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GenomeAdmixR-package Simulate Admixture of Genomes

Description

Individual-based simulations forward in time, simulating how patterns in ancestry along the genome change after admixture. The simulation assumes Wright-Fisher dynamics, e.g. random mating and non-overlapping generations. In the simulation, instead of specific alleles, local ancestry is tracked, thus assuming that local molecular data can always be uniquely traced back to one of the founding individuals (populations). The package provides functionality to perform such simulations, but also to perform post-hoc statistical analyses and to visualize the obtained results.

Version 2.1.7 - Improve documentation

Version 2.1.6 - check classes with inherits

Version 2.1.5 - Removed debugging output

Version 2.1.4 - Only output when verbose = TRUE

Version 2.1.3 - Changed DOI link in description

Version 2.1.2 - Improved testing

Version 2.1.1 - Removed GNU make dependency

Version 2.1 - Removed error in calculate_allele_frequency

Version 2.0.1 - Moved migration outside the modules

Version 2.0 - Added ancestry_module and sequence_module to distinguish between implementations of the model

Version 1.2 - Added example sequencing data

Version 1.2 - Added the option to load sequence data for admixing

Version 1.1 - Fixed a minor bug with plot_joyplot_frequencies

Version 1.1 - Improved tests

Version 1.1 - Improved recombination code (again)

Version 1.0 - Release associated with bioRxiv submission, to be found here: https://doi.org/10.1101/2020.10.19.343491

Version 0.66 - Improved recombination code, about twice as fast

Version 0.65 - Added testing and added logo

Version 0.64 - Reduced cyclomatic complexity

Version 0.63 - Updated random number generation

Version 0.62 - Updated to Roxygen

Version 0.61 - Added plot_over_time

Version 0.60 - Added admixture with migration

Version 0.59 - Updated frequency code under the hood

Version 0.58 - Renamed to GenomeAdmixR

Version 0.58 - Collapsed and improved many functions

Version 0.57 - Added function to generate admixed individuals

Version 0.56 - Added starting frequencies to 'simulate_admixture'

Version 0.55 - Extended 'calculate_marker_frequency' to handle a vector of locations

Version 0.55 - Increased accuracy of choosing a random position for recombination, this should prevent the rare bug fixed in version 0.54

Version 0.54 - Fixed a MAJOR bug regarding recombination: in rare cases, a crossover position could be picked on an existing junction, due to the limited number of digits in uniform()

Version 0.54 - Improved plot_difference_frequencies to handle modified input

Version 0.53 - Added multiplicative_selection

Version 0.52 - Added plot_difference_frequencies

Version 0.51 - Added tajima's d calculation

Version 0.50 - Added simulated_admixture until

Version 0.49 - Added 'simulate' to cpp

Version 0.48 - Added a general 'simulate' function

Version 0.47 - Changed the effect of migration

Version 0.46 - Added joyplot & increase_ancestor

Version 0.45 - Removed create_two_populations

Version 0.44 - Added tracking regions

Version 0.43 - Fixed bugs in select_population

Version 0.42 - Added initial and final frequency tables

Version 0.41 - Added multiple marker support

Version 0.40 - Collapsed selection functions

Version 0.39 - Added support for non-additive selection

Version 0.38 - Added track frequencies

Version 0.37 - Removed selection on regions

Version 0.36 - Added progress_bar option

Version 0.35 - Added calculate_marker_frequency

Version 0.34 - Added selection_markers

Version 0.33 - Fixed bugs in selection

Version 0.32 - Moved Fish.h code to Fish.cpp

Version 0.31 - Changed random number generator to R based

Version 0.30 - Added Recombination = 1 code

Version 0.29 - Changed internal junction representation: removed .left

Version 0.28 - Reverted to Agner Fog Random number generation

Version 0.27 - Speed up return types

Version 0.26 - Added class verification code

Version 0.25 - Squashed plotting bug

Version 0.24 - Removed Output.cpp

Version 0.23 - Removed number_of_founders from calc_allele_spectrum

Version 0.22 - Added save and load functions

Version 0.21 - Changed random-seed management

Version 0.20 - Removed superfluous code

Version 0.19 - Removed number_of_founders from Fst and LD code

Version 0.18 - Start of tracking changes

Author(s)

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References

Janzen, T., Diaz, F. (2020) Individual-based simulations of genome evolution with ancestry: the GenomeAdmixR R package. bioRxiv 2020.10.19.343491; doi: https://doi.org/10.1101/2020.10.19.343491

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ancestry_module

Creates a module to start simulations tracking local ancestry

Description

Module to perform simulations based on local ancestry

Usage

```
ancestry_module(
  input_population = NA,
  number_of_founders = 2,
  initial_frequencies = NA,
  morgan = 1,
 markers = NA,
  track_junctions = FALSE
)
```

Arguments

input_population

Potential earlier simulated population used as starting point for the simulation. If not provided by the user, the simulation starts from scratch.

number_of_founders

Number of unique ancestors / ancestries to be tracked in the simulation

initial_frequencies

A vector describing the initial frequency of each ancestor / ancestry. By default, equal frequencies are assumed. If a vector not summing to 1 is provided, the vector is normalized.

morgan Length of the genomic stretch simulated, expressed in Morgan (e.g. the number

of crossovers during meiosis)

markers A vector of locations of markers, with the location in Morgan. Ancestry at these

marker positions is tracked for every generation.

track_junctions

Tracks the average number of junctions over time if TRUE

Value

list with type = "Ancestry". Can be used in simulate_admixture.

```
calculate_allele_frequencies

Calculate allele frequencies
```

Description

Calculate for a number of regularly spaced markers the relative frequency of each ancestor in the population.

Usage

```
calculate_allele_frequencies(
  source_pop,
  locations = seq(0, 1, length.out = 100),
  progress_bar = FALSE
)
```

Arguments

source_pop Population for which to estimate allele frequencies

locations A vector indicating the locations (in Morgan) where to calculate the allele fre-

quencies.

progress_bar Displays a progress_bar if TRUE. Default value is TRUE

Details

Markers are equidistantly spaced, with a distance of step_size in between them.

Value

A tibble containing the allele frequencies

Examples

calculate_average_ld 7

```
calculate_average_ld Calculates the ld between two alleles
```

Description

calculate the average ld between two loci

Usage

```
calculate_average_ld(alleles_pos_1, alleles_pos_2)
```

Arguments

```
alleles_pos_1 alleles at locus 1 alleles_pos_2 alleles at locus 2
```

Value

```
a list with two entries: LD and r_squared
```

```
calculate_dist_junctions
```

collect the full distribution of junctions in the population

Description

calculates the distribution of junctions across the population

Usage

```
calculate_dist_junctions(pop)
```

Arguments

pop object of the class 'population'

Value

vector with two entries per individual, each indicating the number of junctions in the respective chromosomes

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calculate_fst

Calculate FST

Description

The FST value between two populations is calculated, given a number of markers. Markers are superimposed upon the (known) ancestry along the chromosome for all sampled individuals. Markers can be chosen to be regularly spaced, or randomly distributed.

Usage

```
calculate_fst(
  pop1,
  pop2,
  sampled_individuals = 10,
  number_of_markers = 100,
  random_markers = FALSE
)
```

Arguments

pop1 Population object pop2 Population object sampled_individuals

Number of individuals to base the FST upon. Individuals are randomly drawn from each population, a lower number speeds up calculations.

number_of_markers

Number of markers along the chromosome used to calculate FST metrics.

random_markers If TRUE, markers are randomly spaced along the chromosome, if FALSE, markers are equidistantly spaced along the chromosome.

Details

Uses the function wc from the package hierfstat to calculate the FST. The function wc computes the Weir and Cockerham F statistic.

Value

FST value

Examples

calculate_heterozygosity 9

calculate_heterozygosity

Calculate heterozygosity

Description

Calculate the average population level heterozygosity

Usage

```
calculate_heterozygosity(source_pop, locations, progress_bar = FALSE)
```

Arguments

source_pop	Population for which to estimate allele frequencies, or a list of individuals for which to calculate average heterozygosity
locations	A vector indicating the locations (in Morgan) of markers for which to calculate the heterozygosity
progress_bar	Displays a progress_bar if TRUE. Default value is TRUE

Value

A tibble containing the heterozygosities

calculate_ld	Calculate linkage disequilibrium statistics This function calculates two matrices, once containing all pairwise linkage disequilibrium (ld)
	values, and one matrix containing all pairwise r statistics

Description

Calculate linkage disequilibrium statistics This function calculates two matrices, once containing all pairwise linkage disequilibrium (ld) values, and one matrix containing all pairwise r statistics

```
calculate_ld(pop, sampled_individuals = 10, markers = NA, verbose = FALSE)
```

Arguments

pop focal population

sampled_individuals

Number of individuals randomly sampled to calculate the LD matrices

markers vector of markers. If a single number is used, that number of markers is ran-

domly placed along the genome.

verbose display verbose output, default is FALSE.

Value

An object containing two items:

ld_matrix Pairwise ld statistics for all markers rsq_matrix Pairwise rsq statistics for all markers

Examples

calculate_marker_frequency

Calculate allele frequencies at a specific marker location

Description

Calculate the relative frequency of each ancestor in the population at a specific marker location

Usage

```
calculate_marker_frequency(pop, location)
```

Arguments

pop Population for which to estimate allele frequencies at the given marker

location A vector or scalar of location(s) along the chromosome for which allele frequen-

cies are to be calculated. Locations are in Morgan.

combine_input_data 11

Value

A tibble containing the frequency of each present ancestor at the provided location. Ancestors with frequency = 0 are dropped out of the table. The tibble contains three columns: location, ancestor and frequency.

Examples

Description

Create data in a format that can be used by GenomeAdmixR, entries are sampled randomly from each input data set, with replacement. Probability of sampling from each input data set is driven by the input frequencies, and total number of individuals sampled is driven by pop_size.

Usage

```
combine_input_data(input_data_list, frequencies = NA, pop_size)
```

Arguments

```
input_data_list
list where each entry is the result of create_input_data
frequencies frequency of each entry in the list in the starting population
pop_size intended population size
```

Value

the input data entries are combined to one single population that can be used to seed simulate_admixture_data. Output is identical to create_input_data

12 create_iso_female

Description

function to generate artificial genomeadmixr_data

Usage

```
create_artificial_genomeadmixr_data(
  number_of_individuals,
  marker_locations,
  used_nucleotides = 1:4,
  nucleotide_frequencies = NA
)
```

Arguments

Value

genomeadmixr_data object ready for simulate_admixture_data

create_iso_female

function to simulate creation of an isofemale line

Description

create_isofemale simulates the creation of an isofemale line through extreme inbreeding.

dgrp2.3R.5k.data

Usage

```
create_iso_female(
  module = ancestry_module(),
  n = 1,
  inbreeding_pop_size = 100,
  run_time = 2000,
  num_threads = 1,
  verbose = FALSE
)
```

Arguments

module Source population from which isofemales are generated

n Number of isofemales to be generated

inbreeding_pop_size

Population size of the population used to generate homozygous individuals

run_time Maximum runtime used for inbreeding

num_threads number of threads. Default is 1. Set to -1 to use all available threads

verbose Displays verbose output if TRUE. Default value is FALSE

Details

To create an isofemale, two individuals are randomly picked from the source population. Using these two individuals, a new population is seeded, of size inbreeding_pop_size. Then, this population is allowed to inbreed until either run_time is reached, or until all individuals are homozygous and genetically identical, whatever happens first.

Value

A list of length n, where each entry is a fully homozygous isofemale.

dgrp2.3R.5k.data	A subset of sequencing data from the Drosophila Genetics Reference
	Panel

Description

This data set contains sequences from the 3R chromosome. Included are 4603 SNPs with at least 0.05 minor allele frequency, sequenced across 410 isofemale lines. Sequences were downloaded from http://dgrp2.gnets.ncsu.edu/data.html.

```
data("dgrp2.3R.5k.data")
```

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Format

genomeadmixr_data object

References

Mackay, T., Richards, S., Stone, E. et al. The Drosophila melanogaster Genetic Reference Panel. Nature 482, 173–178 (2012). https://doi.org/10.1038/nature10811>

Examples

iso_female_ancestry

Create isofemale

Description

Creates isofemale individuals, given a population

Usage

```
iso_female_ancestry(
  source_pop = NA,
  n = 1,
  inbreeding_pop_size = 100,
  run_time = 2000,
  morgan = 1,
  num_threads = 1,
  verbose = FALSE
)
```

Arguments

source_pop Source population from which isofemales are generated

n Number of isofemales to be generated

 ${\tt inbreeding_pop_size}$

Population size of the population used to generate homozygous individuals

run_time Maximum runtime used for inbreeding

morgan Size of the chromosome in Morgan (e.g. the number of crossovers during meio-

sis)

num_threads number of threads. Default is 1. Set to -1 to use all available threads

verbose Displays verbose output if TRUE. Default value is FALSE

iso_female_sequence 15

Details

To create an isofemale, two individuals are randomly picked from the source population. Using these two individuals, a new population is seeded, of size inbreeding_pop_size. Then, this population is allowed to inbreed until either run_time is reached, or until all individuals are homozygous and genetically identical, whatever happens first.

Value

A list of length n, where each entry is a fully homozygous isofemale.

Description

Creates isofemale individuals, given a population

Usage

```
iso_female_sequence(
  input_data = NA,
  n = 1,
  inbreeding_pop_size = 100,
  run_time = 2000,
  morgan = 1,
  recombination_rate = NA,
  num_threads = 1,
  verbose = FALSE
)
```

Arguments

input_data Source population from which isofemales are generated

n Number of isofemales to be generated

inbreeding_pop_size

Population size of the population used to generate homozygous individuals

run_time Maximum runtime used for inbreeding

morgan Size of the chromosome in Morgan (e.g. the number of crossovers during meio-

sis)

recombination_rate

rate in cM / Mbp, used to map recombination to the markers. If the recombination_rate is not set, the value for Morgan is used, assuming that the markers

included span an entire chromosome.

verbose Displays verbose output if TRUE. Default value is FALSE

load_population

Details

To create an isofemale, two individuals are randomly picked from the source population. Using these two individuals, a new population is seeded, of size inbreeding_pop_size. Then, this population is allowed to inbreed until either run_time is reached, or until all individuals are homozygous and genetically identical, whatever happens first.

Value

A list of length n, where each entry is a fully homozygous isofemale.

load_population

Load a population from file

Description

Loads a population that has previously been written to file.

Usage

```
load_population(file_name)
```

Arguments

file_name

Name of the file to save the population

Details

This function is a wrapper for readRDS.

Value

A population object

See Also

save_population

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migration_settings

Function to manage settings associated with migration

Description

creates a list with settings associated with migration.

Usage

```
migration_settings(
  migration_rate = NA,
  stop_at_critical_fst = FALSE,
  critical_fst = NA,
  population_size = c(100, 100),
  initial_frequencies = list(c(1, 0), c(0, 1)),
  generations_between_update = 10,
  sampled_individuals = 10,
  number_of_markers = 100,
  random_markers = TRUE
)
```

Arguments

migration_rate Rate of migration between the two populations. Migration is implemented such that with probability m (migration rate) one of the two parents of a new offspring is from the other population, with probability 1-m both parents are of the focal population.

stop_at_critical_fst

option to stop at a critical FST value, default is FALSE

vector of population sizes, one size for each population

initial_frequencies

A list describing the initial frequency of each ancestor in each population. Each entry in the list contains a vector with the frequencies for all ancestor. The length of the vector indicates the number of unique ancestors. If a vector not summing to 1 is provided, the vector is normalized.

generations_between_update

The number of generations after which the simulation has to check again whether the critical Fst value is exceeded

sampled_individuals

Number of individuals to be sampled at random from the population to estimate Fst

number_of_markers

Number of markers to be used to estimate Fst

random_markers Are the markers to estimate Fst randomly distributed, or regularly distributed? Default is TRUE.

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Value

list with migration associated settings. To be used to pass on migration settings to simulate_admixture.

```
plink_to_genomeadmixr_data
function to convert plink style (ped/map) data to genome_admixr_data
```

Description

function to convert plink style (ped/map) data to genome_admixr_data

Usage

```
plink_to_genomeadmixr_data(
   ped_data,
   map_data,
   chosen_chromosome,
   verbose = FALSE
)
```

Arguments

```
\begin{tabular}{lll} ped\_data & result of read.table(ped\_file, header = F) \\ map\_data & result of read.table(map\_file, header = F) \\ chosen\_chromosome & chromosome of choice \\ verbose & verbose output \\ \end{tabular}
```

Value

genomeadmixr_data object ready for simulate_admixture_data

```
plot.individual plot the genome of an individual
```

Description

visualise ancestry blocks on both chromosomes

```
## S3 method for class 'individual'
plot(x, cols = NA, ...)
```

plot_chromosome 19

Arguments

X	object of type individual
cols	colors for the different ancestors
	other arguments

Value

No return value

plot_chromosome plots a chromosome

Description

This function plots a chromosome in the range [xmin, xmax]. Colors indicate different ancestry.

Usage

```
plot_chromosome(chrom, xmin = 0, xmax = 1)
```

Arguments

chrom object of type chromosome, typically a table with two columns. The first column

indicates the start of an ancestry block (location in Morgan), the second column

indicates the ancestry type.

xmin minimum value of the range, default = 0. xmax maximum value of the range, default = 1.

Value

No return value

Examples

plot_difference_frequencies

Plot the change in frequency between the start and end of a simulation

Description

This function plots the change in frequency of one or multiple ancestors after performing a simulation.

Usage

```
plot_difference_frequencies(
  results,
  picked_ancestor = "ALL",
  picked_population = 1
)
```

Arguments

results

An object which is the result of $simulate_admixture$ being a list with four properties: population, frequencies, initial_frequencies and final frequencies

picked_ancestor

Default is "ALL", where different colors indicate different ancestors. Alternatively, for clarity, the user can specify a specific ancestral allele, and only that allele is plotted

picked_population

If multiple populations were simulated (in the case of simulate_admixture_migration), which population should be plotted? Default is population_1.

Value

a ggplot2 object

Examples

plot_dist_junctions 21

plot_dist_junctions

plot the distribution of junctions

Description

plots the distribution of junctions in the population using base R

Usage

```
plot_dist_junctions(pop)
```

Arguments

pop

of the class 'population'

Value

No return value

plot_frequencies

Plot the frequencies of all ancestors along the genome.

Description

This function plots the frequency of all ancestors after performing a simulation.

```
plot_frequencies(
  result,
  locations = seq(0, 1, length.out = 100),
  progress_bar = FALSE
)
```

Arguments

result An object which is the result of select_population or create_population_selection,

being a list with four properties: population, frequencies, initial_frequencies

and final frequencies

locations A vector indicating the locations (in Morgan) where to calculate the allele fre-

quencies.

progress_bar Displays a progress_bar if TRUE. Default value is FALSE

Value

```
a ggplot2 object
```

Examples

```
plot_joyplot_frequencies
```

make a joy plot of the distribution of allele frequencies within a region

Description

This function plots the distribution of allele frequencies within a region over time, making use of a 'joyplot'

Usage

```
plot_joyplot_frequencies(
  frequencies,
  time_points,
  picked_ancestor = "ALL",
  picked_population = 1
)
```

Arguments

frequencies A tibble containing four columns: time, location, ancestor, frequency.

Typically one of the items returned by create_population_selection or select_population

when the user specifies track_frequency.

time_points A sequence of time points for which the user wants to create the joyplot

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```
picked_ancestor
```

Default is "ALL", where different colors indicate different ancestors. Alternatively, for clarity, the user can specify a specific ancestral allele, and only that allele is plotted

picked_population

If multiple populations were simulated (in the case of simulate_admixture_migration), which population should be plotted? Default is population_1.

Value

a ggplot object

Examples

```
s <- 0.01
select_matrix <- matrix(nrow = 1, ncol = 5)</pre>
select_matrix[1, ] \leftarrow c(0.25, 1.0, 1 + 0.5 * s, 1 + s, 0)
markers \leftarrow seq(from = 0.2, to = 0.3, length.out = 100)
selected_pop <- simulate_admixture(</pre>
                    module = ancestry_module(number_of_founders = 10,
                                               morgan = 1,
                                               markers = markers),
                     pop_size = 1000,
                     total_runtime = 11,
                     select_matrix = select_matrix)
require(ggplot2)
plot_joyplot_frequencies(frequencies = selected_pop$frequencies,
                          time_points = 0:11,
                          picked_ancestor = "ALL")
# joyplot frequencies returns a ggplot object, so we can
# add extra elements:
plot_joyplot_frequencies(frequencies = selected_pop$frequencies,
                          time_points = 0:11,
                          picked_ancestor = "ALL") +
 ggplot2::xlab("Location") +
 ggplot2::ylab("Generations")
```

plot_over_time

Plot the frequencies of all ancestors over time

Description

This function plots the frequency of all ancestors over time at a specific location on the chromosome, after performing a simulation.

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Usage

```
plot_over_time(frequencies, focal_location)
```

Arguments

frequencies A tibble containing four columns: time, location, ancestor, frequency. A

fifth colum population can be included if the tibble is the result of simulate_admixture_migration.

focal_location Location (in Morgan) where to plot the allele frequencies.

Value

```
a ggplot2 object
```

Examples

plot_start_end

Plot both the starting frequencies and the final frequencies in one plot

Description

This function plots the distribution of both the starting and the final frequencies in one plot

Usage

```
plot_start_end(results, picked_ancestor = "ALL", picked_population = 1)
```

Arguments

results

An object which is the result of simulate_admixture, being a list with four properties: population, frequencies, initial_frequencies and final frequencies

picked_ancestor

Default is "ALL", where different colors indicate different ancestors. Alternatively, for clarity, the user can specify a specific ancestral allele, and only that allele is plotted

picked_population

If multiple populations were simulated (in the case of simulate_admixture_migration), which population should be plotted? Default is population_1.

Value

```
a ggplot object
```

Examples

```
print.genomeadmixr_data
```

print an individual to the console

Description

prints an object of class genomeadmixr_data to the console

Usage

```
## S3 method for class 'genomeadmixr_data' print(x, ...)
```

Arguments

```
x individual
```

... other arguments

Value

No return value

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print.individual

print an individual to the console

Description

prints an object of class individual to the console

Usage

```
## S3 method for class 'individual' print(x, ...)
```

Arguments

x individual

... other arguments

Value

No return value

print.population

print a population object

Description

prints the contents of a population nicely

Usage

```
## S3 method for class 'population' print(x, ...)
```

Arguments

x input population
... other arguments

Value

No return value

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read_input_data

read sequence data from file to be used in simulation

Description

Create data in a format that can be used by GenomeAdmixR

Usage

```
read_input_data(
    file_names,
    type,
    chosen_chromosome,
    number_of_snps = NA,
    random_snps = TRUE,
    verbose = FALSE
)
```

Arguments

file_names names of input files

type type of data, options are 'ped' and 'vcf'

chosen_chromosome

GenomeAdmixR simulates only a single chromosome.

number_of_snps number of snps to be loaded from file, default is to load all snps

random_snps if a subset of all snps has to be taken, should these be sampled sequentially (e.g.

the first 100 snps) or randomly (100 randomly sampled snps) (examples are for

'number_of_snps' = 100).

verbose give verbose output

Value

list with two properties: genomes a matrix with the sequence translated to numerics, such that [actg] corresponds to [1234], and missing data is represented with "-". Rows in the matrix correspond to chromosomes, and columns represent bases. Two consecutive rows represent an individual, such that rows 1-2 are individual, rows 3-4 are one individual etc. markers corresponds to the locations of the markers (in bp) on the chosen chromosome.

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save_population

Save a population to file

Description

Saves a population to file for later use

Usage

```
save_population(population, file_name, compression = TRUE)
```

Arguments

population Object of class population

file_name Name of the file to save the population

compression By default, the population is compressed to reduce file size. See for more infor-

mation saveRDS

Details

This function functions as a wrapper for the base function saveRDS.

Value

No return value

sequence_module

create sequence module

Description

creates a sequence module, which contains all relevant information in order to perform a simulation based on sequence data.

```
sequence_module(
  molecular_data = NA,
  initial_frequencies = NA,
  morgan = 1,
  recombination_rate = NA,
  markers = NA,
  mutation_rate = 0,
  substitution_matrix = matrix(1/4, 4, 4)
)
```

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Arguments

molecular_data Genomic data used as input, should be of type genomeadmixr_data. Either a single dataset is provided, or a list of multiple genomeadmixr_data objects.

initial_frequencies

A vector describing the initial contribution of each provided input data set to the starting hybrid swarm. By default, equal frequencies are assumed. If a vector not summing to 1 is provided, the vector is normalized.

morgan

Length of the molecular sequence in Morgan (e.g. the number of crossovers during meiosis), alternatively, the recombination rate can be used, see below.

recombination_rate

rate in cM / Mbp, used to map recombination to the markers. If the recombination_rate is not set, the value for Morgan is used, assuming that the markers included span an entire chromosome.

markers

A vector of locations of markers, these markers are tracked for every generation.

mutation_rate

the per base probability of mutation. Default is 0.

substitution_matrix

a 4x4 matrix representing the probability of mutating to another base (where [1/2/3/4] = [a/c/t/g]), conditional on the event of a mutation happening. Default is the JC69 matrix, with equal probabilities for all transitions / transversions.

Value

sequence module object, used as starting point for simulate_admixture.

simulate_admixture

Individual based simulation of the breakdown of contiguous ancestry blocks.

Description

Individual based simulation of the breakdown of contiguous ancestry blocks, with or without selection. Simulations can be started from scratch, or from a predefined input population.

```
simulate_admixture(
  module = ancestry_module(),
  pop_size = 100,
  total_runtime = 100,
  migration = migration_settings(),
  select_matrix = NA,
  multiplicative_selection = TRUE,
  verbose = FALSE,
  num_threads = 1
)
```

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Arguments

module Chosen module to simulate, either created with module_ancestry or module_sequence.

pop_size The number of individuals in the population. If the number is larger than the

number of individuals in the input population (if provided), additional individuals are sampled randomly from the input population to reach the intended size.

total_runtime Number of generations

migration settings associated with migration, should be created with migration_settings

select_matrix Selection matrix indicating the markers which are under selection. If not pro-

vided by the user, the simulation proceeds neutrally. If provided, each row in the matrix should contain five entries: location location of the marker under selection (in Morgan) fitness of wildtype (aa) fitness of heterozygote (aA) fitness of homozygote mutant (AA) Ancestral type that represents the

mutant allele A

multiplicative_selection

Default: TRUE. If TRUE, fitness is calculated for multiple markers by multiplying fitness values for each marker. If FALSE, fitness is calculated by adding

fitness values for each marker.

verbose Verbose output if TRUE. Default value is FALSE

num_threads number of threads. Default is 1. Set to -1 to use all available threads

Value

A list with: population a population object, and three tibbles with allele frequencies (only contain values of a vector was provided to the argument markers: frequencies, initial_frequencies and final_frequencies. Each tibble contains four columns, time, location, ancestor and frequency, which indicates the number of generations, the location along the chromosome of the marker, the ancestral allele at that location in that generation, and finally, the frequency of that allele.

Examples

```
# local ancestry simulation
two_populations <- simulate_admixture(</pre>
                         module = ancestry_module(number_of_founders = 3,
                                                   morgan = 0.8),
                         migration = migration_settings(
                                          migration_rate = 0.01,
                                          population_size = c(100, 100),
                         total_runtime = 10)
# sequence simulation
data(dgrp2.3R.5k.data)
sequence_population <-
      simulate_admixture(
                  module = sequence_module(molecular_data = dgrp2.3R.5k.data,
                           recombination_rate = 0.2,
                           mutation_rate = 1e-5),
                  pop\_size = 1000,
                  total_runtime = 10)
```

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simulate_ancestry	Individual based simulation of the breakdown of contiguous ancestry
	blocks.

Description

Individual based simulation of the breakdown of contiguous ancestry blocks, with or without selection. Simulations can be started from scratch, or from a predefined input population.

Usage

```
simulate_ancestry(
   input_population = NA,
   pop_size = NA,
   number_of_founders = 2,
   initial_frequencies = NA,
   total_runtime = 100,
   morgan = 1,
   num_threads = 1,
   select_matrix = NA,
   markers = NA,
   verbose = FALSE,
   track_junctions = FALSE,
   multiplicative_selection = TRUE
)
```

Arguments

input_population

Potential earlier simulated population used as starting point for the simulation. If not provided by the user, the simulation starts from scratch.

pop_size

The number of individuals in the population. If the number is larger than the number of individuals in the input population (if provided), additional individuals are sampled randomly from the input population to reach the intended size.

number_of_founders

Number of unique ancestors

initial_frequencies

A vector describing the initial frequency of each ancestor. By default, equal frequencies are assumed. If a vector not summing to 1 is provided, the vector is normalized.

total_runtime Number of generations

morgan Length of the chromosome in Morgan (e.g. the number of crossovers during

meiosis)

num_threads number of threads. Default is 1. Set to -1 to use all available threads

select_matrix Selection matrix indicating the markers which are under selection. If not pro-

vided by the user, the simulation proceeds neutrally. If provided, each row in the matrix should contain five entries: location location of the marker under selection (in Morgan) fitness of wildtype (aa) fitness of heterozygote (aA) fitness of homozygote mutant (AA) Ancestral type that represents the

mutant allele A

markers A vector of locations of markers (relative locations in [0, 1]). If a vector is

provided, ancestry at these marker positions is tracked for every generation.

verbose Verbose output if TRUE. Default value is FALSE

track_junctions

Track the average number of junctions over time if TRUE

multiplicative_selection

Default: TRUE. If TRUE, fitness is calculated for multiple markers by multiplying fitness values for each marker. If FALSE, fitness is calculated by adding fitness values for each marker.

Value

A list with: population a population object, and three tibbles with allele frequencies (only contain values of a vector was provided to the argument markers: frequencies, initial_frequencies and final_frequencies. Each tibble contains four columns, time, location, ancestor and frequency, which indicates the number of generations, the location along the chromosome of the marker, the ancestral allele at that location in that generation, and finally, the frequency of that allele.

simulate_ancestry_migration

Individual based simulation of the breakdown of contiguous ancestry blocks in two populations linked by migration

Description

Individual based simulation of the breakdown of contiguous ancestry blocks, with or without selection. Simulations can be started from scratch, or from a predefined input population. Two populations are simulated, connected by migration

```
simulate_ancestry_migration(
  input_population_1 = NA,
  input_population_2 = NA,
  pop_size = c(100, 100),
  initial_frequencies = list(c(1, 0), c(0, 1)),
  total_runtime = 100,
  morgan = 1,
  num_threads = 1,
```

```
select_matrix = NA,
markers = NA,
verbose = FALSE,
track_junctions = FALSE,
multiplicative_selection = TRUE,
migration_rate = 0,
stop_at_critical_fst = FALSE,
critical_fst = 0.1,
generations_between_update = 100,
sampled_individuals = 10,
number_of_markers = 100,
random_markers = TRUE
```

Arguments

input_population_1

Potential earlier simulated population used as starting point for the simulation. If not provided by the user, the simulation starts from scratch.

input_population_2

Potential earlier simulated population used as starting point for the simulation. If not provided by the user, the simulation starts from scratch.

pop_size Vector containing the number of individuals in both populations.

initial_frequencies

A list describing the initial frequency of each ancestor in each population. Each entry in the list contains a vector with the frequencies for all ancestor. The length of the vector indicates the number of unique ancestors. If a vector not summing to 1 is provided, the vector is normalized.

total_runtime Number of generations

morgan Length of the chromosome in Morgan (e.g. the number of crossovers during

meiosis)

num_threads number of threads. Default is 1. Set to -1 to use all available threads

select_matrix Selection matrix indicating the markers which are under selection. If not pro-

vided by the user, the simulation proceeds neutrally. If provided, each row in the matrix should contain five entries: location location of the marker under selection (in Morgan) fitness of wildtype (aa) fitness of heterozygote (aA) fitness of homozygote mutant (AA) Ancestral type that representes the

mutant allele A

markers A vector of locations of markers (relative locations in [0, 1]). If a vector is

provided, ancestry at these marker positions is tracked for every generation.

verbose Verbose output if TRUE. Default value is FALSE

track_junctions

Track the average number of junctions over time if TRUE

multiplicative_selection

Default: TRUE. If TRUE, fitness is calculated for multiple markers by multiplying fitness values for each marker. If FALSE, fitness is calculated by adding fitness values for each marker.

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migration_rate Rate of migration between the two populations. Migration is implemented such that with probability m (migration rate) one of the two parents of a new offspring is from the other population, with probability 1-m both parents are of the focal population.

stop_at_critical_fst

option to stop at a critical FST value, default is FALSE

critical_fst the critical fst value to stop, if stop_simulation_at_critical_fst is TRUE generations_between_update

The number of generations after which the simulation has to check again whether the critical Fst value is exceeded

sampled_individuals

Number of individuals to be sampled at random from the population to estimate Fst

number_of_markers

Number of markers to be used to estimate Fst

random_markers Are the markers to estimate Fst randomly distributed, or regularly distributed?

Default is TRUE.

Value

A list with: population_1, population_2 two population objects, and three tibbles with allele frequencies (only contain values of a vector was provided to the argument markers: frequencies, initial_frequencies and final_frequencies. Each tibble contains five columns, time, location, ancestor, frequency and population, which indicates the number of generations, the location along the chromosome of the marker, the ancestral allele at that location in that generation, the frequency of that allele and the population in which it was recorded (1 or 2). If a critical fst value was used to terminate the simulation, and object FST with the final FST estimate is returned as well.

simulate_sequence

Individual based simulation of the breakdown of contiguous ancestry blocks.

Description

Individual based simulation of the breakdown of contiguous ancestry blocks, with or without selection. Simulations can be started from scratch, or from a predefined input population.

```
simulate_sequence(
  input_data = NA,
  pop_size = NA,
  initial_frequencies = NA,
  total_runtime = 100,
  morgan = 1,
  recombination_rate = NA,
```

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```
num_threads = 1,
select_matrix = NA,
markers = NA,
verbose = FALSE,
multiplicative_selection = TRUE,
mutation_rate = 0,
substitution_matrix = matrix(1/4, 4, 4)
```

Arguments

input_data Ge

Genomic data used as input, should be of type genomeadmixr_data. Either a single dataset is provided, or a list of multiple genomeadmixr_data objects.

pop_size

Vector containing the number of individuals in both populations.

initial_frequencies

A vector describing the initial contribution of each provided input data set to the starting hybrid swarm. By default, equal frequencies are assumed. If a vector not summing to 1 is provided, the vector is normalized.

total_runtime

Number of generations

morgan

Length of the chromosome in Morgan (e.g. the number of crossovers during meiosis)

recombination_rate

rate in cM / Mbp, used to map recombination to the markers. If the recombination_rate is not set, the value for Morgan is used, assuming that the markers included span an entire chromosome.

 $num_threads$

number of threads. Default is 1. Set to -1 to use all available threads

select_matrix

Selection matrix indicating the markers which are under selection. If not provided by the user, the simulation proceeds neutrally. If provided, each row in the matrix should contain five entries: location location of the marker under selection (in Morgan) fitness of wildtype (aa) fitness of heterozygote (aA) fitness of homozygote mutant (AA) Ancestral type that represents the mutant allele A

markers

A vector of locations of markers, these markers are tracked for every generation.

verbose

Verbose output if TRUE. Default value is FALSE

multiplicative_selection

Default: TRUE. If TRUE, fitness is calculated for multiple markers by multiplying fitness values for each marker. If FALSE, fitness is calculated by adding fitness values for each marker.

mutation_rate

the per base probability of mutation. Default is 0.

substitution_matrix

a 4x4 matrix representing the probability of mutating to another base (where [1/2/3/4] = [a/c/t/g]), conditional on the event of a mutation happening. Default is the JC69 matrix, with equal probabilities for all transitions / transversions.

Value

A list with: population a population object, and three tibbles with allele frequencies (only contain values of a vector was provided to the argument markers: frequencies, initial_frequencies and final_frequencies. Each tibble contains four columns, time, location, ancestor and frequency, which indicates the number of generations, the location along the chromosome of the marker, the ancestral allele at that location in that generation, and finally, the frequency of that allele.

```
simulate_sequence_migration
```

Individual based simulation of the breakdown of contiguous ancestry blocks in two populations linked by migration

Description

Individual based simulation of the breakdown of contiguous ancestry blocks, with or without selection. Simulations can be started from scratch, or from a predefined input population. Two populations are simulated, connected by migration

```
simulate_sequence_migration(
  input_data_population_1 = NA,
  input_data_population_2 = NA,
  pop_size = c(100, 100),
  total_runtime = 100,
 morgan = 1,
  recombination_rate = NA,
  num\_threads = 1,
  select_matrix = NA,
 markers = NA,
  verbose = FALSE,
 multiplicative_selection = TRUE,
 migration_rate = 0,
  stop_at_critical_fst = FALSE,
  critical_fst = NA,
  generations_between_update = 100,
  sampled_individuals = 10,
  number_of_markers = 100,
  random_markers = TRUE,
 mutation_rate = 0,
  substitution_matrix = matrix(1/4, 4, 4)
)
```

Arguments

input_data_population_1

Genomic data used as input, should be created by the function create_input_data or by the function combine_input_data

input_data_population_2

Genomic data used as input, should be created by the function create_input_data or by the function combine_input_data

pop_size Vector containing the number of individuals in both populations.

total_runtime Number of generations

morgan Length of the chromosome in Morgan (e.g. the number of crossovers during

meiosis)

recombination_rate

rate in cM / Mbp, used to map recombination to the markers. If the recombination_rate is not set, the value for morgan is used, assuming that the markers included span an entire chromosome.

num_threads number of threads. Default is 1. Set to -1 to use all available threads

select_matrix Selection matrix indicating the markers which are under selection. If not provided by the user the simulation proceeds neutrally. If provided each row in the

vided by the user, the simulation proceeds neutrally. If provided, each row in the matrix should contain five entries: location location of the marker under selection (in Morgan) fitness of wildtype (aa) fitness of heterozygote (aA) fitness of homozygote mutant (AA) Ancestral type that representes the

mutant allele A

markers A vector of locations of markers (relative locations in [0, 1]). If a vector is

provided, ancestry at these marker positions is tracked for every generation.

verbose Verbose output if TRUE. Default value is FALSE

multiplicative_selection

Default: TRUE. If TRUE, fitness is calculated for multiple markers by multiplying fitness values for each marker. If FALSE, fitness is calculated by adding

fitness values for each marker.

migration_rate Rate of migration between the two populations. Migration is implemented such

that with probability m (migration rate) one of the two parents of a new offspring is from the other population, with probability 1-m both parents are of the focal

population.

stop_at_critical_fst

option to stop at a critical FST value, default is FALSE

critical_fst the critical fst value to stop, if stop_simulation_at_critical_fst is TRUE generations_between_update

The number of generations after which the simulation has to check again whether the critical Fst value is exceeded

sampled_individuals

Number of individuals to be sampled at random from the population to estimate

number_of_markers

Number of markers to be used to estimate Fst

random_markers Are the markers to estimate Fst randomly distributed, or regularly distributed?

Default is TRUE.

mutation_rate the per base probability of mutation. Default is 0. substitution_matrix

a 4x4 matrix representing the probability of mutating to another base (where [1/2/3/4] = [a/c/t/g]), conditional on the event of a mutation happening. Default is the JC69 matrix, with equal probabilities for all transitions / transversions.

Value

A list with: population_1, population_2 two population objects, and three tibbles with allele frequencies (only contain values of a vector was provided to the argument markers: frequencies, initial_frequencies and final_frequencies. Each tibble contains five columns, time, location, ancestor, frequency and population, which indicates the number of generations, the location along the chromosome of the marker, the ancestral allele at that location in that generation, the frequency of that allele and the population in which it was recorded (1 or 2). If a critical fst value was used to terminate the simulation, and object FST with the final FST estimate is returned as well.

Description

function to convert ped/map data to genome_admixr_data

Usage

```
simulation_data_to_genomeadmixr_data(
    simulation_data,
    markers = NA,
    verbose = FALSE
)
```

Arguments

simulation_data

result of simulate_admixture

markers vector of locations of markers (in Morgan). If no vector is provided, the function

searches for marker locations in the simulation_data.

verbose provide verbose output (default is FALSE)

Value

genomeadmixr_data object ready for simulate_admixture_data

```
vcfR_to_genomeadmixr_data
```

function to convert a vcfR object to genome_admixr_data

Description

function to convert a vcfR object to genome_admixr_data

Usage

```
vcfR_to_genomeadmixr_data(
  vcfr_object,
  chosen_chromosome,
  number_of_snps = NA,
  random_snps = TRUE,
  verbose = FALSE
)
```

Arguments

```
vcfr_object result of vcfR::read.vcfR
```

chosen_chromosome

chromosome of choice

number_of_snps number of snps to be loaded from the vcf file, default is to load all snps

random_snps if a subset of all snps has to be taken, should these be sampled sequentially (e.g.

the first 100 snps) or randomly (100 randomly sampled snps) (examples are for

'number_of_snps' = 100).

verbose if true, print progress bar

Value

genomeadmixr_data object ready for simulate_admixture_data

write_as_plink

function to write simulation output as PLINK style data

Description

function to write simulation output as PLINK style data

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Usage

```
write_as_plink(
   input_pop,
   marker_locations,
   file_name_prefix,
   chromosome = 1,
   recombination_rate = 1
)
```

Arguments

Value

No return value

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