arguments

graph	The admixture graph.
env	The environment containing the graph parameters.
W	First population/sample.
Х	Second population/sample.
Υ	Third population/sample.
Z	Fourth population/sample.

Value

The f_4 value specified by the graph and the environment.

examine_edge_optimisation_matrix Examine the edge optimisation matrix to detect unfitted admix variables.

Description

If the essential number of equations is not higher than the essential number of edge variables, the quality of edge optimisation will not depend on the admix variables (expect possibly in isolated special cases where the quality can be worse), and a complaint will be given. Note: The admix variable not being fitted does not mean that there is no evidence of an admix event! Isolated values of the admix variables, possibly 0 or 1, might give significantly worse fit than a typical value (but not the other way around).

Usage

```
examine_edge_optimisation_matrix(matrix, tol = 1e-08)
```

Arguments

matrix	Not really a matrix but two (should be an output of build_edge_optimisation_matrix).
tol	Calulating the rank with $qr.solve$ sometimes crashes. Default 10^{-8} .

Value

An indicator of warning (complaint), coding all the possibilities in a way that is interpreted elsewhere (in summary.agraph_fit).

See Also

qr.solve

extract_admixture_proportion_parameters *Extract the admixture proportion parameter from edge specifications.*

Description

This function is simply selecting the edges with admixture proportion specifications so these can be handled when building a graph using agraph. It is not a function you would need to call explicitly, rather it is there to allow people *not* to use it to provide admixture proportions explicitly (which we normally wouldn't recommend).

Usage

extract_admixture_proportion_parameters(parent_edges)

Arguments

parent_edges Matrix created with the agraph_parents function.

Value

The parents edges reduced to the rows with admixture proportions.

extract_graph_parameters

Extract all the parameters a graph contains.

Description

The graph is parameterized by edge lengths and admixture proportions. This function extracts these parameters.

Usage

extract_graph_parameters(graph)

Arguments

graph The admixture graph.

Value

A list containing two values: edges, a vector of edges and admix_prop, a vector containing admixture proportions.

extract_trees Extract trees

Description

Extracts all the trees embedded in an agraph object

Usage

```
extract_trees(graph)
```

Arguments

graph An agraph object

Value

A list of trees

26

Description

Calculate the $f_2(A, B)$ statistics.

Usage

f2(graph, A, B)

Arguments

graph	The admixture graph
A	A leaf node.
В	A leaf node.

Value

A symbolic representation of the equation for the f_2 statistics given by the admixture graph.

f3

Calculate the $f_3(A; B, C)$ statistics.

Description

Calculate the $f_3(A; B, C)$ statistics.

Usage

f3(graph, A, B, C)

Arguments

graph	The admixture graph
A	A leaf node.
В	A leaf node.
С	A leaf node.

Value

A symbolic representation of the equation for the f_3 statistics given by the admixture graph.

Calculate the $f_4(W, X; Y, Z)$ statistics.

Description

Calculate the $f_4(W, X; Y, Z)$ statistics.

Usage

f4(graph, W, X, Y, Z)

Arguments

graph	The admixture graph.
W	A leaf node.
Х	A leaf node.
Y	A leaf node.
Z	A leaf node.

Value

The overlaps between paths from W to X and paths from Y to Z.

f4stats

Make a data frame an f_4 statistics object.

Description

This is mostly just a convinience function to set the class of a data frame such that we plot data as error bars in a meaningful way for statistics for admixture graphs.

Usage

f4stats(x)

Arguments

Х

Data frame with observed $D(f_4)$ statistics.

Value

Something about classes.

f4

fast_fit

Description

Given a table of observed f statistics and a graph, uses Nelder-Mead algorithm to find the graph parameters (edge lengths and admixture proportions) that minimize the value of cost_function, *i*. *e*. maximizes the likelihood of a graph with parameters given the observed data. Like fit_graph but dropping most of the analysis on the result. Intended for use in big iteration loops.

Usage

```
fast_fit(data, graph, point = list(rep(1e-05,
    length(extract_graph_parameters(graph)$admix_prop)), rep(1 - 1e-05,
    length(extract_graph_parameters(graph)$admix_prop))), Z.value = TRUE,
    concentration = calculate_concentration(data, Z.value),
    optimisation_options = NULL, parameters = extract_graph_parameters(graph),
    iteration_multiplier = 3)
```

Arguments

data	The data table, must contain columns W, X, Y, Z for sample names and D for the observed $f_4(W, X; Y, Z)$. May contain an optional column Z.value for the Z scores (the f statistics divided by the standard deviations).
graph	The admixture graph (an agraph object).
point	If the user wants to restrict the admixture proportions somehow, like to fix some of them. A list of two vectors: the lower and the upper bounds. As a default the bounds are just it little bit more than zero and less than one; this is because some- times the infimum of the values of cost function is at a point of non-continuity, and zero and one have reasons to be problematic values in this respect.
Z.value	Whether we calculate the default concentration from Z scores (the default option TRUE) or just use the identity matrix.
concentration	The Cholesky decomposition of the inverted covariance matrix. Default matrix determined by the parameter Z.value.
optimisation_op	otions
	Options to the Nelder-Mead algorithm.
parameters	In case one wants to tweak something in the graph.
iteration_multi	Iplier
	Given to mynonneg.

Value

A list containing only the essentials about the fit: graph is the graph input, best_error is the minimal value of cost_function, obtained when the admixture proportions are best_fit.

fast_fit

See Also

cost_function
agraph
calculate_concentration
optimset
fit_graph

Examples

For example, let's fit the following two admixture graph to an example data on bears:

```
data(bears)
print(bears)
```

```
leaves <- c("BLK", "PB", "Bar", "Chi1", "Chi2", "Adm1", "Adm2", "Denali", "Kenai", "Sweden")
inner_nodes <- c("R", "q", "r", "s", "t", "u", "v", "w", "x", "y", "z", "M", "N")</pre>
edges <- parent_edges(c(edge("BLK", "R"),</pre>
                          edge("PB", "v"),
                          edge("Bar", "x"),
                          edge("Chi1", "y"),
                          edge("Chi2", "y"),
edge("Adm1", "z"),
                          edge("Adm2", "z"),
                          edge("Denali", "t"),
                          edge("Kenai", "s"),
                          edge("Sweden", "r"),
                          edge("q", "R"),
                          edge("r", "q"),
                          edge("s", "r"),
                          edge("t", "s"),
                          edge("u", "q"),
edge("v", "u"),
                          edge("w", "M"),
                          edge("x", "N"),
                          edge("y", "x"),
                          edge("z", "w"),
                          admixture_edge("M", "u", "t"),
                          admixture_edge("N", "v", "w")))
admixtures <- admixture_proportions(c(admix_props("M", "u", "t", "a"),</pre>
                                         admix_props("N", "v", "w", "b")))
bears_graph <- agraph(leaves, inner_nodes, edges, admixtures)</pre>
plot(bears_graph, show_admixture_labels = TRUE)
```

fit <- fast_fit(bears, bears_graph)
print(fit\$best_error)</pre>

The result is just the minimal value of the cost function and the values of admixture proportions # where it's obtained, no deeper analysis of the fit. fast_plot

Description

This is a fast, deterministic and stand-alone function for visualizing the admixture graph. Has the bad habit if sometimes drawing several nodes at the exact same coordinates; for clearer reasults try plot.agraph (which, on the other hand, relies on numerical optimising of a compicated cost function and might be unpredictable).

Usage

```
fast_plot(x, ordered_leaves = NULL, show_admixture_labels = FALSE,
    show_inner_node_labels = FALSE, ...)
```

Arguments

х	The admixture graph.
ordered_leaves	The leaf-nodes in the left to right order they should be drawn.
show_admixture_	labels
	A flag determining if the plot should include the names of admixture propor-
	tions.
show_inner_node	e_labels
	A flag determining if the plot should include the names of inner nodes.
	Additional plotting options.

Value

A plot.

See Also

plot.agraph

Examples

taken from the collection of all the admixture graphs with four leaves and at # most two admixture events:

fast_plot(four_leaves_graphs[[24]](c("A", "B", "C", "D")))

To be fair, here is a graph that looks all right:

```
fast_plot(four_leaves_graphs[[25]](c("A", "B", "C", "D")))
```

filter_on_leaves Filter data so all W, X, Y and Z are leaves in the graph.

Description

Filter data so all W, X, Y and Z are leaves in the graph.

Usage

```
filter_on_leaves(data, graph)
```

Arguments

data	Data frame (or similar) object containing columns W, X, Y, and Z
graph	Admixture graph.

Value

Data frame with rows where W, X, Y, or Z are not leaves are removed.

fitted.agraph_fit *Predicted f statistics for the fitted graph.*

Description

Gets the predicted f statistics F for the fitted graph.

Usage

S3 method for class 'agraph_fit'
fitted(object, ...)

Arguments

object	The fitted object.
	Additional parameters.

See Also

link{summary.agraph_fit}

fit_graph

Description

Given a table of observed f statistics and a graph, uses Nelder-Mead algorithm to find the graph parameters (edge lengths and admixture proportions) that minimize the value of cost_function, *i. e.* maximizes the likelihood of a graph with parameters given the observed data. Like fast_fit but outputs a more detailed analysis on the results.

Usage

```
fit_graph(data, graph, point = list(rep(1e-05,
    length(extract_graph_parameters(graph)$admix_prop)), rep(1 - 1e-05,
    length(extract_graph_parameters(graph)$admix_prop))), Z.value = TRUE,
    concentration = calculate_concentration(data, Z.value),
    optimisation_options = NULL, parameters = extract_graph_parameters(graph),
    iteration_multiplier = 3, qr_tol = 1e-08)
```

Arguments

data	The data table, must contain columns W, X, Y, Z for sample names and D for the observed $f_4(W, X; Y, Z)$. May contain an optional column Z.value for the Z scores (the f statistics divided by the standard deviations).	
graph	The admixture graph (an agraph object).	
point	If the user wants to restrict the admixture proportions somehow, like to fix some of them. A list of two vectors: the lower and the upper bounds. As a default the bounds are just it little bit more than zero and less than one; this is because some- times the infimum of the values of cost function is at a point of non-continuity, and zero and one have reasons to be problematic values in this respect.	
Z.value	Whether we calculate the default concentration from Z scores (the default option TRUE) or just use the identity matrix.	
concentration	The Cholesky decomposition of the inverted covariance matrix. Default matrix determined by the parameter Z.value.	
optimisation_options		
	Options to the Nelder-Mead algorithm.	
parameters	In case one wants to tweak something in the graph.	
iteration_multi	plier	
	Given to mynonneg.	
qr_tol	Given to examine_edge_optimisation_matrix.	

fit_graph

Value

A class agraph_fit list containing a lot of information about the fit: data is the input data, graph is the input graph, matrix is the output of build_edge_optimisation_matrix, containing the full matrix, the column_reduced matrix without zero columns, and graph parameters, complaint coding wchich subsets of admixture proportions are trurly fitted, best_fit is the optimal admixture proportions (might not be unique if they are not trurly fitted), best_edge_fit is an example of optimal edge lengths, homogeneous is the reduced row echelon form of the matrix describing when a vector of edge lengths have no effect on the prediced statistics F, free_edges is one way to choose a subset of edge lengths in such a vector as free variables, bounded_edges is how we calculate the reamining edge lengths from the free ones, best_error is the minimum value of the cost_function, approximation is the predicted statistics F with the optimal graph parameters, parameters is jsut a shortcut for the graph parameters. See summary.agraph_fit for the interpretation of some of these results.

See Also

```
cost_function
agraph
calculate_concentration
optimset
fast_fit
```

Examples

For example, let's fit the following two admixture graph to an example data on bears:

```
data(bears)
print(bears)
```

```
edge("t", "s"),
edge("u", "q"),
edge("v", "u"),
edge("w", "M"),
edge("x", "N"),
edge("z", "w"),
admixture_edge("M", "u", "t"),
admixture_edge("N", "v", "w")))
admixtures <- admixture_proportions(c(admix_props("M", "u", "t", "a"),
admix_props("N", "v", "w", "b")))
bears_graph <- agraph(leaves, inner_nodes, edges, admixtures)
plot(bears_graph, show_admixture_labels = TRUE)
fit <- fit_graph(bears, bears_graph)</pre>
```

summary(fit)

It turned out the values of admixture proportions had no effect on the cost function. This is not # too surprising because the huge graph contains a lot of edge variables compared to the tiny # amount of data we used! Note however that the mere existence of the admixture event with non-# trivial (not zero or one) admixture proportion might still decrease the cost function.

fit_graph_list *Fit lots of graphs to data.*

Description

Fits a list of graphs to given data using parallel computation. This function needs doParallel, foreach and parallel installed.

Usage

```
fit_graph_list(data, graphs, cores)
```

Arguments

data	The data table.
graphs	List of graphs.
cores	Number of cores used.

Value

A list of fast_fit results.

See Also

all_graphs fit_permutations_and_graphs fit_permutations_and_graphs

Fit lots of graphs to data.

Description

Combines a list of (population) permutations and a list of graph topologies to a big list of graphs, then fits those graphs to given data using parallel computation. This function needs doParallel, foreach and parallel installed.

Usage

fit_permutations_and_graphs(data, permutations, graphs, cores)

Arguments

data	The data table.
permutations	List of population permutations.
graphs	List of functions for producing graphs.
cores	Number of cores used.

Value

A list of fast_fit results.

See Also

```
make_permutations
four_leaves_graphs
five_leaves_graphs
six_leaves_graphs
seven_leaves_graphs
eight_leaves_trees
fit_graph_list
```

Examples

Let's experiment by fitting all the graphs with five leaves and at most one admixture # event to a five population subset of the bear data. Note that with three data rows only # we do wisely by not concluding too much about the actual bear family tree; this is to # illustrate the function usage only!

```
data(bears)
data <- bears[16:18, ]</pre>
```

```
print(data)
permutations <- make_permutations(c("PB", "BLK", "Sweden", "Denali", "Kenai"))
graphs <- five_leaves_graphs
# We go with one core only as I don't know what kind of machine you are using.
fitted_graphs <- fit_permutations_and_graphs(data, permutations, graphs, 1)
# Now sort the fitted objects by best_error and see how the best graph looks like.
errors <- sapply(fitted_graphs, function(x) x$best_error)
best_graphs <- fitted_graphs[order(errors)]
plot(best_graphs[[1]]$graph, color = "goldenrod", title = best_graphs[[1]]$best_error)
# The same value for best_error actually occurs in the list 152 times because of our
# unsufficient data.</pre>
```

five_leaves_graphs Five leaves graphs.

Description

Kind of obsolete since the introduction of all_graphs. A comprehensive listing of all the 132 admixture graphs with five leaves and at most two admixture events. Our convention is that the position of the root does not matter (as long as it's not after an admixture event) and that graphs that have *eyes*, two inner nodes with the property that all the paths between any two leaves visits both or neither of them, are excluded. The reason is that the *f* statistics can't detect the exact position of the root or distinguish between an eye and a simple branch. The position of the root can be moved later with the function make_an_outgroup.

Usage

five_leaves_graphs

Format

A list of functions on five leaves and a parameter permutations which is FALSE by default. The outputs of these functions are either single agraph objects with the input vector as leaves, or if permutations is TRUE, lists of all the possible agraph objects with that leaf set up to symmetry.

See Also

all_graphs make_permutations fit_permutations_and_graphs fit_graph_list

36
format_path

add_a_leaf
add_an_admixture
add_an_admixture2
make_an_outgroup
Other graphs: eight_leaves_trees, four_leaves_graphs, seven_leaves_graphs, six_leaves_graphs

Examples

```
# While the usage of this function is pretty self-explanatory, let's plot all the graphs
# just for browsing.
for (i in seq(1, length(five_leaves_graphs))) {
   graph <- five_leaves_graphs[[i]](c("A", "B", "C", "D", "E"))
   # This is how you include quotation marks in strings by the way:
   title <- paste("five_leaves_graphs[[", i, "]](c(\"A\", \"B\", \"C\", \"D\", \"E\"))",
        sep = "")
   plot(graph, color = "purple", title = title)
}</pre>
```

format_path Create a path data frame from a list of nodes.

Description

Creates a path data frame from a list of nodes.

Usage

```
format_path(graph, nodes)
```

Arguments

graph	The admixture graph the path is in.
nodes	A list of nodes on a path.

Value

A data frame capturing the path and the probabilities/weights on the edges.

four_leaves_graphs Four leaves graphs.

Description

Kind of obsolete since the introduction of all_graphs. A comprehensive listing of all the 37 admixture graphs with four leaves and at most two admixture events. Our convention is that the position of the root does not matter (as long as it's not after an admixture event) and that graphs that have *eyes*, two inner nodes with the property that all the paths between any two leaves visits both or neither of them, are excluded. The reason is that the *f* statistics can't detect the exact position of the root or distinguish between an eye and a simple branch. The position of the root can be moved later with the function make_an_outgroup.

Usage

four_leaves_graphs

Format

A list of functions on four leaves and a parameter permutations which is FALSE by default. The outputs of these functions are either single agraph objects with the input vector as leaves, or if permutations is TRUE, lists of all the possible agraph objects with that leaf set up to symmetry.

See Also

all_graphs
make_permutations
fit_permutations_and_graphs
fit_graph_list
add_a_leaf
add_an_admixture
add_an_admixture2
make_an_outgroup
Other graphs: eight_leaves_trees, five_leaves_graphs, seven_leaves_graphs, six_leaves_graphs

Examples

```
# While the usage of this function is pretty self-explanatory, let's plot all the graphs
# just for browsing.
for (i in seq(1, length(four_leaves_graphs))) {
    graph <- four_leaves_graphs[[i]](c("A", "B", "C", "D"))
    # This is how you include quotation marks in strings by the way:
    title <- paste("four_leaves_graphs[[", i, "]](c(\"A\", \"B\", \"C\", \"D\"))", sep = "")
    plot(graph, color = "tomato3", title = title)</pre>
```

get_graph_f4_sign *Extracts the sign for the f_4 statistics predicted by the graph.*

Description

Extracts the sign for the f_4 statistics predicted by the graph.

Usage

get_graph_f4_sign(graph, W, X, Y, Z)

Arguments

graph	The admixture graph.	
W	First population/sample.	
Х	Second population/sample.	
Υ	Third population/sample.	
Z	Fourth population/sample.	

Value

The sign of the f_4 specified by the graph (or NA when it cannot be determined without knowing the graph parameters).

graphs_2_0	Admixture graphs of 2 leaves and 0 admixture events compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_2_0

Format

A data frame with 1 row and 9 variables.

Source

graphs_3_0

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_3_0

Format

A data frame with 1 row and 25 variables.

Source

Calculated using all_graphs and graph_to_vector.

graphs_3_1	Admixture graphs of 3 leaves and 1 admixture event compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_3_1

Format

A data frame with 3 rows and 49 variables.

Source

graphs_4_0

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_4_0

Format

A data frame with 3 rows and 49 variables.

Source

Calculated using all_graphs and graph_to_vector.

graphs_4_1	Admixture graphs of 4 leaves and 1 admixture event compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_4_1

Format

A data frame with 30 rows and 81 variables.

Source

graphs_4_2

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_4_2

Format

A data frame with 486 rows and 121 variables.

Source

Calculated using all_graphs and graph_to_vector.

graphs_5_0	Admixture graphs of 5 leaves and 0 admixture events compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_5_0

Format

A data frame with 15 rows and 81 variables.

Source

graphs_5_1

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_5_1

Format

A data frame with 315 rows and 121 variables.

Source

Calculated using all_graphs and graph_to_vector.

graphs_5_2	Admixture graphs of 5 leaves and 2 admixture events compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_5_2

Format

A data frame with 7710 rows and 169 variables.

Source

graphs_6_0

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_6_0

Format

A data frame with 105 rows and 121 variables.

Source

Calculated using all_graphs and graph_to_vector.

graphs_6_1	Admixture graphs of 6 leaves and 1 admixture event compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_6_1

Format

A data frame with 3780 rows and 169 variables.

Source

graphs_6_2

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_6_2

Format

A data frame with 131400 rows and 225 variables.

Source

Calculated using all_graphs and graph_to_vector.

graphs_7_0	Admixture graphs of 7 leaves and 0 admixture events compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_7_0

Format

A data frame with 945 rows and 169 variables.

Source

graphs_7_1

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_7_1

Format

A data frame with 51975 rows and 225 variables.

Source

Calculated using all_graphs and graph_to_vector.

graphs_8_0	Admixture graphs of 8 leaves and 0 admixture events compressed into
	vectors

Description

Use vector_to_graph on the n:th row to access the n:th graph as an agraph object.

Usage

graphs_8_0

Format

A data frame with 10395 rows and 225 variables.

Source

graph_environment Build an environment in which f statistics can be evaluated.

Description

Constructs an environment in which the f statistics for a graph can be evaluted, based on the parameters in a graph and values for edge lengths and admixture proportions (with defaults if not specified).

Usage

```
graph_environment(parameters, edge_lengths = NULL, admix_prop = NULL)
```

Arguments

parameters	The parameters of a graph as returned by extract_graph_parameters.
edge_lengths	If specified, a vector of edge lengths. Otherwise defaults are used.
admix_prop	If specified, a vector of admixture proportions. Otherwise defaults are used.

Value

A list containing two values: edges, a vector of edges and admix_prop, a vector containing admixture proportions.

graph_to_vector	Graph to vector.	
-----------------	------------------	--

Description

Encodes an agraph object into a logical vector for saving memory. The admixture proportion names will be lost.

Usage

```
graph_to_vector(graph)
```

Arguments

graph A graph.

Value

The logical vector representing the graph.

is_descendant_of Is descendant of.

Description

Tells whether a given node is descendant of another given node in a graph.

Usage

is_descendant_of(graph, offspring, ancestor)

Arguments

graph	A graph.
offspring	Potential offspring.
ancestor	Potential ancestor.

Value

A truth value.

is_negative

All overlaps are either empty or have a negative weight.

Description

All overlaps are either empty or have a negative weight.

Usage

```
is_negative(overlaps)
```

Arguments

overlaps Data frame representing path overlaps, typically generated by all_path_overlaps.

is_positive

Description

All overlaps are either empty or have a positive weight.

Usage

is_positive(overlaps)

Arguments

overlaps Data frame representing path overlaps, typically generated by all_path_overlaps.

is_unknown	Overlapping edges have both positive and negative contributions.	
------------	--	--

Description

Overlapping edges have both positive and negative contributions.

Usage

is_unknown(overlaps)

Arguments

overlaps Data frame representing path overlaps, typically generated by all_path_overlaps.

is_zero

All overlaps are empty.

Description

All overlaps are empty.

Usage

```
is_zero(overlaps)
```

Arguments

overlaps Data frame representing path overlaps, typically generated by all_path_overlaps.

log_likelihood

Description

Or the log likelihood of the observation, given graph with parameters, depending how things are modeled. Basically this is just cost_function that doesn't optimize the edge variables but has them as an argument instead.

Usage

```
log_likelihood(f, concentration, matrix, graph,
    parameters = extract_graph_parameters(graph))
```

Arguments

f	The observed f statistics (the column D from data).
concentration	The Cholesky decomposition of the inverted covariance matrix. So if S is the covariance matrix, this is $C = chol(S^{-1})$ satisfying $S^{-1} = C^t C$.
matrix	A column reduced edge optimisation matrix (typically given by the function build_edge_optimisation_matrix).
graph	The admixture graph. Here to give default value for:
parameters	Just because we need to know variable names.

Value

The output is a function. Given admixture proportions x and edge lengths e, the graph topology T implies an estimate F for the statistics f. This output function calculates

$$l = (F - f)^t S^{-1} (F - f)$$

from x and e. Up to a constant error and multiplier that is a log likelihood function, as

$$\det(2\pi S)^{-1/2} e^{-l/2}$$

can be seen as a likelihood of a graph with parameters, given the observation, or the other way around (possibly up to a normalization constant).

See Also

cost_function
edge_optimisation_function
calculate_concentration

log_sum_of_logs

Computes the log of a sum of numbers all given in log-space.

Description

Given a sequence of numbers $[\log(x_1), \log(x_2), ..., \log(x_n)]$, computes $\log(\sum_{i=1}^n x_i)$. For adding two numbers that are given in log space we use the expression $\max(x, y) + \log \log(\exp(-abs(x - y)))$ which is a good approximation if x and y are of the same order of magnitude, but if they are of very different sizes just returns the maximum of the two. To prevent adding numbers of very different magnitude we iteratively add the numbers pairwise. Because of numerical issues with doing this, the order of the input values can affect the result.

Usage

log_sum_of_logs(log_values)

Arguments

log_values Sequence of numbers in log space $[\log(x_1), \log(x_2), ..., \log(x_n)]$.

Value

 $\log(\sum_{i=1}^{n} x_i).$

make_an_outgroup	Make an outgroup.
------------------	-------------------

Description

Given a graph and a leaf, tries to put the root of the graph on the edge leading to the leaf. If not possible (*i. e.* if the leaf has admixture in its ancestry), puts the root somewhere else.

Usage

```
make_an_outgroup(graph, outgroup = "", all_neutral = FALSE)
```

Arguments

graph	An admixture graph.
outgroup	A leaf we want to be the outgroup.
all_neutral	For when other functions need to root graphs in a neutral way.

Value

An admixture graph with the given leaf as an outgroup, if possible.

See Also

make_permutations
four_leaves_graphs
five_leaves_graphs
six_leaves_graphs
seven_leaves_graphs
eight_leaves_trees
fit_permutations_and_graphs
fit_graph_list
add_a_leaf
add_an_admixture
add_an_admixture2

Examples

Here is a little family tree of some dinosaur-like animals.

```
species <- c("triceratops", "crocodile", "diplodocus", "tyrannosaurus", "chicken")
graph <- five_leaves_graphs[[1]](species)
plot(graph)</pre>
```

Of course we know that while this is correct as an undirected graph, "crocodile"
should really be the outgroup.

```
graph <- make_an_outgroup(graph, "crocodile")
plot(graph)</pre>
```

```
# Strictly speaking the graph is still a little misleading because unfortunately
# the (non-bird) dinosaurs are extinct :-(
```

<pre>make_mcmc_model</pre>	Collect the information about a graph and a data set needed to run an	
	MCMC on it.	

Description

Collect the information about a graph and a data set needed to run an MCMC on it.

Usage

```
make_mcmc_model(graph, data)
```

52

make_permutations

Arguments

graph	The admixture graph to analyse.
data	The data set to compute the posterior over.

Value

A model object wrapping functions and data needed to sample from the MCMC.

make_permutations List of permutations.

Description

List of permutations of given elements.

Usage

make_permutations(populations)

Arguments

populations A vector (of populations for example) of length between 4 and 8.

Value

A list of different permutations of the elements of x.

See Also

four_leaves_graphs
five_leaves_graphs
six_leaves_graphs
seven_leaves_trees
eight_leaves_trees
fit_permutations_and_graphs
add_a_leaf
add_an_admixture
add_an_admixture2

Examples

```
# The number of permutations of n elements is n!. Take 0! = 1, 1! = 1, 2! = 2
# and 3! = 6 for granted. Now we can estimate e:
FOUR <- length(make_permutations(c(1, 2, 3, 4)))
FIVE <- length(make_permutations(c(1, 2, 3, 4, 5)))
SIX <- length(make_permutations(c(1, 2, 3, 4, 5, 6)))
SEVEN <- length(make_permutations(c(1, 2, 3, 4, 5, 6, 7)))
EIGHT <- length(make_permutations(c(1, 2, 3, 4, 5, 6, 7, 8)))
1/1 + 1/1 + 1/2 + 1/6 + 1/FOUR + 1/FIVE + 1/SIX + 1/SEVEN + 1/EIGHT
# Hey that was pretty close!
```

model_bayes_factor_n Computes the Bayes factor between two models from samples from their posterior distributions.

Description

The likelihood of a graph can be computed by integrating over all the graph parameters (with appropriate priors). Doing this by sampling from priors is very inefficient, so we use samples from the posteriors to importance sample the likelihood. Given two graphs, and samples from their posteriors, we can estimate the Bayes factor between them.

Usage

```
model_bayes_factor_n(logL1, logL2, no_samples = 100)
```

Arguments

logL1	Samples of log likelihoods from the posterior distribution of the first graph.
logL2	Samples of log likelihoods from the posterior distribution of the second graph.
no_samples	Number of permutations to sample when computing the result.

Details

The numerical issues with adding a lot of numbers in log space is unstable so we get a better estimate by doing it several times on different permutations of the data. This function calculates the mean of the Bayes factors over different permutations of the input and estimates the standard deviation.

Value

The Bayes factor between the two graphs given as the mean and standard deviation over no_samples different permutations of the input.

54

model_likelihood

Computes the likelihood of a model from samples from its posterior distribution.

Description

The likelihood of a graph can be computed by integrating over all the graph parameters (with appropriate priors). Doing this by sampling from priors is very inefficient, so we use samples from the posteriors to importance sample the likelihood.

Usage

model_likelihood(log_likelihoods)

Arguments

log_likelihoods

Samples of log likelihoods from the posterior distribution of the graph.

Value

The likelihood of a graph where graph parameters are integrated out.

<pre>model_likelihood_n</pre>	Computes the likelihood of a model from samples from its posterior
	distribution.

Description

The likelihood of a graph can be computed by integrating over all the graph parameters (with appropriate priors). Doing this by sampling from priors is very inefficient, so we use samples from the posteriors to importance sample the likelihood.

Usage

model_likelihood_n(log_likelihoods, no_samples = 100)

Arguments

log_likelihoods

Samples of log likelihoods from the posterior distribution of the graph.

no_samples Number of permutations to sample when computing the result.

Details

The numerical issues with adding a lot of numbers in log space is unstable so we get a better estimate by doing it several times on different permutations of the data. This function calculates the mean of the likelihoods over different permutations of the input and estimates the standard devition.

Value

The likelihood of a graph where graph parameters are integrated out given as the mean and standard deviation over no_samples different permutations of the input.

mynonneg

Non negative least square solution.

Description

This is the function lsqnonneg from the package pracma, I just changed qr.solve into using Moore-Penrose inverse instead (ginv from MASS) as qr.solve crashes for some singular inputs. Now it won't crash but it's sometimes running for very long time (forever?), presumably with those problematic inputs. After too many steps the function halts and lies that the fit was terrible. I don't think this will cause problems.

Usage

mynonneg(C, d, iteration_multiplier = 3)

Arguments

С	The matrix.
d	The vector.
iteration_multi	plier
	The definition of "too many steps". Default value is 3 (times 10 times the matrix
	height).

Value

A vector (x) and the error (resid.norm).

See Also

lsqnonneg qr.solve ginv

56

no_admixture_events Get the number of admixture events in a graph.

Description

Get the number of admixture events in a graph.

Usage

```
no_admixture_events(x)
```

Arguments

x The graph.

Value

Number of admixture events in the graph.

no_admixture_events.agraph

Get the number of admixture events in a graph.

Description

Get the number of admixture events in a graph.

Usage

S3 method for class 'agraph'
no_admixture_events(x)

Arguments

x The graph.

Value

Number of admixture events in the graph.

no_admixture_events.agraph_fit

Get the number of admixture events in a fitted graph.

Description

Get the number of admixture events in a fitted graph.

Usage

```
## S3 method for class 'agraph_fit'
no_admixture_events(x)
```

Arguments

x The fitted graph.

Value

Number of admixture events in the graph.

Description

Get the number of admixture events in a list of fitted graph.

Usage

```
## S3 method for class 'agraph_fit_list'
no_admixture_events(x)
```

Arguments

x The graphs.

Value

Number of admixture events in the graphs.

no_poor_fits

Description

Get the number of tests in the fit where the predictions fall outside of the error bars.

Usage

no_poor_fits(fit, sigma = 6)

Arguments

fit	The fitted graph.
sigma	The width of the error bars.

Value

The poorly fitted tests.

```
no_poor_fits.agraph_fit
```

Get the number of tests in the fit where the predictions fall outside of the error bars.

Description

Get the number of tests in the fit where the predictions fall outside of the error bars.

Usage

```
## S3 method for class 'agraph_fit'
no_poor_fits(fit, sigma = 6)
```

Arguments

fit	The fitted graph.
sigma	The width of the error bars

Value

The poorly fitted tests.

no_poor_fits.agraph_fit_list

Get the number of tests in the fit where the predictions fall outside of the error bars.

Description

Get the number of tests in the fit where the predictions fall outside of the error bars.

Usage

```
## S3 method for class 'agraph_fit_list'
no_poor_fits(fit, sigma = 6)
```

Arguments

fit	The fitted graph.
sigma	The width of the error bars.

Value

The poorly fitted tests.

overlaps_sign *Get the sign of overlapping paths.*

Description

Get the sign of overlapping paths.

Usage

```
overlaps_sign(overlaps)
```

Arguments

overlaps Data frame representing path overlaps, typically generated by all_path_overlaps.

parent_edges

Description

Syntactic suggar for constructing edges in an admixture graph.

Usage

parent_edges(edges)

Arguments

edges List of edges.

path_overlap Collect the postive and negative overlap between two paths.

Description

Collects the postive and negative overlap between two paths.

Usage

```
path_overlap(path1, path2)
```

Arguments

path1	The first path.
path2	The second path

Value

The (admixture) probability of seeing the two paths together with the positive and negative edges in the overlap.

plot.agraph

Description

This is a basic drawing routine for visualising the graph. Uses Nelder-Mead algorithm and complicated heuristic approach to find aestethic node coordinates, but due to bad luck or an oversight in the heuristics, especially with larger graphs, might sometimes produce a weird looking result. Usually plotting again helps and if not, use the optional parameters to help the algorithm or try the faster and deterministic function fast_plot (which unfortunately is not very good at handling multiple admixture events).

Usage

```
## S3 method for class 'agraph'
plot(x, show_leaf_labels = TRUE, draw_leaves = TRUE,
    color = "yellowgreen", show_inner_node_labels = FALSE,
    draw_inner_nodes = FALSE, inner_node_color = color,
    show_admixture_labels = FALSE, parent_order = list(),
    child_order = list(), leaf_order = NULL, fix = list(), platform = 1,
    title = NULL, ...)
```

Arguments

Х	The admixture graph.	
<pre>show_leaf_labe</pre>	ls	
	A flag determining if leaf names are shown.	
draw_leaves	A flag determining if leaf nodes are drawn as little circles.	
color	Color of all drawn nodes unless overriden by inner_node_color.	
show_inner_node	e_labels	
	A flag determining if the plot should include the names of inner nodes.	
draw_inner_node	es	
	A flag determining if inner nodes are drawn as little circles.	
<pre>inner_node_col</pre>	or	
	Color of inner node circles, if drawn.	
show_admixture	_labels	
	A flag determining if the plot should include the names of admixture propor- tions.	
parent_order	An optional list of instuctions on which order from left to right to draw the parents of nodes. The list should contain character vectors of parents with the name of the child, <i>e.g.</i> child = c("left_parent", "right_parent"). Using automated heuristics for nodes not specified.	
child_order	An optional list of instuctions on which order from left to right to draw the children of nodes. The list should contain character vectors of children with the name of the parent, <i>e.g.</i> parent = c("left_child", "right_child"). Using automated heuristics for nodes not specified.	

leaf_order	An optional vector describing in which order should the leaves be drawn. Us- ing automated heuristic depending on parent_order and child_order if not specified. Accepts both a character vector of the leaves or a numeric vector interpreted as a permutation of the default order.
fix	If nothing else helps, the list fix can be used to correct the inner node coordinates given by the heuristics. Should contain numeric vectors of length 2 with the name of an inner node, <i>e.g.</i> inner_node = $c(0, 10)$, moving inner_node to the right 10 units where 100 is the plot width. Non-specified inner nodes are left in peace.
platform	By default admixture nodes are drawn with a horizontal platform for proportion labels, the width of which is half the distance between any two leaves. The number platform tells how many default platform widths should the platforms be wide, <i>i. e.</i> zero means no platform.
title	Optional title for the plot.
	Additional plotting options.

Value

A plot.

See Also

agraph

fast_plot

Examples

plot.agraph_fit *Plot the fit of a graph to data.*

Description

Plot the fit of a graph to data.

Usage

```
## S3 method for class 'agraph_fit'
plot(x, sigma = 6, grayscale = FALSE, ...)
```

Arguments

х	Fitted graph object.
sigma	How many standard deviations the error bars should be wide.
grayscale	Should the plot be in black and white?
	Additional parameters.

plot.f4stats

Description

Plot the fit of a graph to data.

Usage

S3 method for class 'f4stats'
plot(x, sigma = 6, ...)

Arguments

Х	Data frame with observed $D(f_4)$ statistics
sigma	How many sigmas the error bars should be wide.
	Additional parameters.

plot_fit_1

A plot of the cost function or number of fitted statistics.

Description

A plot of the cost function with respect to one admix variable specified by the user. Sorry about the name, all the good ones were taken and the fact that the word "graph" means two different things doesn't help any.

Usage

```
plot_fit_1(object, X, resolution = 100, show_fit = FALSE, sigma = 6, ...)
```

Arguments

object	The fitted object.
Х	An admix variable name (remember quotation marks).
resolution	How densely is the function evaluated.
show_fit	Should the function plot the number of statistics where the graph fits the data instead of the cost_function?
sigma	If show_fit is TRUE then each statistic is considered fitted if the difference be- tween a prediction and the observation statistics is no more than $D * \sigma/(2 * Z)$. Notice that even when plotting the number of fitted statistics, we have no guar- antee that the chosen variables maximize this number as the fitting function still optimizes cost_function.
	Additional parameters.

Value

Values for optimal cost function for values of X between zero and one, plotted.

See Also

plot_fit_2

plot_fit_2 A contour plot of the cost function.

Description

A contour plot of the cost function with respect to two admix variables specified by the user.

Usage

```
plot_fit_2(object, X, Y, resolution = 10, show_fit = FALSE, sigma = 6,
grayscale = FALSE, ...)
```

Arguments

object	The fitted object.
Х	An admix variable name (remember quotation marks).
Υ	An admix variable name (remember quotation marks).
resolution	How densely is the function evaluated.
show_fit	Should the function plot the number of statistics where the graph fits the data instead of the cost_function?
sigma	If show_fit is TRUE then each statistic is considered fitted if the difference be- tween a prediction and the observation statistics is no more than $D * \sigma/(2 * Z)$. Notice that even when plotting the number of fitted statistics, we have no guar- antee that the chosen variables maximize this number as the fitting function still optimizes cost_function.
grayscale	Should the figure be plotted in grayscale or in colour?
	Additional parameters passed to the plotting function contour.

Value

The matrix of values computed and plotted.

See Also

contour
plot_fit_1

poor_fits

Description

Get the tests in the fit where the predictions fall outside of the error bars.

Usage

poor_fits(fit, sigma = 6)

Arguments

fit	The fitted graph.
sigma	The width of the error bars.

Value

The poorly fitted tests.

poor_fits.agraph_fit Get the tests in the fit where the predictions fall outside of the error bars.

Description

Get the tests in the fit where the predictions fall outside of the error bars.

Usage

```
## S3 method for class 'agraph_fit'
poor_fits(fit, sigma = 6)
```

Arguments

fit	The fitted graph.
sigma	The width of the error bars.

Value

The poorly fitted tests.

```
poor_fits.agraph_fit_list
```

Get the tests in the fit where the predictions fall outside of the error bars.

Description

Get the tests in the fit where the predictions fall outside of the error bars.

Usage

```
## S3 method for class 'agraph_fit_list'
poor_fits(fit, sigma = 6)
```

Arguments

fit	The fitted graphs.
sigma	The width of the error bars.

Value

The poorly fitted tests.

print.agraph_fit *Print function for the fitted graph.*

Description

Prints the value of cost_function of the fitted graph, and complains if some or all of the admixture proportions aren't trurly fitted. Note: the admixture proportion not being trurly fitted does not necessarily mean that there is no evidence of an admix event!

Usage

S3 method for class 'agraph_fit'
print(x, ...)

Arguments

Х	The fitted object.
	Additional parameters.

See Also

link{summary.agraph_fit}

project_to_population Map sample names to population names.

Description

Map sample names to population names.

Usage

```
project_to_population(data, f)
```

Arguments

data	The data frame to modify.
f	Function mapping sample names to population names.

Details

This function maps the sample names in W, X, Y, and Z to population names (typically what an admixture graph has for leaves) and stores the original sample names so we can map them back again after using the graph for making predictions.

remove_duplicates *Remove duplicate graphs from a list.*

Description

Using canonise_graph to calculate unique characteristic logical vector for each graph in a given list of graphs, then sorts the list according to this attribute and remove repeated graphs. Leaf names count so that graphs with permuted leaves are considered different. Also organises similar graphs next to each other if organise is TRUE, but this is extremely slow.

Usage

```
remove_duplicates(graph_list, organise = FALSE, return_piles = FALSE)
```

Arguments

graph_list	A list of graphs with the same leaf set.
organise	If TRUE also organises isomorphic graphs (now disregarding leaf names) next to each other.
return_piles	If TRUE and organise is also TRUE, the output will be a list of lists of isomorphic graphs instead of one big list.

Value

A list of graphs that are all different (or a list of lists of graphs if both organise and return_piles are TRUE).

rename_nodes Rename nodes.

Description

Changes the names of the nodes of a graph. Capable of giving new standard names to the inner nodes in a way that only depends on the graph topology (without the root) and the leaf names. This is necessary when detecting when graphs are identical up to inner node and admixture proportion names, see canonise_graph and remove_duplicates.

Usage

```
rename_nodes(graph, newnames = list())
```

Arguments

graph	The graph to be renamed.
newnames	A list of new names, given in the form list(old = "new"). Nodes not listed will keep their old name, unless no list is given at all, in which case the leaves keep their old names while the inner nodes get new standardised names.

Value

A graph with new node names.

residuals.agraph_fit Errors of prediction in the fitted graph

Description

Gets f - F, the difference between predicted and observed statistics, for each data point used in the fit.

Usage

S3 method for class 'agraph_fit'
residuals(object, ...)

Arguments

object	The fitted object.
	Additional parameters.

70

See Also

link{summary.agraph_fit}

run_metropolis_hasting

Run a Metropolis-Hasting MCMC to sample graph parameters.

Description

The MCMC performs a random walk in transformed parameter space (edge lengths are log transformed and admixture proportions inverse Normal distribution transformed) and from this explores the posterior distribution of graph parameters.

Usage

```
run_metropolis_hasting(model, initial_state, iterations, no_temperatures = 1,
    cores = 1, no_flips = 1, max_tmp = 100, verbose = TRUE)
```

Arguments

model	Object constructed with make_mcmc_model.
initial_state	The initial set of graph parameters.
iterations	Number of iterations to sample.
no_temperatures	
	Number of chains in the MC3 procedure.
cores	Number of cores to spread the chains across. Best performance is when $cores = no_temperatures$.
no_flips	Mean number of times a flip between two chains should be proposed after each step.
max_tmp	The highest temperature.
verbose	Logical value determining if a progress bar should be shown during the run.

Details

Using the posterior distribution of parameters is one approach to getting parameter estimates and a sense of their variability. Credibility intervals can directly be obtained from sampled parameters; to get confidence intervals from the likelihood maximisation approach requires either estimating the Hessian matrix for the likelihood or a boot-strapping approach to the data.

From sampling the likelihood values for each sample from the posterior we can also compute the model likelihood (the probability of the data when integrating over all the model parameters). This gives us a direct way of comparing graphs since the ratio of likelihoods is the Bayes factor between the models. Comparing models using maximum likelihood estimates is more problematic since usually graphs are not nested models.

Value

A matrix containing the trace of the chain with temperature 1.

seven_leaves_graphs Seven leaves graphs.

Description

Kind of obsolete since the introduction of all_graphs. A comprehensive listing of all the 48 admixture graphs with seven leaves and at most one admixture event. Our convention is that the position of the root does not matter (as long as it's not after an admixture event) and that graphs that have *eyes*, two inner nodes with the property that all the paths between any two leaves visits both or neither of them, are excluded. The reason is that the *f* statistics can't detect the exact position of the root or distinguish between an eye and a simple branch. The position of the root can be moved later with the function make_an_outgroup.

Usage

seven_leaves_graphs

Format

A list of functions on seven leaves and a parameter permutations which is FALSE by default. The outputs of these functions are either single agraph objects with the input vector as leaves, or if permutations is TRUE, lists of all the possible agraph objects with that leaf set up to symmetry.

See Also

all_graphs
make_permutations
fit_permutations_and_graphs
fit_graph_list
add_a_leaf
add_an_admixture
add_an_admixture2
make_an_outgroup

Other graphs: eight_leaves_trees, five_leaves_graphs, four_leaves_graphs, six_leaves_graphs

Examples

```
# While the usage of this function is pretty self-explanatory, let's plot all the graphs
# just for browsing.
for (i in seq(1, length(seven_leaves_graphs))) {
   graph <- seven_leaves_graphs[[i]](c("A", "B", "C", "D", "E", "F", "G"))
   # This is how you include quotation marks in strings by the way:
   title <- paste("seven_leaves_graphs[[", i,
                          "]](c(\"A\", \"B\", \"C\", \"D\", \"E\", \"F\", \"G\"))", sep = "")</pre>
```
```
plot(graph, color = "seagreen", title = title)
}
```

seven_leaves_trees Seven leaves trees.

Description

The function seven_leaves_graphs is better than this as it also contains graphs with one admixture. (This function is only kept for legacy reasons.) Even more obsolete since the introduction of all_graphs.

Usage

seven_leaves_trees

Format

A list of functions on seven leaves. The outputs of these functions are agraph objects.

sf2

Calculate the $f_2(A, B)$ statistics.

Description

Calculate the $f_2(A, B)$ statistics.

Usage

sf2(graph, A, B)

Arguments

graph	The admixture graph
A	A leaf node.
В	A leaf node.

Value

A symbolic representation of the equation for the f_2 statistics given by the admixture graph.

sf3

Description

Calculate the $f_3(A; B, C)$ statistics.

Usage

sf3(graph, A, B, C)

Arguments

graph	The admixture graph.
A	A leaf node.
В	A leaf node.
С	A leaf node.

Value

A symbolic representation of the equation for the f_3 statistics given by the admixture graph.

sf4

Calculate the $f_4(W, X; Y, Z)$ statistics.

Description

Calculate the $f_4(W, X; Y, Z)$ statistics.

Usage

sf4(graph, W, X, Y, Z)

Arguments

graph	The admixture graph
W	A leaf node.
Х	A leaf node.
Υ	A leaf node.
Z	A leaf node.

Value

A symbolic representation of the equation for the f_4 statistics given by the admixture graph.

six_leaves_graphs Six leaves graphs.

Description

Kind of obsolete since the introduction of all_graphs . A comprehensive listing of all the 21 admixture graphs with six leaves and at most one admixture event. Our convention is that the position of the root does not matter (as long as it's not after an admixture event) and that graphs that have *eyes*, two inner nodes with the property that all the paths between any two leaves visits both or neither of them, are excluded. The reason is that the *f* statistics can't detect the exact position of the root or distinguish between an eye and a simple branch. The position of the root can be moved later with the function make_an_outgroup.

Usage

six_leaves_graphs

Format

A list of functions on six leaves and a parameter permutations which is FALSE by default. The outputs of these functions are either single agraph objects with the input vector as leaves, or if permutations is TRUE, lists of all the possible agraph objects with that leaf set up to symmetry.

See Also

all_graphs
make_permutations
fit_permutations_and_graphs
fit_graph_list
add_a_leaf
add_an_admixture
add_an_admixture2
make_an_outgroup

Other graphs: eight_leaves_trees, five_leaves_graphs, four_leaves_graphs, seven_leaves_graphs

Examples

```
plot(graph, color = "yellow4", title = title)
}
```

split_population Reverse a projection of samples to populations.

Description

Reverse a projection of samples to populations.

Usage

split_population(x)

Arguments

Х

The projected data or a fitted object on projected data.

split_population.agraph_fit

Reverse a projection of samples to populations.

Description

Reverse a projection of samples to populations.

Usage

```
## S3 method for class 'agraph_fit'
split_population(x)
```

Arguments

Х

The projected data or a fitted object on projected data.

76

split_population.data.frame

Reverse a projection of samples to populations.

Description

Reverse a projection of samples to populations.

Usage

```
## S3 method for class 'data.frame'
split_population(x)
```

Arguments

х

The projected data or a fitted object on projected data.

summary.agraph_fit *Summary for the fitted graph.*

Description

Prints:

Optimal admixture proportions and a complaint if some of them are not trury fitted, *i. e.* if after fixing a (possibly empty) subset of them, the rest have typically no effect on the cost function. Here typically means that some isolated values of the admixture proportions, like 0 or 1, might actually give a significantly worse fit than the constant fit given by any other values (but not better). Thus, an admixture proportion not being fitted does not always mean that there is no evidence of an admix event, as fixing them at 0 or 1 could make the fit worse while the exact value won't matter otherwise. The optimal edge lengths give one of the solutions for the best fit. It is generally not unique, as after fixing the admixture proportions, the best edge lengths are a non-negative least square solution for a system of linear equations. To get all the solutions one has to add any solution of the corresponding homogeneous system to the given exaple solution (and exclude possible negative values). The solutions of the homogeneous system are given as a set of free edge lengths that may obtain any non-negative value, and bounded edge lengths that linearly depend on the free ones. Minimal error is the value of the $cost_function$ at the fit.

Usage

```
## S3 method for class 'agraph_fit'
summary(object, ...)
```

Arguments

object	The fitted object.
	Additional parameters

sum_of_squared_errors Get the sum of squared errors for a fitted graph.

Description

Get the sum of squared errors for a fitted graph.

Usage

sum_of_squared_errors(x)

Arguments

x The fitted graph.

Value

SSE for the fit.

sum_of_squared_errors.agraph_fit

Get the sum of squared errors for a fitted graph.

Description

Get the sum of squared errors for a fitted graph.

Usage

S3 method for class 'agraph_fit'
sum_of_squared_errors(x)

Arguments

x The fitted graph.

Value

SSE for the fit.

Description

Get the sum of squared errors for a list of fitted graph.

Usage

```
## S3 method for class 'agraph_fit_list'
sum_of_squared_errors(x)
```

Arguments

x The fitted graphs.

Value

SSE for the fits.

thinning

Thins out an MCMC trace.

Description

Thins out an MCMC trace.

Usage

```
thinning(trace, k)
```

Arguments

trace	A trace from an MCMC run.
k	The number of lines to skip over per retained sample.

vector_to_graph Vector to graph.

Description

Interprets a logical vector back to an agraph object. The admixture proportion names are now lost.

Usage

```
vector_to_graph(vector)
```

Arguments

vector A logical vector.

Value

The graph corresponding to the vector.

Index

*Topic datasets bears, 16 eight_leaves_trees, 22 five_leaves_graphs, 36 four_leaves_graphs, 38 graphs_2_0, 39 graphs_3_0, 40 graphs_3_1, 40 graphs_4_0, 41 graphs_4_1, 41 graphs_4_2, 42 graphs_5_0, 42 graphs_5_1, 43 graphs_5_2, 43 graphs_6_0, 44 graphs_6_1, 44 graphs_6_2, 45 graphs_7_0, 45 graphs_7_1, 46 graphs_8_0, 46 seven_leaves_graphs, 72 seven_leaves_trees, 73 six_leaves_graphs, 75 add_a_leaf, 5, 8, 8, 22, 37, 38, 52, 53, 72, 75 add_an_admixture, 5, 7, 8, 22, 37, 38, 52, 53, 72,75 add_an_admixture2, 5, 7, 8, 22, 37, 38, 52, 53, 72, 75 add_graph_f4,9 add_graph_f4_sign, 10 admix_props, 11, 12 admixture_edge, 10, 12 admixture_proportions, 11, 12 admixturegraph-package, 4 agraph, 12, 22, 28, 29, 32, 33, 36, 38-47, 63, 72, 73, 75, 80 agraph_children, 13, 14 agraph_parents, 13, 13 agraph_weights, 14

all_graphs, 5, 8, 14, 22, 34, 36, 38-46, 72, 73.75 all_path_overlaps, 15, 48, 49, 60 all_paths, 15 bears. 16 build_edge_optimisation_matrix, 16, 20, 21, 24, 33, 50 burn_in, 17 calculate_concentration, 17, 29, 33, 50 canonise_expression, 18 canonise_graph, 18, 69, 70 character, 18 coef.agraph_fit, 19 contour, 66 cost_function, 19, 21, 28, 29, 32, 33, 50, 65, 66.68.77 edge, 12, 20 edge_optimisation_function, 19, 20, 21, 50 eight_leaves_trees, 22, 35, 37, 38, 52, 53, 72.75 eval, 16 evaluate_f4, 23 examine_edge_optimisation_matrix, 23, 32 extract_admixture_proportion_parameters, 24 extract_graph_parameters, 16, 25, 47 extract_trees, 25 f2, 26 f3, 26 f4, 18, 27 f4stats, 27 fast_fit, 28, 32-35 fast_plot, 30, 62, 63

filter_on_leaves, 31

fit_graph, 28, 29, 32 fit_graph_list, 5, 8, 15, 22, 34, 35, 36, 38, 52, 72, 75 fit_permutations_and_graphs, 5, 8, 22, 34, 35, 36, 38, 52, 53, 72, 75 fitted.agraph_fit, 31 five_leaves_graphs, 22, 35, 36, 38, 52, 53, 72.75 format_path, 37 four_leaves_graphs, 22, 35, 37, 38, 52, 53, 72.75 get_graph_f4_sign, 39 ginv, 56 graph_environment, 47 graph_to_vector, 39-46, 47 graphs_2_0, 39 graphs_3_0, 40 graphs_3_1, 40 graphs_4_0, 41 graphs_4_1, 41 graphs_4_2, 42 graphs_5_0, 42 graphs_5_1, 43 graphs_5_2, 43 graphs_6_0, 44 graphs_6_1, 44 graphs_6_2, 45 graphs_7_0, 45 graphs_7_1, 46 graphs_8_0, 46 is_descendant_of, 48 is_negative, 48 is_positive, 49 is_unknown, 49 is_zero, 49 log_likelihood, 20, 21, 50 log_sum_of_logs, 51 lsqnonneg, 56 make_an_outgroup, 5, 8, 22, 36-38, 51, 72, 75 make_mcmc_model, 52, 71 make_permutations, 22, 35, 36, 38, 52, 53, 72.75 model_bayes_factor_n, 54 model_likelihood, 55 model_likelihood_n, 55

mynonneg, 20, 21, 28, 32, 56 no_admixture_events, 57 no_admixture_events.agraph, 57 no_admixture_events.agraph_fit, 58 no_admixture_events.agraph_fit_list, 58 no_poor_fits, 59 no_poor_fits.agraph_fit, 59 no_poor_fits.agraph_fit_list, 60 optimset, 29, 33 overlaps_sign, 60 parent_edges, 12, 61 parse, 16 path_overlap, 61 plot.agraph, 12, 30, 62 plot.agraph_fit, 64 plot.f4stats, 65 plot_fit_1, 65, 66 plot_fit_2, 66, 66 poor_fits, 67 poor_fits.agraph_fit, 67 poor_fits.agraph_fit_list, 68 print.agraph_fit, 68 project_to_population, 69 gr.solve, 24, 56 remove_duplicates, 69, 70 rename_nodes, 70 residuals.agraph_fit,70 run_metropolis_hasting, 71 seven_leaves_graphs, 22, 35, 37, 38, 52, 72, 73.75 seven_leaves_trees, 53, 73 sf2, 73 sf3,74 sf4, 74 six_leaves_graphs, 22, 35, 37, 38, 52, 53, 72.75 split_population, 76 split_population.agraph_fit, 76 split_population.data.frame,77 sum_of_squared_errors, 78 sum_of_squared_errors.agraph_fit, 78 sum_of_squared_errors.agraph_fit_list, 79

82

INDEX

summary.agraph_fit, 24, 33, 77

thinning, 79

vector_to_graph, *39*–*46*, 80