Package 'dartR.popgen'

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Type Package

Title Analysing 'SNP' and 'Silicodart' Data Generated by Genome-Wide Restriction Fragment Analysis

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Description Facilitates the analysis of SNP (single nucleotide polymorphism) and silicodart (presence/absence) data. 'dartR.popgen' provides a suit of functions to analyse such data in a population genetics context. It provides several functions to calculate population genetic metrics and to study population structure. Quite a few functions need additional software to be able to run (gl.run.structure(), gl.blast(), gl.LDNe()). You find detailed description in the help pages how to download and link the packages so the function can run the software. 'dartR.popgen' is part of the the 'dartRverse' suit of packages. Gruber et al. (2018) <doi:10.1111/1755-0998.12745>. Mijangos et al. (2022) <doi:10.1111/2041-210X.13918>.

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- Depends R (>= 3.5), adegenet (>= 2.0.0), dartR.base, dartR.data
- **Imports** methods, utils, MASS, dplyr, patchwork, crayon, ggplot2, data.table, stringr, furrr, future, ggdendro
- **Suggests** SIBER, expm, fields, gplots, gridExtra, igraph, iterpc, label.switching, leaflet, plyr, proxy, purrr, qvalue, raster, reshape2, scales, snpStats, tidyr, viridis, zoo, gsubfn, sp

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gl.blast

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gl.blast

Aligns nucleotides sequences against those present in a target database using blastn

gl.blast

Description

Basic Local Alignment Search Tool (BLAST; Altschul et al., 1990 & 1997) is a sequence comparison algorithm optimized for speed used to search sequence databases for optimal local alignments to a query. This function creates fasta files, creates databases to run BLAST, runs blastn and filters these results to obtain the best hit per sequence.

This function can be used to run BLAST alignment of short-read (DArTseq data) and long-read sequences (Illumina, PacBio... etc). You can use reference genomes from NCBI, genomes from your private collection, contigs, scaffolds or any other genetic sequence that you would like to use as reference.

Usage

```
gl.blast(
    x,
    ref_genome,
    task = "megablast",
    Percentage_identity = 70,
    Percentage_overlap = 0.8,
    bitscore = 50,
    number_of_threads = 2,
    verbose = NULL
)
```

x	Either a genlight object containing a column named 'TrimmedSequence' con- taining the sequence of the SNPs (the sequence tag) trimmed of adapters as provided by DArT; or a path to a fasta file with the query sequences [required].				
ref_genome	Path to a reference genome in fasta of fna format [required].				
task	Four different tasks are supported: 1) "megablast", for very similar sequences (e.g, sequencing errors), 2) "dc-megablast", typically used for inter-species comparisons, 3) "blastn", the traditional program used for inter-species comparisons, 4) "blastn-short", optimized for sequences less than 30 nucleotides [default 'megablast'].				
Percentage_identity					
	Not a very sensitive or reliable measure of sequence similarity, however it is a reasonable proxy for evolutionary distance. The evolutionary distance associated with a 10 percent change in Percentage_identity is much greater at longer distances. Thus, a change from $80 - 70$ percent identity might reflect divergence 200 million years earlier in time, but the change from 30 percent to 20 percent might correspond to a billion year divergence time change [default 70].				
Percentage_overlap					
	Calculated as alignment length divided by the query length or subject length (whichever is shortest of the two lengths, i.e. length / $min(qlen,slen)$) [default 0.8].				
bitscore	A rule-of-thumb for inferring homology, a bit score of 50 is almost always sig- nificant [default 50].				

number_of_threa	ds
	Number of threads (CPUs) to use in blastn search [default 2].
verbose	verbose= 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2 or as specified using gl.set.verbosity]

Details

Installing BLAST

You can download the BLAST installs from: https://ftp.ncbi.nlm.nih.gov/blast/executables/ blast+/LATEST/

It is important to install BLAST in a path that does not contain spaces for this function to work.

Running BLAST

Four different tasks are supported:

- "megablast", for very similar sequences (e.g, sequencing errors)
- "dc-megablast", typically used for inter-species comparisons
- "blastn", the traditional program used for inter-species comparisons
- "blastn-short", optimized for sequences less than 30 nucleotides

If you are running a BLAST alignment of similar sequences, for example Turtle Genome Vs Turtle Sequences, the recommended parameters are: task = "megablast", Percentage_identity = 70, Percentage_overlap = 0.8 and bitscore = 50.

If you are running a BLAST alignment of highly dissimilar sequences because you are probably looking for sex linked hits in a distantly related species, and you are aligning for example sequences of Chicken Genome Vs Bassiana, the recommended parameters are: task = "dc-megablast", Percentage_identity = 50, Percentage_overlap = 0.01 and bitscore = 30.

Be aware that running BLAST might take a long time (i.e. days) depending of the size of your query, the size of your database and the number of threads selected for your computer.

BLAST output

The BLAST output is formatted as a table using output format 6, with columns defined in the following order:

- qseqid Query Seq-id
- sacc Subject accession
- stitle Subject Title
- qseq Aligned part of query sequence
- sseq Aligned part of subject sequence
- nident Number of identical matches
- mismatch Number of mismatches
- pident Percentage of identical matches
- length Alignment length
- evalue Expect value
- bitscore Bit score

gl.blast

- qstart Start of alignment in query
- · qend End of alignment in query
- sstart Start of alignment in subject
- send End of alignment in subject
- gapopen Number of gap openings
- gaps Total number of gaps
- qlen Query sequence length
- slen Subject sequence length
- PercentageOverlap length / min(qlen,slen)

Databases containing unfiltered aligned sequences, filtered aligned sequences and one hit per sequence are saved to the working directory (plot.dir tempdir if not set).

BLAST filtering

BLAST output is filtered by ordering the hits of each sequence first by the highest percentage identity, then the highest percentage overlap and then the highest bitscore. Only one hit per sequence is kept based on these selection criteria.

Value

If the input is a genlight object: returns a genlight object with one hit per sequence merged to the slot \$other\$loc.metrics. If the input is a fasta file: returns a dataframe with one hit per sequence.

Author(s)

Berenice Talamantes Becerra & Luis Mijangos (Post to https://groups.google.com/d/forum/ dartr)

References

- Altschul, S. F., Gish, W., Miller, W., Myers, E. W., & Lipman, D. J. (1990). Basic local alignment search tool. Journal of molecular biology, 215(3), 403-410.
- Altschul, S. F., Madden, T. L., Schäffer, A. A., Zhang, J., Zhang, Z., Miller, W., & Lipman, D. J. (1997). Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic acids research, 25(17), 3389-3402.
- Pearson, W. R. (2013). An introduction to sequence similarity ("homology") searching. Current protocols in bioinformatics, 42(1), 3-1.

See Also

gl.print.history

Examples

```
## Not run:
res <- gl.blast(x = testset.gl, ref_genome = "sequence.fasta")
# display of reports saved in the temporal directory
# open the reports saved in the temporal directory
## End(Not run)
```

gl.collapse

Collapses a distance matrix by amalgamating populations with pairwise fixed difference count less that a threshold

Description

This script takes a file generated by gl.fixed.diff and amalgamates populations with distance less than or equal to a specified threshold. The distance matrix is generated by gl.fixed.diff().

The script then applies the new population assignments to the genlight object and recalculates the distance and associated matrices.

Usage

gl.collapse(fd, tpop = 0, tloc = 0, pb = FALSE, verbose = NULL)

Arguments

fd	Name of the list of matrices produced by gl.fixed.diff() [required].
tpop	Threshold number of fixed differences above which populations will not be amalgamated [default 0].
tloc	Threshold defining a fixed difference (e.g. 0.05 implies 95:5 vs 5:95 is fixed) [default 0].
pb	If TRUE, show a progress bar on time consuming loops [default FALSE].
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2 or as specified using gl.set.verbosity]

Value

A list containing the gl object x and the following square matrices:

- 1. \$gl the new genlight object with populations collapsed;
- 2. \$fd raw fixed differences;
- 3. \$pcfd percent fixed differences;
- 4. \$nobs mean no. of individuals used in each comparison;
- 5. \$nloc total number of loci used in each comparison;
- 6. \$expfpos NA's, populated by gl.fixed.diff [by simulation]
- 7. \$expfpos NA's, populated by gl.fixed.diff [by simulation]
- 8. \$prob NA's, populated by gl.fixed.diff [by simulation]

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gl.evanno

Author(s)

Custodian: Arthur Georges – Post to https://groups.google.com/d/forum/dartr

Examples

```
fd <- gl.fixed.diff(testset.gl,tloc=0.05)
fd
fd2 <- gl.collapse(fd,tpop=1)
fd3
fd <- gl.collapse(fd2,tpop=1)
fd3
fd <- gl.fixed.diff(testset.gl,tloc=0.05)
fd2 <- gl.collapse(fd)</pre>
```

```
gl.evanno
```

Creates an Evanno plot from a STRUCTURE run object

Description

This function takes a genlight object and runs a STRUCTURE analysis based on functions from strataG

Usage

gl.evanno(sr, plot.out = TRUE)

Arguments

sr	structure run object from gl.run.structure [required].					
plot.out	TRUE: all four plots are shown. FALSE: all four plots are returned as a ggplot but not shown [default TRUE].					

Details

The function is basically a convenient wrapper around the beautiful strataG function evanno (Archer et al. 2016). For a detailed description please refer to this package (see references below).

Value

An Evanno plot is created and a list of all four plots is returned.

Author(s)

Bernd Gruber (Post to https://groups.google.com/d/forum/dartr)

References

- Pritchard, J.K., Stephens, M., Donnelly, P. (2000) Inference of population structure using multilocus genotype data. Genetics 155, 945-959.
- Archer, F. I., Adams, P. E. and Schneiders, B. B. (2016) strataG: An R package for manipulating, summarizing and analysing population genetic data. Mol Ecol Resour. doi:10.1111/1755-0998.12559
- Evanno, G., Regnaut, S., and J. Goudet. 2005. Detecting the number of clusters of individuals using the software STRUCTURE: a simulation study. Molecular Ecology 14:2611-2620.

See Also

gl.run.structure, clumpp,

Examples

```
# examples need structure to be installed on the system (see above)
## Not run:
    bc <- bandicoot.gl[,1:100]
    sr <- gl.run.structure(bc, k.range = 2:5, num.k.rep = 3, exec = './structure.exe')
    ev <- gl.evanno(sr)
    ev
    qmat <- gl.plot.structure(sr, K=3)
    head(qmat)
    gl.map.structure(qmat, bc, K=3, scalex=1, scaley=0.5)
## End(Not run)</pre>
```

gl.ld.distance

Plots linkage disequilibrium against distance by population disequilibrium patterns

Description

The function creates a plot showing the pairwise LD measure against distance in number of base pairs pooled over all the chromosomes and a red line representing the threshold (R.squared = 0.2) that is commonly used to imply that two loci are unlinked (Delourme et al., 2013; Li et al., 2014).

Usage

```
gl.ld.distance(
    ld.report,
    ld.resolution = 1e+05,
    pop.colors = NULL,
    plot.title = " ",
    plot.theme = NULL,
    plot.out = TRUE,
    plot.file = NULL,
```

```
plot.dir = NULL,
verbose = NULL
)
```

Arguments

ld.report	Output from function gl.report.ld.map [required].					
ld.resolution	Resolution at which LD should be reported in number of base pairs [default NULL].					
pop.colors	A color palette for box plots by population or a list with as many colors as there are populations in the dataset [default NULL].					
plot.title	Title of tyh plot [default " "].					
plot.theme	User specified theme [default NULL].					
plot.out	Specify if plot is to be produced [default TRUE].					
plot.file	Name for the RDS binary file to save (base name only, exclude extension) [de-fault NULL]					
plot.dir	Directory in which to save files [default = working directory]					
verbose Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, p and results summary; 5, full report [default 2, unless specified using gl.set						

Value

A dataframe with information of LD against distance by population.

Author(s)

Custodian: Luis Mijangos - Post to https://groups.google.com/d/forum/dartr

References

- Delourme, R., Falentin, C., Fomeju, B. F., Boillot, M., Lassalle, G., André, I., . . . Marty, A. (2013). High-density SNP-based genetic map development and linkage disequilibrium assessment in Brassica napusL. BMC genomics, 14(1), 120.
- Li, X., Han, Y., Wei, Y., Acharya, A., Farmer, A. D., Ho, J., . . . Brummer, E. C. (2014). Development of an alfalfa SNP array and its use to evaluate patterns of population structure and linkage disequilibrium. PLoS One, 9(1), e84329.

See Also

Other ld functions: gl.ld.haplotype()

Examples

```
if ((requireNamespace("snpStats", quietly = TRUE)) & (requireNamespace("fields", quietly = TRUE))) {
    require("dartR.data")
```

x <- platypus.gl

x <- gl.filter.callrate(x, threshold = 1)</pre>

```
x <- gl.filter.monomorphs(x)
x$position <- x$other$loc.metrics$ChromPos_Platypus_Chrom_NCBIv1
x$chromosome <- as.factor(x$other$loc.metrics$Chrom_Platypus_Chrom_NCBIv1)
ld_res <- gl.report.ld.map(x, ld.max.pairwise = 1000000)
ld_res_2 <- gl.ld.distance(ld_res, ld.resolution = 1000000)</pre>
```

gl.ld.haplotype

Visualize patterns of linkage disequilibrium and identification of haplotypes

Description

This function plots a Linkage disequilibrium (LD) heatmap, where the colour shading indicates the strength of LD. Chromosome positions (Mbp) are shown on the horizontal axis, and haplotypes appear as triangles and delimited by dark yellow vertical lines. Numbers identifying each haplotype are shown in the upper part of the plot.

The heatmap also shows heterozygosity for each SNP.

The function identifies haplotypes based on contiguous SNPs that are in linkage disequilibrium using as threshold ld_threshold_haplo and containing more than min_snps SNPs.

Usage

```
gl.ld.haplotype(
  х,
  pop_name = NULL,
  chrom_name = NULL,
  ld_max_pairwise = 1e+07,
  maf = 0.05,
  ld_stat = "R.squared",
  ind.limit = 10,
  haplo_id = FALSE,
  min_snps = 10,
  ld_threshold_haplo = 0.5,
  target_snp = NULL,
  coordinates = NULL,
  color_haplo = "viridis",
  color_het = "deeppink",
  plot.out = TRUE,
  plot.save = FALSE,
  plot.dir = NULL,
  verbose = NULL
)
```

}

Arguments

-							
х	Name of the genlight object containing the SNP data [required].						
pop_name	Name of the population to analyse. If NULL all the populations are analised [default NULL].						
chrom_name	Nme of the chromosome to analyse. If NULL all the chromosomes are analised [default NULL].						
ld_max_pairwise	9						
	Maximum distance in number of base pairs at which LD should be calculated [default 10000000].						
maf	Minor allele frequency (by population) threshold to filter out loci. If a value > 1 is provided it will be interpreted as MAC (i.e. the minimum number of times an allele needs to be observed) [default 0.05].						
ld_stat	The LD measure to be calculated: "LLR", "OR", "Q", "Covar", "D.prime", "R.squared", and "R". See ld (package snpStats) for details [default "R.squared"].						
ind.limit	Minimum number of individuals that a population should contain to take it in account to report loci in LD [default 10].						
haplo_id	Whether to identify haplotypes [default FALSE].						
min_snps	Minimum number of SNPs that should have a haplotype to call it [default 10].						
ld_threshold_ha	aplo						
	Minimum LD between adjacent SNPs to call a haplotype [default 0.5].						
target_snp	Position of target SNP [default NULL].						
coordinates	A vector of two elements with the start and end coordinates in base pairs to which restrict the analysis e.g. $c(1,1000000)$ [default NULL].						
color_haplo	Color palette for haplotype plot. See details [default "viridis"].						
color_het	Color for heterozygosity [default "deeppink"].						
plot.out	Specify if heatmap plot is to be produced [default TRUE].						
plot.save	Whethwr to save the plot in pdf format [default FALSE].						
plot.dir	Directory in which to save files [default = working directory]						
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2, unless specified using gl.set.verbosity].						

Details

The information for SNP's position should be stored in the genlight accessor "@position" and the SNP's chromosome name in the accessor "@chromosome" (see examples). The function will then calculate LD within each chromosome.

The output of the function includes a table with the haplotypes that were identified and their location.

Colors of the heatmap (color_haplo) are based on the function scale_fill_viridis from package viridis. Other color palettes options are "magma", "inferno", "plasma", "viridis", "cividis", "rocket", "mako" and "turbo". A table with the haplotypes that were identified.

Author(s)

Custodian: Luis Mijangos - Post to https://groups.google.com/d/forum/dartr

See Also

Other ld functions: gl.ld.distance()

Examples

```
require("dartR.data")
x <- platypus.gl
x <- gl.filter.callrate(x, threshold = 1)
# only the first 15 individuals because of speed during tests
x <- gl.keep.pop(x, pop.list = "TENTERFIELD")[1:15, ]
x$chromosome <- as.factor(x$other$loc.metrics$Chrom_Platypus_Chrom_NCBIv1)
x$position <- x$other$loc.metrics$ChromPos_Platypus_Chrom_NCBIv1
ld_res <- gl.ld.haplotype(x,
    chrom_name = "NC_041728.1_chromosome_1",
    ld_max_pairwise = 10000000
)</pre>
```

gl.LDNe

Estimates effective population size using the Linkage Disequilibrium method based on NeEstimator (V2)

Description

This function is basically a convenience function that runs the LD Ne estimator using Neestimator2 (http://www.molecularfisherieslaboratory.com.au/neestimator-software/) within R using the provided genlight object. To be able to do so, the software has to be downloaded from their website and the appropriate executable Ne2-1 has to be copied into the path as specified in the function (see example below).

Usage

```
gl.LDNe(
    x,
    outfile = "genepopLD.txt",
    outpath = tempdir(),
    neest.path = getwd(),
    critical = 0,
    singleton.rm = TRUE,
    mating = "random",
```

gl.LDNe

```
pairing = "all",
Waples.correction = NULL,
Waples.correction.value = NULL,
naive = FALSE,
plot.out = TRUE,
plot_theme = theme_dartR(),
plot_colors_pop = gl.select.colors(x, verbose = 0),
plot.file = NULL,
plot.dir = NULL,
verbose = NULL
)
```

x	Name of the genlight object containing the SNP data [required].					
outfile	File name of the output file with all results from Neestimator 2 [default 'genepopLD.txt'].					
outpath	Path where to save the output file. Use outpath=getwd() or outpath='.' when calling this function to direct output files to your working directory [default tempdir(), mandated by CRAN].					
neest.path	Path to the folder of the NE2-1 file. Please note there are 3 different executa- bles depending on your OS: Ne2-1.exe (=Windows), Ne2-1M (=Mac), Ne2-1L (=Linux). You only need to point to the folder (the function will recognise which OS you are running) [default getwd()].					
critical	(vector of) Critical values that are used to remove alleles based on their minor allele frequency. This can be done before using the gl.filter.maf function, there- fore the default is set to 0 (no loci are removed). To run for MAF 0 and MAF 0.05 at the same time specify: critical = $c(0,0.05)$ [default 0].					
singleton.rm	Whether to remove singleton alleles [default TRUE].					
mating	Formula for Random mating='random' or monogamy= 'monogamy' [default 'random'].					
pairing	'all' [default] if all possible loci should be paired, or 'separate' if only loci on different chromosomes should be used.					
Waples.correcti						
	The type of Waples et al 2016 correction to apply. This is ignored if pairing is set to 'separate'. Options are 'nChromosomes', for eq 1a, or 'genomeLength' for eq 1b. NULL if none should be applied [default NULL].					
Waples.correcti	on.value					
	The number of chromosomes or the genome length in cM. See Waples et al 2016 for details.					
naive	Whether the naive (uncorrected for samples size - see eq 7 and eq 8 in Waples 2006) should also be reported. This is mostly to diagnose the source of Inf estimate.					
plot.out	Specify if plot is to be produced [default TRUE].					
plot_theme	User specified theme [default theme_dartR()].					

<pre>plot_colors_pop</pre>	
	population colors with as many colors as there are populations in the dataset [default discrete_palette].
plot.file	Name for the RDS binary file to save (base name only, exclude extension) [de-fault NULL] temporary directory (tempdir) [default FALSE].
plot.dir	Directory in which to save files [default = working directory]
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2, unless specified using gl.set.verbosity]

Value

Dataframe with the results as table

Author(s)

Custodian: Bernd Gruber (Post to https://groups.google.com/d/forum/dartr)

References

- Waples, R. S. (2006). "A bias correction for estimates of effective population size based on linkage disequilibrium at unlinked gene loci*." Conservation Genetics 7(2): 167-184.
- Waples, R. K., et al. (2016). "Estimating contemporary effective population size in non-model species using linkage disequilibrium across thousands of loci." Heredity 117(4): 233-240.

Examples

```
## Not run:
# SNP data (use two populations and only the first 100 SNPs)
pops <- possums.gl[1:60, 1:100]</pre>
nes <- gl.LDNe(pops,</pre>
  outfile = "popsLD.txt", outpath = tempdir(),
 neest.path = "./path_to Ne-21",
  critical = c(0, 0.05), singleton.rm = TRUE, mating = "random"
)
nes
# Using only pairs of loci on different chromosomes
# make up some chromosome location
pops@chromosome <- as.factor(sample(1:10, size = nLoc(pops), replace = TRUE))</pre>
nessep <- gl.LDNe(pops,</pre>
              outfile = "popsLD.txt", outpath = "./TestNe", pairing="separate",
              neest.path = "./path_to Ne-21",
              critical = c(0, 0.05), singleton.rm = TRUE, mating = "random"
nessep
```

End(Not run)

gl.map.structure

Description

This function takes the output of plotstructure (the q matrix) and maps the q-matrix across using the population centers from the genlight object that was used to run the structure analysis via gl.run.structure) and plots the typical structure bar plots on a spatial map, providing a barplot for each subpopulation. Therefore it requires coordinates from a genlight object. This kind of plots should support the interpretation of the spatial structure of a population, but in principle is not different from gl.plot.structure

Usage

```
gl.map.structure(
  qmat,
  x,
  K,
  provider = "Esri.NatGeoWorldMap",
  scalex = 1,
  scaley = 1,
  movepops = NULL,
  pop.labels = TRUE,
  pop.labels.cex = 12
)
```

qmat	Q-matrix from a structure run followed by a clumpp run object [from gl.run.structure and gl.plot.structure] [required].					
x	Name of the genlight object containing the coordinates in the \@other\$latlon slot to calculate the population centers [required].					
К	The number for K to be plotted [required].					
provider	Provider passed to leaflet. Check providers for a list of possible backgrounds [default "Esri.NatGeoWorldMap"].					
scalex	Scaling factor to determine the size of the bars in x direction [default 1].					
scaley	Scaling factor to determine the size of the bars in y direction [default 1].					
movepops	A two-dimensional data frame that allows to move the center of the barplots manually in case they overlap. Often if populations are horizontally close to each other. This needs to be a data.frame of the dimensions [rows=number of populations, columns = 2 (lon/lat)]. For each population you have to specify the x and y (lon and lat) units you want to move the center of the plot, (see example for details) [default NULL].					
pop.labels	Switch for population labels below the parplots [default TRUE].					
<pre>pop.labels.cex</pre>	Size of population labels [default 12].					

Details

Creates a mapped version of structure plots. For possible background maps check as specified via the provider: http://leaflet-extras.github.io/leaflet-providers/preview/index. html. You may need to adjust scalex and scaley values [default 1], as the size depends on the scale of the map and the position of the populations.

Value

An interactive map that shows the structure plots broken down by population.

returns the map and a list of the qmat split into sorted matrices per population. This can be used to create your own map.

Author(s)

Bernd Gruber (Post to https://groups.google.com/d/forum/dartr)

References

- Pritchard, J.K., Stephens, M., Donnelly, P. (2000) Inference of population structure using multilocus genotype data. Genetics 155, 945-959.
- Archer, F. I., Adams, P. E. and Schneiders, B. B. (2016) strataG: An R package for manipulating, summarizing and analysing population genetic data. Mol Ecol Resour. doi:10.1111/1755-0998.12559
- Evanno, G., Regnaut, S., and J. Goudet. 2005. Detecting the number of clusters of individuals using the software STRUCTURE: a simulation study. Molecular Ecology 14:2611-2620.
- Mattias Jakobsson and Noah A. Rosenberg. 2007. CLUMPP: a cluster matching and permutation program for dealing with label switching and multimodality in analysis of population structure. Bioinformatics 23(14):1801-1806. Available at clumpp

See Also

gl.run.structure, clumpp, gl.plot.structure

Examples

```
# examples need structure to be installed on the system (see above)
## Not run:
bc <- bandicoot.gl[,1:100]
sr <- gl.run.structure(bc, k.range = 2:5, num.k.rep = 3, exec = './structure.exe')
ev <- gl.evanno(sr)
ev
qmat <- gl.plot.structure(sr, k=2:4)#' #head(qmat)
gl.map.structure(qmat, bc,K=3)
gl.map.structure(qmat, bc,K=4)
# move population 4 (out of 5) 0.5 degrees to the right and populations 1
# 0.3 degree to the north of the map.
mp <- data.frame(lon=c(0,0,0.5,0), lat=c(-0.3,0,0,0,0))
gl.map.structure(qmat, bc,K=4, movepops=mp)</pre>
```

End(Not run)

gl.nhybrids

Creates an input file for the program NewHybrids and runs it if NewHybrids is installed

Description

This function compares two sets of parental populations to identify loci that exhibit a fixed difference, returns an genlight object with the reduced data, and creates an input file for the program NewHybrids using the top 200 (or hard specified loc.limit) loci. In the absence of two identified parental populations, the script will select a random set 200 loci only (method='random') or the first 200 loci ranked on information content (method='AvgPIC').

A fixed difference occurs when a SNP allele is present in all individuals of one population and absent in the other. There is provision for setting a level of tolerance, e.g. threshold = 0.05 which considers alleles present at greater than 95 a fixed difference. Only the 200 loci are retained, because of limitations of NewHybids.

If you specify a directory for the NewHybrids executable file, then the script will create the input file from the SNP data then run NewHybrids. If the directory is set to NULL, the execution will stop once the input file (default='nhyb.txt') has been written to disk. Note: the executable option will not work on a Mac; Mac users should generate the NewHybrids input file and run this on their local installation of NewHybrids.

Refer to the New Hybrids manual for further information on the parameters to set - http://ib.berkeley.edu/labs/slatkin/eriq/soft

It is important to stringently filter the data on RepAvg and CallRate if using the random option. One might elect to repeat the analysis (method='random') and combine the resultant posterior probabilities should 200 loci be considered insufficient.

The F1 individuals should be homozygous at all loci for which the parental populations are fixed and different, assuming parental populations have been specified. Sampling errors can result in this not being the case, especially where the sample sizes for the parental populations are small. Alternatively, the threshold for posterior probabilities used to determine assignment (pprob) or the definition of a fixed difference (threshold) may be too lax. To assess the error rate in the determination of assignment of F1 individuals, a plot of the frequency of homozygous reference, heterozygotes and homozygous alternate (SNP) can be produced by setting plot=TRUE (the default).

Usage

```
gl.nhybrids(
  gl,
  outpath = tempdir(),
  p0 = NULL,
  p1 = NULL,
  threshold = 0,
  method = "random",
  plot = TRUE,
  plot_theme = theme_dartR(),
  plot_colors = gl.select.colors(ncolors = 2, verbose = 0),
  pprob = 0.95,
```

```
nhyb.directory = NULL,
BurnIn = 10000,
sweeps = 10000,
GtypFile = "TwoGensGtypFreq.txt",
AFPriorFile = NULL,
PiPrior = "Jeffreys",
ThetaPrior = "Jeffreys",
verbose = NULL
)
```

Arguments

gl	Name of the genlight object containing the SNP data [required].
outpath	Path where to save the output file [default tempdir()].
p0	List of populations to be regarded as parental population 0 [default NULL].
p1	List of populations to be regarded as parental population 1 [default NULL].
threshold	Sets the level at which a gene frequency difference is considered to be fixed [default 0].
method	Specifies the method (random) to select 200 loci for NewHybrids [default ran- dom]. Previous AvgPic does not work anymore!
plot	If TRUE, a plot of the frequency of homozygous reference, heterozygotes and homozygous alternate (SNP) is produced for the F1 individuals [default TRUE, applies only if both parental populations are specified].
plot_theme	User specified theme [default theme_dartR()].
plot_colors	Vector with two color names for the borders and fill [default two colors].
pprob	Threshold level for assignment to likelihood bins [default 0.95, used only if plot=TRUE].
nhyb.directory	Directory that holds the NewHybrids executable file e.g. C:/NewHybsPC [de-fault NULL].
BurnIn	Number of sweeps to use in the burn in [default 10000].
sweeps	Number of sweeps to use in computing the actual Monte Carlo averages [default 10000].
GtypFile	Name of a file containing the genotype frequency classes [default TwoGensG-typFreq.txt].
AFPriorFile	Name of the file containing prior allele frequency information [default NULL].
PiPrior	Jeffreys-like priors or Uniform priors for the parameter pi [default Jeffreys].
ThetaPrior	Jeffreys-like priors or Uniform priors for the parameter theta [default Jeffreys].
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2 or as specified using gl.set.verbosity].

Value

The reduced genlight object, if parentals are provided; output of NewHybrids is saved to the working directory.

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gl.outflank

Author(s)

Custodian: Arthur Georges – Post to https://groups.google.com/d/forum/dartr

References

Anderson, E.C. and Thompson, E.A.(2002). A model-based method for identifying species hybrids using multilocus genetic data. Genetics. 160:1217-1229.

Examples

```
## Not run:
m <- gl.nhybrids(testset.gl,
    p0 = NULL, p1 = NULL,
    nhyb.directory = "D:/workspace/R/NewHybsPC", # Specify as necessary
    outpath = "D:/workspace", # Specify as necessary, usually getwd() [= workspace]
    BurnIn = 100,
    sweeps = 100,
    verbose = 3
)
## End(Not run)
```

gl.outflank	Identifies loci	under	selection	per	population	using	the	outflank
method of Whitlock and Lotterhos (2015)								

Description

Identifies loci under selection per population using the outflank method of Whitlock and Lotterhos (2015)

Usage

```
gl.outflank(
   gi,
   plot = TRUE,
   LeftTrimFraction = 0.05,
   RightTrimFraction = 0.05,
   Hmin = 0.1,
   qthreshold = 0.05,
   ...
)
```

gi	A genlight or genind object, with a defined population structure [required].
plot	A switch if a barplot is wanted [default TRUE].

LeftTrimFraction	
	The proportion of loci that are trimmed from the lower end of the range of Fst
	before the likelihood function is applied [default 0.05].
RightTrimFracti	on
	The proportion of loci that are trimmed from the upper end of the range of Fst before the likelihood function is applied [default 0.05].
Hmin	The minimum heterozygosity required before including calculations from a locus [default 0.1].
qthreshold	The desired false discovery rate threshold for calculating q-values [default 0.05].
	additional parameters (see documentation of outflank on github).

Details

This function is a wrapper around the outflank function provided by Whitlock and Lotterhos. To be able to run this function the packages qvalue (from bioconductor) and outflank (from github) needs to be installed. To do so see example below.

Value

Returns an index of outliers and the full outflank list

References

Whitlock, M.C. and Lotterhos K.J. (2015) Reliable detection of loci responsible for local adaptation: inference of a neutral model through trimming the distribution of Fst. The American Naturalist 186: 24 - 36.

Github repository: Whitlock & Lotterhos: https://github.com/whitlock/OutFLANK (Check the readme.pdf within the repository for an explanation. Be aware you now can run OufFLANK from a genlight object)

See Also

utils.outflank,utils.outflank.plotter,utils.outflank.MakeDiploidFSTMat

Examples

gl.outflank(bandicoot.gl, plot = TRUE)

gl.plot.faststructure Plots fastStructure analysis results (Q-matrix)

Description

This function takes a fastStructure run object (output from gl.run.faststructure) and plots the typical structure bar plot that visualize the q matrix of a fastStructure run.

Usage

```
gl.plot.faststructure(
    sr,
    k.range,
    met_clumpp = "greedyLargeK",
    iter_clumpp = 100,
    clumpak = TRUE,
    plot_theme = NULL,
    colors_clusters = NULL,
    ind_name = TRUE,
    border_ind = 0.15,
    den = FALSE,
    x = NULL
)
```

sr	fastStructure run object from gl.run.faststructure [required].	
k.range	The number for K of the q matrix that should be plotted. Needs to be within you simulated range of K's in your sr structure run object. If NULL, all the K's are plotted [default NULL].	
<pre>met_clumpp</pre>	The algorithm to use to infer the correct permutations. One of 'greedy' or 'greedyLargeK' or 'stephens' [default "greedyLargeK"].	
iter_clumpp	The number of iterations to use if running either 'greedy' 'greedyLargeK' [default 100].	
clumpak	Whether use the Clumpak method (see details) [default TRUE].	
plot_theme	Theme for the plot. See Details for options [default NULL].	
colors_clusters		
	A color palette for clusters (K) or a list with as many colors as there are clusters (K) [default NULL].	
ind_name	Whether to plot individual names [default TRUE].	
border_ind	The width of the border line between individuals [default 0.25].	
den	Whether to include a dendrogram. It is necessary to include the original genlight object used in gl.run.structure in the parameter x [default FALSE].	
х	The original genlight object used in gl.run.structure description [default NULL].	

The function outputs a barplot which is the typical output of fastStructure.

This function is based on the methods of CLUMPP and Clumpak as implemented in the R package starmie (https://github.com/sa-lee/starmie).

The Clumpak method identifies sets of highly similar runs among all the replicates of the same K. The method then separates the distinct groups of runs representing distinct modes in the space of possible solutions.

The CLUMPP method permutes the clusters output by independent runs of clustering programs such as structure, so that they match up as closely as possible.

This function averages the replicates within each mode identified by the Clumpak method.

Examples of other themes that can be used can be consulted in

- https://ggplot2.tidyverse.org/reference/ggtheme.html and
- https://yutannihilation.github.io/allYourFigureAreBelongToUs/ggthemes/

Value

List of Q-matrices

Author(s)

Bernd Gruber & Luis Mijangos (Post to https://groups.google.com/d/forum/dartr)

References

- Raj, A., Stephens, M., & Pritchard, J. K. (2014). fastSTRUCTURE: variational inference of population structure in large SNP data sets. Genetics, 197(2), 573-589.
- Pritchard, J.K., Stephens, M., Donnelly, P. (2000) Inference of population structure using multilocus genotype data. Genetics 155, 945-959.
- Kopelman, Naama M., et al. "Clumpak: a program for identifying clustering modes and packaging population structure inferences across K." Molecular ecology resources 15.5 (2015): 1179-1191.
- Mattias Jakobsson and Noah A. Rosenberg. 2007. CLUMPP: a cluster matching and permutation program for dealing with label switching and multimodality in analysis of population structure. Bioinformatics 23(14):1801-1806. Available at clumpp

See Also

gl.run.faststructure

Examples

```
## Not run:
t1 <- gl.filter.callrate(platypus.gl, threshold = 1)
res <- gl.run.faststructure(t1,
    exec = "./fastStructure", k.range = 2:3,
    num.k.rep = 2, output = paste0(getwd(), "/res_str")
```

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```
)
qmat <- gl.plot.faststructure(res, k.range = 2:3)
gl.map.structure(qmat, K = 2, t1, scalex = 1, scaley = 0.5)
## End(Not run)</pre>
```

gl.plot.structure Plots STRUCTURE analysis results (Q-matrix)

Description

This function takes a structure run object (output from gl.run.structure) and plots the typical structure bar plot that visualize the q matrix of a structure run.

Usage

```
gl.plot.structure(
  sr,
 K = NULL,
 met_clumpp = "greedyLargeK",
  iter_clumpp = 100,
  clumpak = TRUE,
  plot_theme = NULL,
  color_clusters = NULL,
  ind_name = TRUE,
  k_name = NULL,
  border_ind = 0.15,
  den = FALSE,
  dis.mat = NULL,
  x = NULL,
  plot.out = TRUE,
  plot.file = NULL,
  plot.dir = NULL,
  verbose = NULL
)
```

sr	Structure run object from gl.run.structure [required].
К	The number for K of the q matrix that should be plotted. Needs to be within you simulated range of K's in your sr structure run object. If NULL, all the K's are plotted [default NULL].
<pre>met_clumpp</pre>	The algorithm to use to infer the correct permutations. One of 'greedy' or 'greedyLargeK' or 'stephens' [default "greedyLargeK"].
iter_clumpp	The number of iterations to use if running either 'greedy' 'greedyLargeK' [default 100].

clumpak	Whether use the Clumpak method (see details) [default TRUE].
plot_theme	Theme for the plot. See Details for options [default NULL].
color_clusters	A color palette for clusters (K) or a list with as many colors as there are clusters (K) [default NULL].
ind_name	Whether to plot individual names [default TRUE].
k_name	Name of the structure plot to plot. It should be character [default NULL].
border_ind	The width of the border line between individuals [default 0.25].
den	Whether to include a dendrogram. It is necessary to include the original genlight object used in gl.run.structure in the parameter x [default FALSE].
dis.mat	A dis object (distance matrix) to be used to order structure plot which is plotted together with structure plot [default NULL].
х	The original genlight object used in gl.run.structure description [default NULL].
plot.out	Specify if plot is to be produced [default TRUE].
plot.file	Name for the RDS binary file to save (base name only, exclude extension) [de-fault NULL]
plot.dir	Directory in which to save files [default = working directory]
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default NULL, unless specified using gl.set.verbosity]

Details

The function outputs a barplot which is the typical output of structure. For a Evanno plot use gl.evanno.

This function is based on the methods of CLUMPP and Clumpak as implemented in the R package starmie (https://github.com/sa-lee/starmie).

The Clumpak method identifies sets of highly similar runs among all the replicates of the same K. The method then separates the distinct groups of runs representing distinct modes in the space of possible solutions.

The CLUMPP method permutes the clusters output by independent runs of clustering programs such as structure, so that they match up as closely as possible.

This function averages the replicates within each mode identified by the Clumpak method.

Plots and table are saved to the working directory specified in plot.dir (tempdir) if plot.file is set.

Examples of other themes that can be used can be consulted in

- https://ggplot2.tidyverse.org/reference/ggtheme.html and
- https://yutannihilation.github.io/allYourFigureAreBelongToUs/ggthemes/

Value

List of Q-matrices

Author(s)

Bernd Gruber & Luis Mijangos (Post to https://groups.google.com/d/forum/dartr)

gl.run.epos

References

- Pritchard, J.K., Stephens, M., Donnelly, P. (2000) Inference of population structure using multilocus genotype data. Genetics 155, 945-959.
- Kopelman, Naama M., et al. "Clumpak: a program for identifying clustering modes and packaging population structure inferences across K." Molecular ecology resources 15.5 (2015): 1179-1191.
- Mattias Jakobsson and Noah A. Rosenberg. 2007. CLUMPP: a cluster matching and permutation program for dealing with label switching and multimodality in analysis of population structure. Bioinformatics 23(14):1801-1806. Available at clumpp

See Also

gl.run.structure, gl.plot.structure

Examples

```
# examples need structure to be installed on the system (see above)
## Not run:
bc <- bandicoot.gl[,1:100]
sr <- gl.run.structure(bc, k.range = 2:5, num.k.rep = 3, exec = './structure')
ev <- gl.evanno(sr)
ev
qmat <- gl.plot.structure(sr, K=3)
head(qmat)
gl.map.structure(qmat, K=3, bc, scalex=1, scaley=0.5)
## End(Not run)</pre>
```

gl.run.epos

Run EPOS for Inference of Historical Population-Size Changes

Description

This function runs EPOS (based on Lynch et al. 2019) to estimate historical population-size https://github.com/EvolBioInf/epos. It relies on a compiled version of the software epos, epos2plot and if a bootstrap output is required bootSfs. For more information on the approach check the publication (Lynch at al. 2019), the github repository https://github.com/EvolBioInf/epos and look out for the manual epos.pdf (https://github.com/EvolBioInf/epos/blob/master/doc/epos.pdf. The binaries need to be provided in a single folder and can be downloaded via the gl.download.binary function (including the necessary dlls for windows; under Linux gls, blas need to be installed on your system). Please note: if you use this method, make sure you cite the original publication in your work. EPOS (Estimation of Population Size changes) is a software tool developed based on the theoretical framework outlined by Lynch et al. (2019). It is designed to infer historical changes in population size using allele-frequency data obtained from population-genomic surveys. Below is a brief summary of the main concepts of EPOS:

EPOS (Estimation of Population Size changes) is a software tool that infers historical changes

in population size using allele-frequency data from population-genomic surveys. The method relies on the site-frequency spectrum (SFS) of nearly neutral polymorphisms. The underlying theory uses coalescence models, which describe how gene sequences have originated from a common ancestor. By analyzing the probability distributions of the starting and ending points of branch segments over all possible coalescence trees, EPOS can estimate historic population sizes.

The function uses a model-flexible approach, meaning it estimates historic population sizes, without the necessity to provide a candidate scenario. An efficient statistical procedure is employed, to estimate historic effective population sizes.

For all the possible settings, please refer to the manual of EPOS.

The main parameters that are necessary to run the function are a genlight/dartR object, L (length of sequences), u (mutation rate), and the path to the epos binaries. For details check the example below.

Please note: There is currently not really a good way to estimate L, the length of all sequences. Often users of dart data use the number of loci multiplied by 69, but this is definitely an underestimate as monomorphic loci need to be included (also the length of the restriction site should be added for each loci). For mutation rate u, the default value is set to 5e-9, but should be adapted to the species of interest. The good news is, that settings of L and mu affects only the axis of the inferred history, but not the shape of the history. So users can infer the shape, but need to be careful with a temporal interpretation as both x and y axis are affected by the mutation rate and L.

Usage

```
gl.run.epos(
  х,
  epos.path,
  sfs = NULL,
 minbinsize = 1,
  folded = TRUE,
 L = NULL,
  u = NULL,
 boot = 0,
  upper = 0.975,
  lower = 0.025,
 method = "greedy",
  depth = 2,
  other.options = ""
  cleanup = TRUE,
  plot.display = TRUE,
  plot.theme = theme_dartR(),
 plot.dir = NULL,
  plot.file = NULL,
  verbose = NULL
)
```

x	dartR/genlight object
epos.path	path to epos and other required programs (epos, epos2plot are always required
	and bootSfs in case a bootstrap and confidence estimate is required)

sfs	if no sfs is provided function gl.sfs(x, minbinsize=1, singlepop=TRUE) is used to calculate the sfs that is provided to epos
minbinsize	remove bins from the left of the sfs. if you run epos from a genlight object the sfs is calculated by the function (using gl.sfs) and as default minbinsize is set to 1 (the monomorphic loci of the sfs are removed). This parameter is ignored if sfs is provide via the sfs parameter (see below). Be aware even if you genlight object has more than one population the sfs is calculated with singlepop set to true (one sfs for all individuals) as epos does not work with multidimensional sfs)
folded	if set to TRUE (default) a folded sfs (minor allele frequency sfs) is returned. If set to FALSE then an unfolded (derived allele frequency sfs) is returned. It is assumed that 0 is homozygote for the reference and 2 is homozygote for the derived allele. So you need to make sure your coding is correct. option -U in epos.
L	length of sequences (including monomorphic and polymorphic sites). If the sfs is provided with minbinsize=1 (default) then L needs to be specified. option -l in epos
u	mutation rate. If not provided the default value of epos is used (5e-9). option -u in epos
boot	if set to a value >0 the programm bootSfs is used to provide multiple boot- strapped sfs, which allows to calculate confidence intervals of the historic Ne sizes. Be aware the runtime can be extended. default:0 no bootstrapped simula- tions are run, otherwise boot number of bootstraps are run (option -i in bootSfs)
upper	upper quantile of the bootstrap (only used if boot>0). default 0.975. (option -u in epos2plot)
lower	lower quantile of the bootstrap (only used if boot>0). default 0.025. (option -1 in epos2plot)
method	either "exhaustive" or "greedy". check the epos manual for details. If method="exhaustive" then the paramter depth is used. default: "greedy".
depth	if method="exhaustive" then this parameter is used to set the search depth, de- fault is 2. If method is set to greedy this is setting is ignored.
other.options	additional options for epos (e.g -m, -x etc.)
cleanup	if set to true intermediate tempfiles are deleted after the run
plot.display	Specify if plot is to be produced [default TRUE].
plot.theme	User specified theme [default theme_dartR()].
plot.dir	Directory to save the plot RDS files [default as specified by the global working directory or tempdir()]
plot.file	Filename (minus extension) for the RDS plot file [Required for plot save]
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2, unless specified using gl.set.verbosity].

returns a list with two components:

- history: Ne estimates of over generations (generation, median, low and high)
- plot: a ggplot of history

Author(s)

Custodian: Bernd Gruber - Post to https://groups.google.com/d/forum/dartr

References

Lynch, Michael, Bernhard Haubold, Peter Pfaffelhuber, and Takahiro Maruki. 2019. Inference of Historical Population-Size Changes with Allele-Frequency Data. G3: Genes|Genomes|Genetics 10, no. 1: 211–23. doi:10.1534/g3.119.400854.

Examples

```
## Not run:
#gl.download.binary("epos",os="windows")
require(dartR.data)
epos <- gl.run.epos(possums.gl, epos.path = file.path(tempdir(),"epos"), L=1e5, u = 1e-8)
epos$history
```

End(Not run)

gl.run.faststructure Runs a faststructure analysis using a genlight object

Description

This function takes a genlight object and runs a faststructure analysis.

Usage

```
gl.run.faststructure(
    x,
    k.range,
    num.k.rep = 1,
    exec = "./fastStructure",
    exec.plink = getwd(),
    output = getwd(),
    tol = 1e-05,
    prior = "simple",
    cv = 0,
    seed = NULL
)
```

gl.run.faststructure

Arguments

х	Name of the genlight object containing the SNP data [required].
k.range	Range of the number of populations [required].
num.k.rep	Number of replicates [default 1].
exec	Full path and name+extension where the fastStructure executable is located [de-fault working directory "./fastStructure"].
exec.plink	path to plink executable [default working directory].
output	Path to output file [default getwd()].
tol	Convergence criterion [default 10e-6].
prior	Choice of prior: simple or logistic [default "simple"].
cv	Number of test sets for cross-validation, 0 implies no CV step [default 0].
seed	Seed for random number generator [default NULL].

Details

Download faststructure binary for your system from here (only runs on Mac or Linux):

https://github.com/StuntsPT/Structure_threader/tree/master/structure_threader/bins

Move faststructure file to working directory. Make file executable using terminal app.

system(paste0("chmod u+x ",getwd(), "/faststructure"))

Download plink binary for your system from here:

https://www.cog-genomics.org/plink/

Move plink file to working directory. Make file executable using terminal app.

system(paste0("chmod u+x ",getwd(), "/plink"))

To install fastStructure dependencies follow these directions: https://github.com/rajanil/fastStructure

fastStructure performs inference for the simplest, independent-loci, admixture model, with two choices of priors that can be specified using the –prior parameter. Thus, unlike Structure, fast-Structure does not require the mainparams and extraparam files. The inference algorithm used by fastStructure is fundamentally different from that of Structure and requires the setting of far fewer options.

To identify the number of populations that best approximates the marginal likelihood of the data, the marginal likelihood is extracted from each run of K, averaged across replications and plotted.

Value

A list in which each list entry is a single faststructure run output (there are k.range * num.k.rep number of runs).

Author(s)

Luis Mijangos (Post to https://groups.google.com/d/forum/dartr)

References

 Raj, A., Stephens, M., & Pritchard, J. K. (2014). fastSTRUCTURE: variational inference of population structure in large SNP data sets. Genetics, 197(2), 573-589.

Examples

```
## Not run:
# Please note: faststructure needs to be installed
# Please note: faststructure is not available for windows
t1 <- gl.filter.callrate(platypus.gl, threshold = 1)
res <- gl.run.faststructure(t1,
    exec = "./fastStructure", k.range = 2:3,
    num.k.rep = 2, output = paste0(getwd(), "/res_str")
)
qmat <- gl.plot.faststructure(res, k.range = 2:3)
gl.map.structure(qmat, K = 2, t1, scalex = 1, scaley = 0.5)
## End(Not run)
```

gl.run.stairway2 Run Stairway Plot 2 for Demographic History Inference

Description

This function runs Stairway Plot 2 to infer demographic history using folded SNP frequency spectra. Stairway Plot 2 is a method for inferring demographic history using folded SNP frequency spectra. The key features and methodology of Stairway Plot 2 include:

- Folded SNP Frequency Spectra: The method uses folded SNP frequency spectra, which are less sensitive to errors in ancestral state inference compared to unfolded spectra.
- **Demographic Inference**: By analyzing the SNP frequency spectra, Stairway Plot 2 can infer changes in population size over time, providing insights into historical demographic events.
- Bootstrap Replicates: The method employs bootstrap replicates to estimate confidence intervals for the inferred demographic history, ensuring robust and reliable results.
- Flexible Modeling: Stairway Plot 2 allows for flexible modeling of demographic history without assuming a specific parametric form for population size changes.

To be able to run Stairway Plot 2, the binaries need to be provided in a single folder and can be downloaded via the gl.download.binary function. In this case your system need to have Java installed as well. for more details on the method and how to install on your system refer to the githubh repository: https://github.com/xiaoming-liu/stairway-plot-v2. Please also refer to the original publication for more details on the method: doi:10.1186/s1305902002196-9. **Also if you use this method, make sure you cite the original publication in your work.** This function implements the theoretical and computational procedures described by Liu and Fu (2020), making it suitable for a wide range of population-genomic datasets to uncover historical demographic patterns. Please note: There is currently not really a good way to estimate L, the length of all sequences. Often users of dart data use the number of loci multiplied by 69, but

gl.run.stairway2

this is definitely an underestimate as monomorphic loci need to be included (also the length of the restriction site should be added for each loci). For mutation rate u, the default value is set to 5e-9, but should be adapted to the species of interest. The good news is, that settings of L and mu affects only the axis of the inferred history, but not the shape of the history. So users can infer the shape, but need to be careful with a temporal interpretation as both x and y axis are affected by the mutation rate and L.

Usage

```
gl.run.stairway2(
 х,
 L = NULL,
 mu = NULL,
 stairway2.path,
 minbinsize = 1,
 maxbinsize = NULL,
 gentime = 1,
  sfs = NULL,
  parallel = 1,
  run = TRUE,
 blueprint = "blueprint",
  filename = "sample",
  pct_training = 0.67,
  nrand = NULL,
  stairway_plot_dir = "stairway_plot_es",
  nreps = 200,
  seed = NULL,
  plot_title = "Ne",
  xmin = 0,
 xmax = 0,
  ymin = 0,
 ymax = 0,
  xspacing = 2,
 yspacing = 2,
  fontsize = 12,
  cleanup = TRUE,
  plot.display = TRUE,
 plot.theme = theme_dartR(),
  plot.dir = NULL,
 plot.file = NULL,
  verbose = NULL
```

)

х	A genlight/dartR object containing SNP data.
L	the length of the sequence in base pairs. (see notes below)
mu	the mutation rate per base pair per generation. (see notes below)

stairway2.path	the path to the Stairway Plot 2 executable. (check the example)	
minbinsize	the minumum bin size for the SFS that should be used. (default=1)	
maxbinsize	the maximum bin size for the SFS that should be used. (default=NULL, so the maximum bin size is set to the number of samples in the dataset)	
gentime	the generation time in years. (default=1)	
sfs	the folded site frequency spectrum (SFS) to be used for the analysis. If not provided the SFS is created from the genlight/dartR object (default=NULL)	
parallel	the number of parallel processes to use for the analysis. (default=1)	
run	logical. If TRUE, the analysis is run immediately. Otherwise only the blueprint files are created [might be useful to run on a cluster]. (default=FALSE)	
blueprint	the name of the blueprint file. (default="blueprint")	
filename	the name of the filename. Also used for the plot. (default="sample")	
<pre>pct_training</pre>	the percentage of the data to use for training. (default=0.67)	
nrand	the number of breakpoint to use for the analysis. (default=NULL)	
stairway_plot_dir		
	the name of the directory where the stairway plot is saved. (default="stairway_plot_es")	
nreps	the number of bootstrap replicates to use for the analysis. (default=200)	
seed	the random seed to use for the analysis. (default=NULL)	
<pre>plot_title</pre>	the title of the plot. (default="Ne"+filename)	
xmin	minimum x value for the plot. (default=0)	
xmax	maximum x value for the plot. (default=0)	
ymin	minimum y value for the plot. (default=0)	
ymax	maximum y value for the plot. (default=0)	
xspacing	spacing between x values for the plot. (default=2)	
yspacing	spacing between y values for the plot. (default=2)	
fontsize	the font size for the plot. (default=12)	
cleanup	logical. If TRUE, the stairway 2 plot output files are removed. (default=TRUE)	
plot.display	Specify if plot is to be produced [default TRUE].	
plot.theme	User specified theme [default theme_dartR()].	
plot.dir	Directory to save the plot RDS files [default as specified by the global working directory or tempdir()]	
plot.file	Filename (minus extension) for the RDS plot file [Required for plot save]	
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2, unless specified using gl.set.verbosity].	

Value

returns a list with two components:

- history: Ne estimates of over generations (generation, median, low and high)
- plot: a ggplot of history

gl.run.structure

References

Liu, X., & Fu, Y. X. (2020). Stairway Plot 2: demographic history inference with folded SNP frequency spectra. Genome Biology, 21(1), 280.

Liu, X., Fu, YX. Stairway Plot 2: demographic history inference with folded SNP frequency spectra. Genome Biol 21, 280 (2020). doi:10.1186/s13059020021969

Examples

End(Not run)

gl.run.structure Runs a STRUCTURE analysis using a genlight object

Description

This function takes a genlight object and runs a STRUCTURE analysis based on functions from strataG

Usage

```
gl.run.structure(
 х,
 exec = "./structure",
 k.range = NULL,
  num.k.rep = 1,
 burnin = 1000,
  numreps = 1000,
  noadmix = TRUE,
  freqscorr = FALSE,
  randomize = TRUE,
  seed = 0,
  pop.prior = NULL,
  locpriorinit = 1,
 maxlocprior = 20,
  gensback = 2,
 migrprior = 0.05,
  pfrompopflagonly = TRUE,
  popflag = NULL,
```

```
inferalpha = FALSE,
alpha = 1,
unifprioralpha = TRUE,
alphamax = 20,
alphapriora = 0.05,
alphapriorb = 0.001,
plot.out = TRUE,
plot_theme = theme_dartR(),
plot.dir = tempdir(),
plot.file = NULL,
verbose = NULL
)
```

Arguments

х	Name of the genlight object containing the SNP data [required].
exec	Full path and name+extension where the structure executable is located. E.g. 'c:/structure/structure.exe' under Windows. For Mac and Linux it might be something like './structure/structure' if the executable is in a subfolder 'structure' in your home directory [default working directory "."].
k.range	Range of the number of populations [required].
num.k.rep	Number of replicates [default 1].
burnin	Number of iterations for MCMC burnin [default 1000].
numreps	Number of MCMC replicates [default 1000].
noadmix	Logical. No admixture? [default TRUE].
freqscorr	Logical. Correlated frequencies? [default FALSE].
randomize	Randomize [default TRUE].
seed	Set random seed [default 0].
pop.prior	A character specifying which population prior model to use: "locprior" or "use-popinfo" [default NULL].
locpriorinit	Parameterizes locprior parameter r - how informative the populations are. Only used when pop.prior = "locprior" [default 1].
maxlocprior	Specifies range of locprior parameter r. Only used when pop.prior = "locprior" [default 20].
gensback	Integer defining the number of generations back to test for immigrant ancestry. Only used when pop.prior = "usepopinfo" [default 2].
migrprior	Numeric between 0 and 1 listing migration prior. Only used when pop.prior = "usepopinfo" [default 0.05].
pfrompopflagon	ly
	Logical. update allele frequencies from individuals specified by popflag. Only used when pop.prior = "usepopinfo" [default TRUE].
popflag	A vector of integers (0, 1) or logicals identifying whether or not to use strata information. Only used when pop.prior = "usepopinfo" [default NULL].

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f t f	Logical. Infer the value of the model parameter # from the data; otherwise is fixed at the value alpha which is chosen by the user. This option is ignored under the NOADMIX model. Small alpha implies that most individuals are essentially from one population or another, while alpha > 1 implies that most individuals are admixed [default FALSE].
	Dirichlet parameter for degree of admixture. This is the initial value if inferalpha = TRUE [default 1].
i	Logical. Assume a uniform prior for alpha which runs between 0 and alphamax. This model seems to work fine; the alternative model (when unfprioralpha = 0) is to take alpha as having a Gamma prior, with mean alphapriora × alphapriorb, and variance alphapriora × alphapriorb^2 [default TRUE].
alphamax N	Maximum for uniform prior on alpha when unifprioralpha = TRUE [default 20].
	Parameters of Gamma prior on alpha when unifprioralpha = FALSE [default 0.05].
	Parameters of Gamma prior on alpha when unifprioralpha = FALSE [default 0.001].
	Create an Evanno plot once finished. Be aware k.range needs to be at least three different k steps [default TRUE].
plot_theme 7	Theme for the plot. See details for options [default theme_dartR()].
	Directory to save the plot RDS files [default as specified by the global working directory or tempdir()]
	Name for the RDS binary file to save (base name only, exclude extension) [de-fault NULL]
	Set verbosity for this function (though structure output cannot be switched off currently) [default NULL].

Details

The function is basically a convenient wrapper around the beautiful strataG function structureRun (Archer et al. 2016). For a detailed description please refer to this package (see references below).

Before running STRUCTURE, we suggest reading its manual (see link below) and the literature in mentioned in the references section.

https://web.stanford.edu/group/pritchardlab/structure_software/release_versions/v2.3.4/structure_doc.pdf To make use of this function you need to download STRUCTURE for you system (**non GUI version**) from here **STRUCTURE**.

Format note

For this function to work, make sure that individual and population names have no spaces. To substitute spaces by underscores you could use the R function gsub as below.

popNames(gl) <- gsub(" ","_",popNames(gl)); indNames(gl) <- gsub(" ","_",indNames(gl))</pre>

It's also worth noting that Structure truncates individual names at 11 characters. The function will fail if the names of individuals are not unique after truncation. To avoid this possible problem, a number sequence, as shown in the code below, might be used instead of individual names. indNames(g1) <- as.character(1:length(indNames(g1)))

Value

An sr object (structure.result list output). Each list entry is a single structurerun output (there are k.range * num.k.rep number of runs). For example the summary output of the first run can be accessed via sr[[1]]\$summary or the q-matrix of the third run via sr[[3]]\$q.mat. To conveniently summarise the outputs across runs (clumpp) you need to run gl.plot.structure on the returned sr object. For Evanno plots run gl.evanno on your sr object.

Author(s)

Bernd Gruber (Post to https://groups.google.com/d/forum/dartr)

References

- Pritchard, J.K., Stephens, M., Donnelly, P. (2000) Inference of population structure using multilocus genotype data. Genetics 155, 945-959.
- Archer, F. I., Adams, P. E. and Schneiders, B. B. (2016) strataG: An R package for manipulating, summarizing and analysing population genetic data. Mol Ecol Resour. doi:10.1111/1755-0998.12559
- Wang, Jinliang. "The computer program structure for assigning individuals to populations: easy to use but easier to misuse." Molecular ecology resources 17.5 (2017): 981-990.
- Lawson, Daniel J., Lucy Van Dorp, and Daniel Falush. "A tutorial on how not to over-interpret STRUCTURE and ADMIXTURE bar plots." Nature communications 9.1 (2018): 3258.
- Porras-Hurtado, Liliana, et al. "An overview of STRUCTURE: applications, parameter settings, and supporting software." Frontiers in genetics 4 (2013): 98.

Examples

```
# examples need structure to be installed on the system (see above)
## Not run:
bc <- bandicoot.gl[,1:100]
sr <- gl.run.structure(bc, k.range = 2:5, num.k.rep = 3,
exec = './structure.exe')
ev <- gl.evanno(sr)
ev
qmat <- gl.plot.structure(sr, K=3)
head(qmat)
gl.map.structure(qmat, bc, scalex=1, scaley=0.5)
## End(Not run)</pre>
```

gl.sfs

Creates a site frequency spectrum based on a dartR or genlight object

Description

Creates a site frequency spectrum based on a dartR or genlight object

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gl.sfs

Usage

```
gl.sfs(
    x,
    minbinsize = 0,
    folded = TRUE,
    singlepop = FALSE,
    plot.out = TRUE,
    plot.file = NULL,
    verbose = NULL
)
```

Arguments

х	dartR/genlight object
minbinsize	remove bins from the left of the sfs. For example to remove singletons (alleles only occurring once among all individuals) set minbinsize to 2. If set to zero, also monomorphic (d0) loci are returned.
folded	if set to TRUE (default) a folded sfs (minor allele frequency sfs) is returned. If set to FALSE then an unfolded (derived allele frequency sfs) is returned. It is assumed that 0 is homozygote for the reference and 2 is homozygote for the derived allele. So you need to make sure your coding is correct.
singlepop	switch to force to create a one-dimensional sfs, even though the genlight/dartR object contains more than one population
plot.out	Specify if plot is to be produced [default TRUE].
plot.file	Name for the RDS binary file to save (base name only, exclude extension) [de-fault NULL]
plot.dir	Directory in which to save files [default = working directory]
verbose	Verbosity: 0, silent or fatal errors; 1, begin and end; 2, progress log; 3, progress and results summary; 5, full report [default 2, unless specified using gl.set.verbosity].

Value

returns a site frequency spectrum, either a one dimensional vector (only a single population in the dartR/genlight object or singlepop=TRUE) or an n-dimensional array (n is the number of populations in the genlight/dartR object). If the dartR/genlight object consists of several populations the multidimensional site frequency spectrum for each population is returned [=a multidimensional site frequency spectrum]. Be aware the multidimensional spectrum works only for a limited number of population and individuals [if too high the table command used internally will through an error as the number of populations and individuals (and therefore dimensions) are too large]. To get a single sfs for a genlight/dartR object with multiple populations, you need to set singlepop to TRUE. The returned sfs can be used to analyse demographics, e.g. using fastsimcoal2.

Author(s)

Custodian: Bernd Gruber & Carlo Pacioni (Post to https://groups.google.com/d/forum/dartr)

References

Excoffier L., Dupanloup I., Huerta-Sánchez E., Sousa V. C. and Foll M. (2013) Robust demographic inference from genomic and SNP data. PLoS genetics 9(10)

Examples

```
gl.sfs(bandicoot.gl, singlepop = TRUE)
gl.sfs(possums.gl[c(1:5, 31:33), ], minbinsize = 1)
```

utils.outflank

OutFLANK: An Fst outlier approach by Mike Whitlock and Katie Lotterhos, University of British Columbia.

Description

This function is the original implementation of Outflank by Whitlock and Lotterhos. dartR simply provides a convenient wrapper around their functions and an easier install being an r package (for information please refer to their github repository)

Usage

```
utils.outflank(
   FstDataFrame,
   LeftTrimFraction = 0.05,
   RightTrimFraction = 0.05,
   Hmin = 0.1,
   NumberOfSamples,
   qthreshold = 0.05
)
```

Arguments

FstDataFrame A data frame that includes a row for each locus, with columns as follows:

- \$LocusName: a character string that uniquely names each locus.
- \$FST: Fst calculated for this locus. (Kept here to report the unbased Fst of the results)
- \$T1: The numerator of the estimator for Fst (necessary, with \$T2, to calculate mean Fst)
- \$T2: The denominator of the estimator of Fst
- \$FSTNoCorr: Fst calculated for this locus without sample size correction. (Used to find outliers)
- \$T1NoCorr: The numerator of the estimator for Fst without sample size correction (necessary, with \$T2, to calculate mean Fst)
- \$T2NoCorr: The denominator of the estimator of Fst without sample size correction

utils.outflank

	• \$He: The heterozygosity of the locus (used to screen out low heterozygosity	
	loci that have a different distribution)	
LeftTrimFraction		
	The proportion of loci that are trimmed from the lower end of the range of Fst before the likelihood funciton is applied [default 0.05].	
RightTrimFraction		
	The proportion of loci that are trimmed from the upper end of the range of Fst before the likelihood funciton is applied [default 0.05].	
Hmin	The minimum heterozygosity required before including calculations from a lo- cus [default 0.1].	
NumberOfSamples		
	The number of spatial locations included in the data set.	
qthreshold	The desired false discovery rate threshold for calculating q-values [default 0.05].	

Details

This method looks for Fst outliers from a list of Fst's for different loci. It assumes that each locus has been genotyped in all populations with approximately equal coverage.

OutFLANK estimates the distribution of Fst based on a trimmed sample of Fst's. It assumes that the majority of loci in the center of the distribution are neutral and infers the shape of the distribution of neutral Fst using a trimmed set of loci. Loci with the highest and lowest Fst's are trimmed from the data set before this inference, and the distribution of Fst df/(mean Fst) is assumed to'follow a chi-square distribution. Based on this inferred distribution, each locus is given a q-value based on its quantile in the inferred null'distribution.

The main procedure is called OutFLANK – see comments in that function immediately below for input and output formats. The other functions here are necessary and must be uploaded, but are not necessarily needed by the user directly.

Steps:

Value

The function returns a list with seven elements:

- FSTbar: the mean FST inferred from loci not marked as outliers
- FSTNoCorrbar: the mean FST (not corrected for sample size -gives an upwardly biased estimate of FST)
- dfInferred: the inferred number of degrees of freedom for the chi-square distribution of neutral FST
- numberLowFstOutliers: Number of loci flagged as having a significantly low FST (not reliable)
- numberHighFstOutliers: Number of loci identified as having significantly high FST
- results: a data frame with a row for each locus. This data frame includes all the original columns in the data set, and six new ones:
 - \$indexOrder (the original order of the input data set),
 - \$GoodH (Boolean variable which is TRUE if the expected heterozygosity is greater than the Hemin set by input),

- \$OutlierFlag (TRUE if the method identifies the locus as an outlier, FALSE otherwise), and
- \$q (the q-value for the test of neutrality for the locus)
- \$pvalues (the p-value for the test of neutrality for the locus)
- \$pvaluesRightTail the one-sided (right tail) p-value for a locus

Author(s)

Bernd Gruber (bugs? Post to https://groups.google.com/d/forum/dartr); original implementation of Whitlock & Lotterhos

utils.outflank.MakeDiploidFSTMat Creates OutFLANK input file from individual genotype info.

Description

Creates OutFLANK input file from individual genotype info.

Usage

utils.outflank.MakeDiploidFSTMat(SNPmat, locusNames, popNames)

Arguments

SNPmat	This is an array of genotypes with a row for each individual. There should be a column for each SNP, with the number of copies of the focal allele (0, 1, or 2) for that individual. If that individual is missing data for that SNP, there should be a 9, instead.
locusNames	A list of names for each SNP locus. There should be the same number of locus names as there are columns in SNPmat.
popNames	A list of population names to give location for each individual. Typically mul- tiple individuals will have the same popName. The list popNames should have the same length as the number of rows in SNPmat.

Value

Returns a data frame in the form needed for the main OutFLANK function.

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utils.outflank.plotter

Plotting functions for Fst distributions after OutFLANK

Description

This function takes the output of OutFLANK as input with the OFoutput parameter. It plots a histogram of the FST (by default, the uncorrected FSTs used by OutFLANK) of loci and overlays the inferred null histogram.

Usage

```
utils.outflank.plotter(
    OFoutput,
    withOutliers = TRUE,
    NoCorr = TRUE,
    Hmin = 0.1,
    binwidth = 0.005,
    Zoom = FALSE,
    RightZoomFraction = 0.05,
    titletext = NULL
)
```

Arguments

OFoutput	The output of the function OutFLANK()	
withOutliers	Determines whether the loci marked as outliers (with \$OutlierFlag) are included in the histogram.	
NoCorr	Plots the distribution of FSTNoCorr when TRUE. Recommended, because this is the data used by OutFLANK to infer the distribution.	
Hmin	The minimum heterozygosity required before including a locus in the plot.	
binwidth	The width of bins in the histogram.	
Zoom	If Zoom is set to TRUE, then the graph will zoom in on the right tail of the distirbution (based on argument RightZoomFraction)	
RightZoomFraction		
	Used when Zoom = TRUE. Defines the proportion of the distribution to plot.	
titletext	Allows a test string to be printed as a title on the graph	

Value

produces a histogram of the FST

```
utils.structure.evanno
```

Util function for evanno plots

Description

These functions were copied from package strataG, which is no longer on CRAN (maintained by Eric Archer)

Usage

utils.structure.evanno(sr, plot = TRUE)

Arguments

sr	structure run object
plot	should the plots be returned

Value

returns a list of dataframes (structure results) and a list of plots

Author(s)

Bernd Gruber (bugs? Post to https://groups.google.com/d/forum/dartr); original implementation of Eric Archer https://github.com/EricArcher/strataG

utils.structure.genind2gtypes structure util functions

Description

These functions were copied from package strataG, which is no longer on CRAN (maintained by Eric Archer)

Usage

utils.structure.genind2gtypes(x)

Arguments

x a genind object

utils.structure.run

Value

a gtypes object

Author(s)

Bernd Gruber (bugs? Post to https://groups.google.com/d/forum/dartr); original implementation of Eric Archer https://github.com/EricArcher/strataG

utils.structure.run Utility function to run Structure

Description

These functions were copied from package strataG, which is no longer on CRAN (maintained by Eric Archer)

Usage

utils.structure.run(g, k.range, num.k.rep, label, delete.files = TRUE, exec, burnin, numreps, noadmix, freqscorr, randomize, seed, pop.prior, locpriorinit, maxlocprior, gensback, migrprior, pfrompopflagonly, popflag, inferalpha, alpha, unifprioralpha, alphamax, alphapriora, alphapriorb)

g	a gtypes object [see strataG].
k.range	vector of values to for maxpop in multiple runs. If set to NULL, a single STRUC- TURE run is conducted with maxpops groups. If specified, do not also specify maxpops.
num.k.rep	number of replicates for each value in k.range.
label	label to use for input and output files
delete.files	logical. Delete all files when STRUCTURE is finished?
exec	name of executable for STRUCTURE. Defaults to "structure".
burnin	Number of burnin reps [default 10000].
numreps	Number of MCMC replicates [default 1000].
noadmix	Logical. No admixture? [default TRUE].
freqscorr	Logical. Correlated frequencies? [default FALSE].
randomize	Randomize [default TRUE].
seed	Set random seed [default 0].
pop.prior	A character specifying which population prior model to use: "locprior" or "use-popinfo" [default NULL].
locpriorinit	Parameterizes locprior parameter r - how informative the populations are. Only used when pop.prior = "locprior" [default 1].
maxlocprior	Specifies range of locprior parameter r. Only used when pop.prior = "locprior" [default 20].
gensback	Integer defining the number of generations back to test for immigrant ancestry. Only used when pop.prior = "usepopinfo" [default 2].
migrprior	Numeric between 0 and 1 listing migration prior. Only used when pop.prior = "usepopinfo" [default 0.05].
pfrompopflagonl	
	Logical. update allele frequencies from individuals specified by popflag. Only used when pop.prior = "usepopinfo" [default TRUE].
popflag	A vector of integers (0, 1) or logicals identifying whether or not to use strata information. Only used when pop.prior = "usepopinfo" [default NULL].
inferalpha	Logical. Infer the value of the model parameter # from the data; otherwise is fixed at the value alpha which is chosen by the user. This option is ignored under the NOADMIX model. Small alpha implies that most individuals are essentially from one population or another, while alpha > 1 implies that most individuals are admixed [default FALSE].
alpha	Dirichlet parameter for degree of admixture. This is the initial value if inferalpha = TRUE [default 1].
unifprioralpha	Logical. Assume a uniform prior for alpha which runs between 0 and alphamax. This model seems to work fine; the alternative model (when unfprioralpha = 0) is to take alpha as having a Gamma prior, with mean alphapriora × alphapriorb, and variance alphapriora × alphapriorb^2 [default TRUE].

alphamax	Maximum for uniform prior on alpha when unifprioralpha = TRUE [default 20].
alphapriora	Parameters of Gamma prior on alpha when unifprioralpha = FALSE [default 0.05].
alphapriorb	Parameters of Gamma prior on alpha when unifprioralpha = FALSE [default 0.001].

Value

- structureRun a list where each element is a list with results from structureRead and a vector of the filenames used
- structureWrite a vector of the filenames used by STRUCTURE
- structureRead a list containing:
 - summary new locus name, which is a combination of loci in group
 - q.mat data.frame of assignment probabilities for each id
 - prior.anc list of prior ancestry estimates for each individual where population priors were used
 - files vector of input and output files used by STRUCTURE
 - label label for the run

Author(s)

Bernd Gruber (bugs? Post to https://groups.google.com/d/forum/dartr); original implementation of Eric Archer https://github.com/EricArcher/strataG

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