Package 'PopGenome'

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```
Type Package
```

Title An Efficient Swiss Army Knife for Population Genomic Analyses

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Imports methods

Suggests parallel, bigmemory, BASIX, WhopGenome, BlockFeST

Description Provides efficient tools for population genomics data analysis, able to process individ-

ual loci, large sets of loci, or whole genomes. PopGenome <DOI:10.1093/molbev/msu136> not only implements a wide range of population genetics statistics, but also facilitates the easy implementation of new algorithms by other researchers. PopGenome is optimized for speed via the seamless integration of C code.

License GPL-3

URL http://popgenome.weebly.com

LazyLoad yes

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SystemRequirements zlib headers and library.

Repository CRAN

NeedsCompilation yes

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${\sf R}$ topics documented:

Achaz.stats-methods	. 3
BayeScanR	. 4
ealc.fixed.shared-methods	. 6
calc.R2-methods	. 7
codontable	. 8
concatenate.classes	. 9
concatenate.regions	. 10
count.unknowns-methods	
create.PopGenome.method	. 11
letail.stats-methods	. 12
liversity.stats-methods	. 14
liversity.stats.between-methods	. 16
asta_file	. 17
F_ST.stats-methods	. 18
F_ST.stats.2-methods	. 20
GENOME-class	. 22
get.biallelic.matrix-methods	. 27
get.codons-methods	. 28
get.feature.names	. 29
get.individuals-methods	. 30
get.status-methods	. 31
getBayes-methods	. 31
get_gff_info	. 32
gff_file	. 33
GFF_split_into_scaffolds	. 33
ntrogression.stats-methods	. 34
ack.knife.transform	. 36
inkage.stats-methods	. 37
oad.session	. 38
MKT-methods	. 39
MS	. 41
MS_getStats	. 42
nult.linkage.stats-methods	. 43
neutrality.stats-methods	
PG_plot.biallelic.matrix-methods	. 46
PopGenome	
PopGplot	. 48
ead.big.fasta	. 49
eadData	. 50
eadHapMap	. 53
eadMS	. 54
eadSNP	. 55
eadVCF	. 56
recomb.stats-methods	. 58
region.as.fasta-methods	. 59
gaya sassion	60

Achaz.stats-methods 3

	set.filter-methods	ıΙ
	set.outgroup-methods	52
	set.populations-methods	
	set.ref.positions-methods	
	set.synnonsyn-methods	54
	show.slots-methods	
	sliding.window.transform-methods	56
	snp_file	
	splitting.data-methods	57
	split_data_into_GFF_attributes	58
	split_data_into_GFF_features	59
	sweeps.stats-methods	70
	test.params-class	72
	vcf_file	73
	VCF_split_into_scaffolds	74
	weighted.jackknife	75
	Whop_readVCF	76
Index		78
mucx		U
Acha	z.stats-methods Achaz statistic	

Description

Achaz statistic

Usage

```
## S4 method for signature 'GENOME'
Achaz.stats(object,new.populations=FALSE,new.outgroup=FALSE,subsites=FALSE)
```

Arguments

```
object an object of class "GENOME"

new.populations

list of populations. default:FALSE

new.outgroup outgroup vector. default:FALSE

subsites "transitions": SNPs that are transitions.

"transversions": SNPs that are transversions.

"syn": synonymous sites.

"nonsyn": nonsynonymous sites.

"exon": SNPs in exon regions.

"intron": SNPs in intron regions.
```

4 BayeScanR

```
"coding": SNPs in coding regions (CDS).
"utr": SNPs in UTR regions.
"gene": SNPs in genes.
default:FALSE
```

Value

returned value is a modified object of class "GENOME"

The following Slots will be modified in the "GENOME" object

Yach Achaz Y statistic

References

Achaz G.,2008 Testing for neutrality in samples with sequencing errors. Genetics 179: 1409.

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class <- Achaz.stats(GENOME.class)
# GENOME.class <- Achaz.stats(GENOME.class,list(1:7,8:12))
# show the result:
# GENOME.class@Yach</pre>
```

BayeScanR

An R implementation of BayeScan (Foll\& Gagiotti 2008)

Description

BayeScanR is an R implementation of BayeScan for analysis of codominant markers.

Usage

BayeScanR(input,nb.pilot=10,pilot.runtime=2500,main.runtime=100000, discard=50000)

BayeScanR 5

Arguments

input textfile or an R-object returned by getBayes()

nb.pilot number of pilot runs
pilot.runtime length of pilot runs
main.runtime length of main runs

discard how many runs in the main.loop should be discarded?

Value

returned value is an object of class "BAYESRETURN"

The following Slots will be filled

alpha alpha effects beta beta effects

var_alpha variance of alpha values

a_inc which alpha is included in the model

fst FST values
P P-value

References

[1] Foll M and OE Gaggiotti (2008). A genome scan method to identify selected loci appropriate for both dominant and codominant markers: A Bayesian perspective. Genetics 180: 977-993

```
# GENOME.class <- readData("...\Alignments")
# GENOME.class <- F_ST.stats(GENOME.class,list(1:5,6:10))
# Bayes.input <- getBayes(GENOME.class)
# BAYES.class <- BayeScanR(Bayes.input)
# BAYES.class</pre>
```

6 calc.fixed.shared-methods

```
calc.fixed.shared-methods
```

Fixed and shared polymorphisms

Description

A generic function to calculate the number of fixed and shared polymorphisms.

Usage

```
## S4 method for signature 'GENOME'
calc.fixed.shared(object,
subsites=FALSE,
new.populations=FALSE,
fixed.threshold=1,
fixed.threshold.fst=1)
```

Arguments

```
object
                 An object of class "GENOME"
                  "transitions": SNPs that are transitions.
subsites
                  "transversions": SNPs that are transversions.
                  "syn": synonymous sites.
                  "nonsyn": nonsynonymous sites.
                  "exon": SNPs in exon regions.
                  "intron": SNPs in intron regions.
                  "coding": SNPs in coding regions (CDS).
                  "utr": SNPs in UTR regions.
                  "gene": SNPs in genes.
                  "intergenic": SNPs in intergenic regions.
new.populations
                 list of populations. default=FALSE
fixed.threshold
                  Polymorphisms are considered as fixed >= threshold value
fixed.threshold.fst
                  Polymorphisms are considered as fixed >= threshold value
```

Details

The nucleotide diversities have to be devided by GENOME.class@n.sites to give diversities per site.

calc.R2-methods 7

Value

Returned value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

	Slot	Reference	Description
1.	n.fixed.sites	[x]	Number of fixed sites
2.	n.shared.sites	[x]	Number of shared sites
3.	n.monomorphic.sites	[x]	Number of monomorphic sites

References

[x]

Examples

```
# GENOME.class <- readData("\home\Alignments")</pre>
# set.populations
# GENOME.class <- calc.fixed.shared(GENOME.class)</pre>
```

calc.R2-methods

Linkage statistics (R2, P-value, Distance)

Description

This generic function calculates some linkage disequilibrium statistics.

Usage

```
## S4 method for signature 'GENOME'
calc.R2(object, subsites=FALSE, lower.bound=0, upper.bound=1)
```

Arguments

object an object of class "GENOME" subsites same as in the other modules

lower.bound sites with minor-allele-frequency>=lower.bound are considered upper.bound sites with minor-allele-frequency<=upper.bound are considered 8 codontable

Details

Note, the pairwise comparisons are computed via combn(n.snps, 2).

Value

The slot GENOME.class@region.stats@linkage.disequilibrium will be filled. (R2,P-value,Distance)
Fisher's Exact Test is used for the P-values.

Examples

```
# GENOME.class <- readData("...\Alignments")
# GENOME.class
# GENOME.class <- calc.R2(GENOME.class)
# show the result:
# GENOME.class@region.stats@linkage.disequilibrium
# [[x]][[y]] x:region, y:population</pre>
```

codontable

Prints the codon table which is used in the PopGenome framework

Description

This functions prints the nucleotide triplets (as numerical values) and the corresponding protein character strings.

Usage

codontable()

Arguments

no arguments

Details

The returned value is a list including two matrices.

The first matrix contains the amino acids and the second matrix the corresponding nucleotide triplets. In the PopGenome Vignette you can see how to manipulate these tables to use alternative genetic codes.

concatenate.classes 9

Examples

```
# table <- codontable()
# table$Proteins
# table$Triplets</pre>
```

concatenate.classes

Concatenate GENOME classes

Description

This function concatenates objects of class GENOME, allowing to stitch together larger datasets from smaller objects.

Usage

```
concatenate.classes(classlist)
```

Arguments

```
classlist a list of GENOME objects
```

Value

The function creates an object of class "GENOME".

```
# a <- readData("Three_Alignments/")
# b <- readData("Two_Alignments/")
# ab <- concatenate.classes(list(a,b))
# ab <- neutrality.stats(ab)
# ab@Tajima.D
# ab@region.names</pre>
```

10 count.unknowns-methods

concatenate.regions Concatenate regions

Description

This function concatenates the regions/chunks contained in one GENOME object.

Usage

```
concatenate.regions(object)
```

Arguments

object of class GENOME

Value

The function creates an object of class "GENOME".

Examples

```
# GENOME.class <- readData("Three_Alignments/")
# WHOLE <- concatenate.regions(GENOME.class)
# WHOLE <- neutrality.stats(WHOLE)
# WHOLE@Tajima.D</pre>
```

count.unknowns-methods

Calculate missing nucleotide frequencies

Description

A generic function to calculate the missing nucleotide frequencies.

Usage

```
## S4 method for signature 'GENOME'
count.unknowns(object)
```

Arguments

```
object An object of class "GENOME"
```

Value

Returned value is a modified object of class "GENOME"

The slot GENOME.class@missing.freqs for the missing frequencies for the whole region. The slot GENOME.class@region.stats@missing.freqs for the missing frequencies for each SNP in a given region

Examples

```
# GENOME.class <- readData("VCF", format="VCF", include.unknown=TRUE)
# GENOME.class@region.stats
# GENOME.class <- count.unknowns(GENOME.class)
# GENOME.class@missing.freqs
# GENOME.class@region.stats@missing.freqs</pre>
```

create.PopGenome.method

Integration of own functions into the PopGenome-framework

Description

This function generates a skeleton for a PopGenome function. It thereby facilitates the effortless integration of new methods into the PopGenome framework.

Usage

```
create. Pop Genome.method (function.name, population.specific=TRUE)\\
```

Arguments

```
function.name name of your function population.specific
```

TRUE:function returns one value per population.FALSE:function returns one value calculated across all populations (as in the case of FST measurements)

12 detail.stats-methods

Details

This mechanism enables you to use your own functions in the PopGenome environment. The functions can also be applied to sliding windows or subsites.

Please look at the generated function, which documents where to place your own function in detail.

Examples

```
# GENOME.class <- readData(".../Alignments")
# create.PopGenome.method("myFunction")
# edit myFunction.R
# source("myFunction")
# value <- myFunction(test)
# value</pre>
```

```
detail.stats-methods Several statistics
```

Description

This generic function calculates some mixed statistics.

Usage

Arguments

```
object an object of class "GENOME" new.populations list of populations.
```

detail.stats-methods 13

new.outgroup outgroup sequences. "transitions": SNPs that are transitions. subsites "transversions": SNPs that are transversions. "syn": synonymous sites. "nonsyn": nonsynonymous sites. "exon": SNPs in exon regions. "intron": SNPs in intron regions. "coding": SNPs in coding regions (CDS). "utr": SNPs in UTR regions. "gene": SNPs in genes. biallelic.structure fixed and shared polymorphisms (stored in GENOME.class@region.stats). mismatch.distribution statistics based on mismatch distribution site.spectrum minor allele frequency of each SNP site.FST computes FST for each SNP Value The return value is a modified object of class "GENOME" The following Slots will be modified in the "GENOME" object **MDSD** MDG1 MDG2 region.stats the slot biallelic.structure and minor.allele.freqs will be filled The function get.detail(GENOME.class, biallelic.structure=TRUE) returns a matrix for each region, where 0 population is polymorphic, the remaining individuals are polymorphic population is polymorphic, the remaining individuals are monomorphic 1 2 population is monomorphic, the remaining individuals are polymorphic

population is monomorphic, the remaining individuals are monomorphic with

3

the same value

4 population is monomorphic, the remaining individuals are monomorphic with different values

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class <- set.populations(GENOME.class,list(1:10))
# GENOME.class <- detail.stats(GENOME.class)
# show the result:
# mismatch.values <- get.detail(GENOME.class)
# bial.struc.values <- get.detail(GENOME.class, biallelic.structure=TRUE)
# GENOME.class@region.stats@biallelic.structure
# GENOME.class@region.stats@biallelic.structure[[1]]</pre>
```

diversity.stats-methods

Diversities

Description

A generic function to calculate nucleotide & haplotype diversities.

Usage

```
## S4 method for signature 'GENOME'
diversity.stats(object,new.populations=FALSE,subsites=FALSE,pi=FALSE, keep.site.info=TRUE)
```

Arguments

```
object An object of class "GENOME"

new.populations

list of populations. default=FALSE

subsites "transitions": SNPs that are transitions.

"transversions": SNPs that are transversions.

"syn": synonymous sites.

"nonsyn": nonsynonymous sites.

"exon": SNPs in exon regions.

"intron": SNPs in intron regions.

"coding": SNPs in coding regions (CDS).

"utr": SNPs in UTR regions.

"gene": SNPs in genes.
```

diversity.stats-methods 15

"intergenic": SNPs in intergenic regions.

```
Nei's calculation of pi
рi
```

keep.site.info stores site specific values in GENOME.class@region.stats

Details

The nucleotide diversities have to be devided by GENOME.class@n.sites to give diversities per

Value

Returned value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

	Slot	Reference	Description
1.	nuc.diversity.within	[1,3]	Nucleotide diversity (within the population)
2.	Pi	[2]	Diversity from Nei (within the population)
3.	hap.diversity.within	[1]	Haplotype diversity (within the population)

References

- [1] Hudson, R. R., M. Slatkin, and W.P. Maddison (1992). Estimating of levels of gene flow from DNA sequence data. Gentics 13(2),583-589
- [2] Nei, M. (1987). Molecular Evolutionary Genetics. Columbia Univ. Press, New York.
- [3] Wakeley, J. (1996). The Variance of Pairwise Nucleotide Differences in Two Populations with Migration. THEORETICAL POPULATION BIOLOGY. 49, 39-57.

```
# GENOME.class <- readData("\home\Alignments")</pre>
# GENOME.class
# GENOME.class <- diversity.stats(GENOME.class)</pre>
# GENOME.class <- diversity.stats(GENOME.class,list(1:4,5:10))</pre>
# GENOME.class <- diversity.stats(GENOME.class,</pre>
# list(c("seq1","seq5","seq3"),c("seq2","seq8")))
# show the result:
# GENOME.class@nuc.diversity.within
```

```
diversity.stats.between-methods

Diversities
```

Description

A generic function to calculate nucleotide & haplotype diversities between populations (dxy).

Usage

```
## S4 method for signature 'GENOME'
diversity.stats.between(object,new.populations=FALSE,subsites=FALSE,keep.site.info=FALSE,
haplotype.mode=FALSE, nucleotide.mode=TRUE)
```

Arguments

An object of class "GENOME" object new.populations list of populations. default=FALSE "transitions": SNPs that are transitions. subsites "transversions": SNPs that are transversions. "syn": synonymous sites. "nonsyn": nonsynonymous sites. "exon": SNPs in exon regions. "intron": SNPs in intron regions. "coding": SNPs in coding regions (CDS). "utr": SNPs in UTR regions. "gene": SNPs in genes. "intergenic": SNPs in intergenic regions. keep.site.info Store SNP specific values in the region.stats haplotype.mode Haplotype Diversities nucleotide.mode **Nucleotide Diversities**

Details

The nucleotide diversities have to be devided by GENOME.class@n.sites to give diversities per site.

fasta_file 17

Value

Returned value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

```
Slot
                               Reference
                                           Description
1. nuc.diversity.between
                               [1,3]
                                           Nucleotide diversity (between the population)
2. hap.diversity.between
                               [1]
                                           Haplotype diversity (between the population)
```

References

- [1] Hudson, R. R., M. Slatkin, and W.P. Maddison (1992). Estimating of levels of gene flow from DNA sequence data. Gentics 13(2),583-589
- [2] Wakeley, J. (1996). The Variance of Pairwise Nucleotide Differences in Two Populations with Migration. THEORETICAL POPULATION BIOLOGY. 49, 39-57.

Examples

```
# GENOME.class <- readData("\home\Alignments")</pre>
# GENOME.class
# GENOME.class <- diversity.stats.between(GENOME.class)</pre>
# GENOME.class <- set.populations(GENOME.class, list(...))</pre>
# GENOME.class <- diversity.stats.between(GENOME.class)</pre>
# GENOME.class <- diversity.stats(GENOME.class,</pre>
# list(c("seq1","seq5","seq3"),c("seq2","seq8")))
# show the result:
# GENOME.class@nuc.diversity.within
```

fasta_file FASTA file (subdirectory "data")

Description

The FASTA files (unpacked) in the subdirectory "data" of the PopGenome package have to be stored in a folder (multiple files can be stored in this folder). The folder name is then used as the input for the readData function.

F_ST.stats-methods

F_ST.stats-methods Fixation Index

Description

A generic function to calculate some F-statistics and nucleotide/haplotype diversities.

Usage

```
## S4 method for signature 'GENOME'
F_ST.stats(
object,
new.populations=FALSE,
subsites=FALSE,
detail=TRUE,
mode="ALL",
only.haplotype.counts=FALSE,
FAST=FALSE
)

## S4 method for signature 'GENOME'
get.diversity(object,between=FALSE)
## S4 method for signature 'GENOME'
get.F_ST(object,mode=FALSE,pairwise=FALSE)
```

Arguments

```
An object of class "GENOME"
object
new.populations
                  list of populations. default:FALSE
                  "transitions": SNPs that are transitions.
subsites
                  "transversions": SNPs that are transversions.
                  "syn": synonymous sites.
                  "nonsyn": nonsynonymous sites.
                  "exon": SNPs in exon regions.
                  "intron": SNPs in intron regions.
                  "coding": SNPs in coding regions (CDS).
                  "utr": SNPs in UTR regions.
                  "gene": SNPs in genes.
                  "intergenic": SNPs in intergenic regions.
                  detail statistics. Note: slower!
detail
                  TRUE: show between-diversities. FALSE: show within-diversities
between
                 mode="haplotype" or mode="nucleotide"
mode
```

F_ST.stats-methods

only.haplotype.counts

only calculate the haplotype counts

FAST if TRUE only calculate a subset of statistics. see details!

pairwise show paiwise comparisons. default:FALSE

Details

If FAST is switched on, this module only calculates nuc.diversity.within, hap.diversity.within, haplotype.F_ST, nucleotide.F_ST and pi.

Note:

- 1) The nucleotide diversities have to be devided by the size of region considered (e.g. GENOME@n.sites) to give diversities per site.
- 2) When missing or unknown nucleotides are included (include.unknown=TRUE) those sites are completely deleted in case of haplotype based statistics.
- 3) The function detail.stats(..., site.FST=TRUE) will compute SNP specific FST values which are then stored in the slot GENOME.class@region.stats@site.FST.
- 4) We recommend to use mode="nucleotide" in case you have many unknowns included in your dataset.

Value

	Slot	Reference	Description
1.	haplotype.F_ST	[1]	Fixation Index based on haplotype frequencies
2.	nucleotide.F_ST	[1]	Fixation Index based on minor.allele frequencies
3.	Nei.G_ST	[2]	Nei's Fixation Index
4.	Hudson.G_ST	[3]	see reference
5.	Hudson.H_ST	[3]	see reference
6.	Hudson.K_ST	[3]	see reference
7.	nuc.diversity.within	[1,5]	Nucleotide diversity (within the population)
8.	hap.diversity.within	[1]	Haplotype diversity (within the population)
9.	Pi	[4]	Nei's diversity (within the population)
10.	hap.F_ST.vs.all	[1]	Fixation Index for each population against all other individuals (haplotype)
11.	nuc.F_ST.vs.all	[1]	Fixation Index for each population against tall other individuals (nucleotide)
12.	hap.diversity.between	[1]	Haplotype diversities between populations
13.	nuc.diversity.between	[1,5]	Nucleotide diversities between populations
14.	nuc.F_ST.pairwise	[1]	Fixation Index for every pair of populations (nucleotide)
15.	hap.F_ST.pairwise	[1]	Fixation Index for every pair of populations (haplotype)
16.	Nei.G_ST.pairwise	[2]	Fixation Index for every pair of populations (Nei)
17.	region.stats		an object of class "region.stats" for detailed statistics

References

[1] Hudson, R. R., M. Slatkin, and W.P. Maddison (1992). *Estimating levels of gene flow from DNA sequence data*. Gentics 13(2),583-589

20 F_ST.stats.2-methods

[2] Nei, M. (1973). Analysis of gene diversity in subdivided populations. Proc.Natl. Acad. Sci. USA 70: 3321-3323

- [3] Hudson, R. R., Boos, D.D. and N. L. Kaplan (1992). A statistical test for detecting population subdivison. Mol. Biol. Evol. 9: 138-151.
- [4] Nei, M. (1987). Molecular Evolutionary Genetics. Columbia Univ. Press, New York.
- [5] Wakeley, J. (1996). The Variance of Pairwise Nucleotide Differences in Two Populations with Migration. THEORETICAL POPULATION BIOLOGY. 49, 39-57.

See Also

```
# methods?F_ST.stats.2 #F_ST.stats.2
```

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class <- F_ST.stats(GENOME.class)
# GENOME.class <- F_ST.stats(GENOME.class,list(1:4,5:10),subsites="syn")
# GENOME.class <- F_ST.stats(GENOME.class,list(c("seq1","seq5","seq3"),c("seq2","seq8")))
# show the result:
# get.F_ST(GENOME.class)
# get.F_ST(GENOME.class, pairwise=TRUE)
# get.diversity(GENOME.class, between=TRUE)
# GENOME.class@Pi --> population specific view
# GENOME.class@region.stats
```

```
F\_ST.stats.2-methods Fixation Index (2)
```

Description

A generic function to calculate some FST measurenments.

Usage

```
## S4 method for signature 'GENOME'
F_ST.stats.2(object,new.populations="list",subsites=FALSE,snn=TRUE,Phi_ST=FALSE)
```

F_ST.stats.2-methods 21

Arguments

object An object of class "GENOME"

new.populations

list of populations. default=FALSE

subsites "transitions": SNPs that are transitions.

"transversions": SNPs that are transversions.

"syn": synonymous sites.

"nonsyn": nonsynonymous sites.
"exon": SNPs in exon regions.
"intron": SNPs in intron regions.

"coding": SNPs in coding regions (CDS).

"utr": SNPs in UTR regions.

"gene": SNPs in genes.

"intergenic": SNPs in intergenic regions.

snn Snn statistic from Hudson
Phi_ST Statistic from Excoffier et al.

Value

Returned value is an modified object of class "GENOME"

Following slots will be modified in the "GENOME" object

Slot Reference Description

Hudson. Snn [1] Snn statistic from Hudson (2000)
 Phi_ST [2] Phi_ST from Excoffier (1992)

References

[1] Hudson, R. R. (2000). A new statistic for detecting genetic differentiation. Genetics 155: 2011-2014.

[2] Excoffier, L., Smouse, P., Quattro, J. (1992), Analysis of molecular variance inferred from metric distances among DNA haplotypes: application to human mitochondrial DNA restriction data. Genetics 131: 479-91

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME alace</pre>
```

GENOME.class

GENOME.class <- F_ST.stats.2(GENOME.class)</pre>

```
# GENOME.class <- F_ST.stats.2(GENOME.class,list(1:4,5:10))
# GENOME.class <- F_ST.stats.2(GENOME.class,
# list(c("seq1","seq5","seq3"),c("seq2","seq8")))
# show the result:
# GENOME.class@Hudson.Snn</pre>
```

GENOME-class

Class "GENOME"

Description

A class where all data and calculated values are stored

Slots

```
BIG.BIAL: Biallelic matrix as an ff-object
SLIDE.POS: Positions of biallelic sites (Sliding window mode)
big.data: ff-package?
gff.info: Gff information?
snp.data: SNP data?
basepath: The basepath of the data
project: —
populations: Populations definded before reading data
poppairs: —
outgroup: A vector of outgroup sequences
region.names: Names/identifier of each region
feature.names: Feature attributes of a given region
genelength: Number of regions
keep.start.pos: Start positions for sliding window
n.sites: Total number of sites
n.sites2: Total number of sites
n.biallelic.sites: Number of biallelic sites (SNPs)
n.gaps: Number of gaps observed in the data
n.unknowns: Number of unknown.positions
n.valid.sites: Sites without gaps
n.polyallelic.sites: Sites with more than two variants
trans.transv.ratio: Transition-transversion ratio
Coding. region: Number of nucleotides in CDS regions
UTR. region: Number of nucleotides in UTR regions
```

Intron. region: Number of nucleotides in Intron regions Exon. region: Number of nucleotides in Exon regions Gene.region: Number of nucleotides in Gene regions Pop_Neutrality: Populations defined in the neutrality module Pop_FSTN: Populations defined in the FST (nucleotide) module Pop_FSTH: Populations defined in the FST (haplotype) module Pop_Linkage: Populations defined in the Linkage module Pop_Slide: — Pop_MK: Populations defined in the MK module Pop_Detail: Populations defined in the Detail module Pop_Recomb: Populations defined in the Recombination module Pop_Sweeps: Populations defined in the Selective sweeps module FSTNLISTE: nucleotide.F_ST: Nucleotide FST nucleotide.F ST2: nuc.diversity.between: Nucleotide diversity between the populations nuc.diversity.within: Nucleotide diversity within the populations nuc.F_ST.pairwise: FST for each pair of populations nuc.F_ST.vs.all: FST for one population vs. all other individuals n.haplotypes: hap.diversity.within: Haplotype diversity withing the populations hap.diversity.between: Haplotype diversity between the populations Pi: Pi from Nei PIA_nei: Pi between the populations haplotype.counts: Counts of the haplotypes observed haplotype.F_ST: Haplotype FST hap.F_ST.pairwise: Haplotype diversity for each pair of populations Nei.G_ST.pairwise: Haplotype diversity for each pair of populations hap.F_ST.vs.all: FST for one population vs. all other individuals Nei.G_ST: GST from Nei Hudson. G_ST: GST from Hudson Hudson. H_ST: HST from Hudson Hudson.K_ST: KST from Hudson Hudson. Snn: Snn from Hudson Phi_ST: Fixation index from Excoffier hap.pair.F_ST: — MKT: Mcdonald-Kreitman values

```
Tajima.D: Tajima's D
SLIDE: —
Fay.Wu.H:
Zeng.E:
theta_Tajima:
theta_Watterson:
theta_Fu.Li:
theta_Achaz.Watterson:
theta_Achaz.Tajima:
theta_Fay.Wu:
theta_Zeng:
Fu.Li.F:
Fu.Li.D:
Yach:
n.segregating.sites: Total number of segregating sites
Rozas.R_2:
Fu.F_S:
Strobeck.S:
Kelly.Z_nS:
Rozas.ZZ:
Rozas.ZA:
Wall.B:
Wall.Q:
mult.Linkage: Linkage disequilibrium between regions
RM: Minimum number of recombination events (Hudson)
CL: Composite likelihood of SNPs (Nielsen et. al)
CLmax: Max. composite likelihood of SNPs (Nielsen et.al)
CLR: Composite likelihood ratio test (Nielsen et. al)
MDSD:
MDG1:
MDG2:
genes:
region.data: Detailed information about the data
region.stats: Detailed (site-specific) statistics
D Pattersons D statistic
f the fraction of the genome that is admixed
jack.knife jacknife mode
```

```
missing.freqs: Missing nucleotide frequency
n.fixed.sites: ...
n.shared.sites: ...
n.monomorphic.sites: ...
BD: ...
BDF: ...
BDF_bayes: ...
alpha_ABBA: ...
alpha_BABA: ...
beta_BBAA: ...
Bd_clr: ...
Bd_dir: ...
D.pval: ...
D.z: ...
D.SE: ...
BDF.pval: ...
BDF.z: ...
BDF.SE: ...
P.Bd_clr: ...
RNDmin: ...
```

Methods

```
detail.stats Several misc. statistics
diversity.stats Haplotype and nucleotide diversities
diversity.between Haplotype and nucleotide diversities
F_ST.stats.2 Snn from Hudson
F_ST.stats Fixation index
getBayes Get the input for BayeScanR
get.detail Get the results from the Detail module
get.codons Get information about the nature of codon changes
get.diversity Get diversities from the FST module
get.F_ST Get FST values from the FST module
get.linkage Get the values from the Linkage module
get.MKT Get Mcdonald-Kreitman values
getMS —
get.neutrality Get the values from the Neutrality module
get.status Status of calculations
```

get.sum.data Get some data observed from the alignments linkage.stats Linkage disequilibrium calc.R2 Linkage disequilibrium mult.linkage.stats Linkage disequilibrium between regions recomb.stats Recombination statistics sweeps.stats Selective sweeps Achaz.stats Achaz's statistics **get.recomb** Get the values from the Recombination module **get.sweeps** Get the values frome the Selective Sweep module **set.ref.positions** Set the SNP positions set.synnonsyn Verify synonymous positions **splitting.data** Split the data into subsites MKT MKT Test neutrality.stats Neutrality statistics popFSTN Internal function get.biallelic.matrix Print the biallelic.matrix set.populations Define the populations set.outgroup Define the outgroup get.individuals get the names/IDs of individuals region.as.fasta Extract the region as a fasta file show show.slots Show slots of the class GENOME sliding.window.transform Transform a GENOME object into a new object suitable for sliding window analysis usage — **PG_plot.biallelic.matrix** Plot the biallelic matrix introgression.stats Methods to measure archaic admixture **count.unknowns** Calculates the frequencies of missing nucleotides calc.fixed.shared Calculates the frequencies of missing nucleotides set.filter SNP Filtering weighted.jackknife weighted jackknife

Author(s)

Bastian Pfeifer

References

See the documentation for each module

Examples

```
#GENOME.class <- readData("Alignments")
#GENOME.class@n.sites
#GENOME.class@region.names</pre>
```

Description

This function returns the biallelic matrix of a specific region.

Usage

```
## S4 method for signature 'GENOME'
get.biallelic.matrix(object,region)
```

Arguments

object An object of class "GENOME"

region ID of the region

Value

Biallelic matrix rows: names of individuals columns: biallelic sites

```
# GENOME.class <- readData("\home\Alignments")
# get.biallelic.matrix(GENOME.class,7) # biallelic matrix of the 7th alignment</pre>
```

28 get.codons-methods

get.codons-methods

Detailed information about the nature of codon changes

Description

This generic function returns some information about the codon changes resulting from the observed SNPs.

Usage

```
## S4 method for signature 'GENOME'
get.codons(object, regionID)
```

Arguments

object an object of class "GENOME"

regionID what region/alignment should be analyzed?

Details

The slot GENOME.class@region.data@synonymous and GENOME.class@region.data@codons have to be set.

The data have to be read in with the correponding GFF file.

The function set.synnonsyn(..., save.codons=TRUE) sets the syn/nonsny sites in case of SNP data and stores the corresponding codon changes.

Value

The function get. codons returns a data.frame with the following information

1	Position of the SNPs
2	Major Codon
3	Minor Codon
4	Major amino acid
5	Minor amino acid
6	synonymous (TRUE/FALSE)
7	Polarity of the major amino acid
8	Polarity of the minor amino acid

get.feature.names 29

Examples

```
# Alignments
# GENOME.class <- readData("FASTA",gffpath="GFF")
# get.codons(GENOME.class,1)
# SNP data
# GENOME.class <- readData("VCF",gffpath="GFF")
# GENOME.class <- set.synnonsyn(GENOME.class, ref.chr="ref.fas",save.codons=TRUE)
# get.codons(GENOME.class,1)</pre>
```

get.feature.names

Feature informations and GFF-attributes

Description

Returns feature names and additional attributes for a given region

Usage

```
get.feature.names(object, gff.file, chr)
```

Arguments

object An object of class GENOME gff.file The corresponding GFF file

chr The chromosome/scaffold identifier

Details

The algorithm uses the information stored in GENOME.class.split@region.names to iterate over the GFF file and returns attribute plus feature informations for each given region. Note, the functions splitting.data, split_data_into_GFF_attributes or sliding.window.transform should be performed prior to that.

The slot region. names must have the following form: "pos1 - pos2".

Value

The returned value is a character vector of length length(GENOME.class.split@region.names)

Examples

```
# GENOME.class <- readVCF("chr1.vcf.gz",1000,"1",1,100000)
# GENOME.class.split <- split_data_into_GFF_attributes(GENOME.class,"Homo_sapiens.GRCh37.73.gtf",
# "1", "gene_name")
# GENOME.class.split@region.names
# info <- get.feature.names(GENOME.class.split, gff.file="Homo_sapiens.GRCh37.73.gtf", chr="1")
# GENOME.class.split <- splitting.data(GENOME.class, subsites="gene")
# GENOME.class.split@region.names
# info <- get.feature.names(GENOME.class.split, gff.file="Homo_sapiens.GRCh37.73.gtf", chr="1")</pre>
```

```
get.individuals-methods
```

Print the names/IDs of individuals

Description

Extract the names/IDs of individuals.

Usage

```
## S4 method for signature 'GENOME'
get.individuals(object,region=FALSE)
```

Arguments

object an object of class "GENOME"
region a vector of regions. Default: ALL

```
# GENOME.class <- readData("\home\Alignments")
# get.individuals(GENOME.class)</pre>
```

get.status-methods 31

get.status-methods State of calculations

Description

Some information about the definitions of populations and subsites.

Usage

```
## S4 method for signature 'GENOME'
get.status(object)
```

Arguments

object

An object of class "GENOME"

Examples

```
# get.status(GENOME.class)
```

getBayes-methods

Get values for BayeScanR

Description

This function returns the values that are necessary to run BayeScanR.

Usage

```
## S4 method for signature 'GENOME'
getBayes(object,snps=FALSE)
```

Arguments

object An object of class "GENOME" snps SNPs are considered seperately

Value

coming soon!

get_gff_info

References

Foll M and OE Gaggiotti (2008). A genome scan method to identify selected loci appropriate for both dominant and codominant markers: A Bayesian perspective. Genetics 180: 977-993

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class <- F_ST.stats(GENOME.class,list(1:4,5:10))
# Bayes.input <- getBayes(GENOME.class)
# Bayes.class <- BayeScanR(Bayes.input)</pre>
```

get_gff_info

Annotation info

Description

This function extracts annotation information from a GTF/GFF file.

Usage

```
get_gff_info(object=FALSE,gff.file,chr,position,feature=FALSE,extract.gene.names=FALSE)
```

Arguments

 $object \qquad object \ of \ class \ {\tt GENOME}$

gff.file basepath of the GTF/GFF file

chr the chromosome

position reference positions or region id (when object is specified) feature feature to search for in the gff-file. returns a list of positions

extract.gene.names

returns the gene names of the chromosome

Details

This function extracts annotation information from a GTF/GFF file.

```
# get_gff_info("Arabidopsis.gff",chr=1,200202)
# get_gff_info(GENOME.class,"Arabidopsis.gff",chr=1,position=3)
```

gff_file 33

gff_file

GFF file (subdirectory "data")

Description

A typical GFF file which should be stored in a folder (for example in "GFF"). This folder is the input for the readData(...,gffpath="GFF") function. The corresponding FASTA file is stored in the "data" subdirectory of the PopGenome package. It has to be stored in a folder with the SAME NAME as the GFF file (for example in "FASTA"). readData("FASTA", gffpath="GFF")

```
{\tt GFF\_split\_into\_scaffolds}
```

Split a GFF file into multiple scaffold-GFFs

Description

This function splits a GFF file into multiple GFFs including data for exactly one scaffold each.

Usage

```
GFF_split_into_scaffolds(GFF.file, output.folder)
```

Arguments

```
GFF.file the basepath of the GFF file output.folder name of the folder where the GFFs should be stored
```

Details

The algorithm splits the GFF into multiple scaffold based GFFs and stores the files in a given folder. This folder can be used as an input for readData(,gffpath="")

Value

TRUE

```
# GFF_split_into_scaffolds("GFFfile.gff","scaffoldGFFs")
# test <- readData("scaffoldVCFs", format="VCF", gffpath="scaffoldGFFs")</pre>
```

introgression.stats-methods

Introgression statistics

Description

A generic function to estimate archaic admixture.

Usage

```
## $4 method for signature 'GENOME'
introgression.stats(object,
subsites=FALSE,
do.D=TRUE,
do.BDF=TRUE,
keep.site.info=TRUE,
block.size=FALSE,
do.RNDmin=FALSE,
l.smooth=FALSE)
```

Arguments

	biect	An object of class "GENOME"
--	-------	-----------------------------

subsites "transitions": SNPs that are transitions.

"transversions": SNPs that are transversions.

"syn": synonymous sites.

"nonsyn": nonsynonymous sites.
"exon": SNPs in exon regions.
"intron": SNPs in intron regions.

"coding": SNPs in coding regions (CDS).

"utr": SNPs in UTR regions. "gene": SNPs in genes.

"intergenic": SNPs in intergenic regions.

do.D Pattersons D and Martin's f statistic

do.BDF Bd-fraction

keep.site.info keep site specific values (GENOME.class@region.stats)

block.size the block size for jackknife
do.RNDmin RNDmin (Rosenzweig, 2016)

1.smooth laplace smoothing for Bd-fraction

Details

To perform the D and f statistic one needs to define 3 populations via the function set.populations, where the third population represent the archaic population. In addition, an outgroup is required and have to be set via the function set.outgroup. Here, only SNPs where the outgroup is monomorphic are considered. f is the fraction of the genome that is admixed [2].

Value

Returned value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

	Slot	Reference	Description
1.	D	[1;eq. 2]	Pattersons D statistic
2.	f	[2]	f statistic
3.	BDF	[x]	Bd-fraction
4.	RNDmin	[x]	RNDmin
5.	D.z	[x]	z values (jackknife)
6.	D.pval	[x]	P values (jackknife)
7.	BDF.z	[x]	z values (jackknife)
8.	BDF.pval	[x]	P values (jackknife)

References

[1] Durand, E. Y., Patterson, N. J., Reich, D., & Slatkin, M. (2011). Testing for ancient admixture between closely related populations.

Molecular Biology and Evolution, 28(8), 2239–2252. doi:10.1093/molbev/msr048

[2] Simon H Martin, Kanchon K Dasmahapatra, Nicola J Nadeau, et al. (2013). Genome-wide evidence for speciation with gene flow in Heliconius butterflies.

Genome Res. doi:10.1101/gr.159426.113

```
# GENOME.class <- readData("\home\Alignments")</pre>
# GENOME.class <- set.populations(GENOME.class, list(1:3,4:8,9:12))
# GENOME.class <- set.outgroup(GENOME.class,13)</pre>
# GENOME.class <- introgression.stats(GENOME.class, do.D=TRUE)</pre>
# show the result:
# GENOME.class@D
# GENOME.class@f
# GENOME.class <- introgression.stats(GENOME.class, do.BDF=TRUE)
# show the result:
# GENOME.class@BDF
```

36 jack.knife.transform

```
jack.knife.transform Jacknife Transformation
```

Description

This generic function transforms an existing object of class "GENOME" into another object of class "GENOME", in which each region corresponds to the (JACKNIFE!) window. Each jacknife window will be excluded from the analyses and the calculation will be applied to the union of all other windows.

Usage

```
## S4 method for signature 'GENOME'
jack.knife.transform(object,
width=7, jump=5,
type=1,
start.pos=FALSE,end.pos=FALSE
)
```

Arguments

```
object an object of class "GENOME"
width window size. default:7
jump jump size. default:5
type 1 scan only biallelic positions (SNPs), 2 scan the genome. default:1
```

start.pos start position end.pos end position

Value

The function creates a transformed object of class "GENOME".

Note

This function currently is only available for SNP data formats. PopGenome will scan the data from position 1 to the last observed SNP if start or end-positions are not specified. This mechanism can also be applied to the splitting.data() function. Just set split.GENOME.class@jack.knife <- TRUE after splitting the data.

```
# GENOME.class <- readData("...", format="VCF")
# jack.GENOME.class <- jack.knife.transform(GENOME.class,100,100)
# jack.GENOME.class <- neutrality.stats(jack.GENOME.class)
# jack.GENOME.class@Tajima.D</pre>
```

linkage.stats-methods 37

linkage.stats-methods Linkage Disequilibrium

Description

A generic function to calculate some linkage disequilibrium statistics.

Usage

```
## S4 method for signature 'GENOME'
linkage.stats(object,new.populations=FALSE,subsites=FALSE,detail=FALSE,
do.ZnS,do.WALL=TRUE)
## S4 method for signature 'GENOME'
get.linkage(object)
```

Arguments

An object of class "GENOME" object new.populations list of populations. default=FALSE "transitions": SNPs that are transitions. subsites "transversions": SNPs that are transversions. "syn": synonymous sites. "nonsyn": nonsynonymous sites. "exon": SNPs in exon regions. "intron": SNPs in intron regions. "coding": SNPs in coding regions (CDS). "utr": SNPs in UTR regions. "gene": SNPs in genes. default:FALSE detail if you want to calculate some detailed statistics. This can be considerably slower! default:FALSE do.ZnS calculate ZnS, ZA and ZZ do.WALL calculate Wall's B/Q

Details

Note, the pairwise comparisons are computed via combn(n.snps, 2).

Value

The return value is a modified object of class "GENOME"

38 load.session

The following slots will be modified in the "GENOME" object

	Slot	Reference	Description
1.	Wall.B	[2]	Wall \$B\$ statistic (only adjacent positions are considered)
2.	Wall.Q	[2]	Wall \$Q\$ statistic (only adjacent positions are considered)
3.	Kelly.Z_nS	[3]	Kelly \$Z_nS\$ statistic (if detail==TRUE)
4.	Rozas.ZA	[1]	Rozas \$ZA\$ statistic (adjacent positions, if detail==TRUE)
5.	Rozas.ZZ	[1]	Rozas \$ZZ\$ statistic (\$ZZ=ZA-Z_nS\$, if detail==TRUE)

References

- [1] Rozas, J., M.Gullaud, G.Blandin, and M.Aguade(2001). DNA variation at the rp49 gene region of Drosophila simulans: evolutionary inferences from an unusual haplotype structure. Genetics 158(3),1147-1155
- [2] Wall, J.(1999). Recombination and the power of statistical tests of neutrality. Genet Res 74, 65-79
- [3] Kelly,J.K. (1997). A test of neutrality based on interlocus associations. Genetics 146: 1197-1206

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class <- linkage.stats(GENOME.class)
# GENOME.class <- linkage.stats(GENOME.class,list(1:4,5:10),subsites="syn")
# GENOME.class <- linkage.stats(GENOME.class,list(c("seq1","seq5","seq3"),
# c("seq2","seq8")))
# GENOME.class <- linkage.stats(GENOME.class, detail=TRUE)
# show the result:
# get.linkage(GENOME.class)
# GENOME.class@Wall.B --> population specific view
# GENOME.class@region.stats
```

load.session

Loading a PopGenome session

Description

This function loads a PopGenome session (more precisely: the corresponding "GENOME" object) from the current workspace.

MKT-methods 39

Usage

```
load.session(folder)
```

Arguments

folder

name of the folder/object

Details

This function has to be used in the same workspace (folder) where the object of class "GENOME" was saved.

Value

An object of class "GENOME".

Examples

```
# GENOME.class <- readData("...\Alignments")
# save.session(GENOME.class,folder="GENOME.class")
# q()
# R
# library(PopGenome)
# load.session("GENOME.class")</pre>
```

MKT-methods

McDonald-Kreitman Test (McDonald \& Kreitman 1991)

Description

This generic function calculates an approximate version of the McDonald-Kreitman Test.

Usage

```
## S4 method for signature 'GENOME'
MKT(object,
new.populations=FALSE,
do.fisher.test=FALSE,
fixed.threshold.fst=FALSE,
subsites=FALSE)
## S4 method for signature 'GENOME'
get.MKT(object)
```

40 MKT-methods

Arguments

object an object of class "GENOME"

new.populations

list of populations. default:FALSE

do.fisher.test P-value calculation out of the Dn,Ds,Pn,Ps table

fixed.threshold.fst

Fixed threshold

subsites Subsites

Details

This approximate version of the McDonald-Kreitman test assumes that the probability that two single nucleotide polymorphisms (SNPs) occur in the same codon is very small. Thus, only codons with a single SNP are examined.

If no gff-file was specified when the data was read in, it is assumed that the alignment is in the correct reading frame (starting at a first codon position).

The outgroup has to be defined as a population!

Value

The return value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

MKT a matrix which includes the following values:

Columns Description

P_nonsyn nonsynonymous sites
 P_syn synonymous sites

3. D_nonsyn fixed nonsynonymous sites4. D_syn fixed synonymous sites

5. neutrality.index \$(P_nonsyn/P_syn)/(D_nonsyn/D_syn)\$

6. alpha 1-neutrality.index

References

McDonald, J. H.; Kreitman, M. (1991). *Adaptive protein evolution at the Adh locus in Drosophila*. Nature 351 (6328): 652-654

MS 41

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class <- MKT(GENOME.class)
# GENOME.class <- MKT(GENOME.class,list(1:7,8:12))
# show the result:
# get.MKT(GENOME.class)</pre>
```

MS

Coalescent simulation with or without selection

Description

This function uses Hudson's MS and Ewing's MSMS to compare simulated data with the observed data.

Usage

```
MS(GENO, niter=10, thetaID="user", params=FALSE, detail=FALSE, neutrality=FALSE, linkage=FALSE, F_ST=FALSE, MSMS=FALSE, big. data=FALSE)
```

Arguments

GENO	an object of class "GENOME"
niter	number of samples per locus
thetaID	"Tajima","Watterson" or "user". default:"user"
neutrality	Calculate neutrality tests. default=FALSE
linkage	Calculate linkage disequilibrium. default=FALSE
F_ST	Calculate fixation index. default=FALSE
params	an object of class "test.params". see ?test.params
detail	detailed statistics. Note: slower computations! default=FALSE
MSMS	specify parameter for MSMS simulation with selection (has to be specified as a string)
big.data	if TRUE the ff-package is used

Details

You can choose different mutation rate estimators to generate simulation data. When thetaID="user", you have to define the theta values in an object of class "test.params". The "test.params" class can also be used to specify some additional parameter like migration and/or recombination rates... (?test.params).

Please read the MSMS documentation for the correct use of coalescent simulations to assess statistical significance.

42 MS_getStats

Value

The function creates an object of class "cs.stats"

Note

The executable file ms has to be stored in the current workspace.

If you want to use the MSMS application, put the msms folder including the corresponding executable files in the current workspace.

Both programs can be obtained from their websites (see references).

References

Hudson, R. R. (2002). Generating samples under a Wright-Fisher neutral model of genetic variation. Bioinformatics 18: 337-338

Gregory Ewing and Joachim Hermisson, MSMS: A Coalescent Simulation Program Including Recombination, Demographic Structure, and Selection at a Single Locus. Bioinformatics 2010, doi: 10.1093/bioinformatics/btq322

Examples

```
# GENOME.class <- readData("...\Alignments")
# GENOME.class <- neutrality.stats(GENOME.class,list(1:6))
# MS.class <- MS(GENOME.class,thetaID="Tajima",neutrality=TRUE)
# MS.class <- MS(GENOME.class,thetaID="Tajima",neutrality=TRUE,
# MSMS="-N 1000 -SAA 200 -SaA 100 -SF 1e-2")
# MS.class
# MS.class@obs.val
# MS.class@locus[[1]]</pre>
```

MS_getStats

Get the simulated MS/MSMS statistics

Description

This function extracts the simulated values from the class cs.stats

Usage

```
MS_getStats(object,locus=1,population=1)
```

Arguments

object of class "cs.stats"

locus the locus ID

population the population ID

Value

The return value is a matrix containing the simulation results of different statistical tests. (see MS())

Examples

```
# GENOME.class <- readData("...\Alignments")
# GENOME.class <- neutrality.stats(GENOME.class)
# ms <- MS(GENOME.class,thetaID="Tajima",neutrality=TRUE)
# MS_getStats(ms)</pre>
```

```
mult.linkage.stats-methods
```

Multilocus linkage statistics

Description

This generic function calculates the linkage disequilibrium between regions.

Usage

```
## S4 method for signature 'GENOME'
mult.linkage.stats(object,lower.bound=0,upper.bound=1,pairs=FALSE)
```

Arguments

object an object of class "GENOME"

lower.bound sites with minor-allele-frequency>=lower.bound are considered upper.bound sites with minor-allele-frequency<=upper.bound are considered

pairs permutation matrix of pairwise comparisons

Details

pairs is a matrix. Each column contains the pairwise comparison region IDs.

11

23

compares region 1 with 2, and region 1 with 3.

Value

The return value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

mult.Linkage Some linkage statistics for each pair of regions (R2, P-value, Distance)

The Fisher-Exact-Test is used to calculate the P-values.

Examples

```
# GENOME.class <- readData("...\Alignments")
# GENOME.class
# GENOME.class <- mult.linkage.stats(GENOME.class)
# show the result:
# GENOME.class@mult.Linkage</pre>
```

neutrality.stats-methods

Neutrality Statistics

Description

This generic function calculates some neutrality statistics.

Usage

```
## S4 method for signature 'GENOME'
neutrality.stats(object,new.populations=FALSE,new.outgroup=FALSE,
subsites=FALSE,detail=FALSE, FAST=FALSE, do.R2=FALSE)
## S4 method for signature 'GENOME'
get.neutrality(object,theta=FALSE,stats=TRUE)
```

neutrality.stats-methods 45

Arguments

an object of class "GENOME" object new.populations list of populations. default:FALSE vector of outgroup sequences. default:FALSE new.outgroup subsites "transitions": SNPs that are transitions. "transversions": SNPs that are transversions. "syn": synonymous sites. "nonsyn": non-synonymous sites.

"exon": SNPs in exon regions. "intron": SNPs in intron regions.

"coding": SNPs in coding regions (CDS).

"utr": SNPs in UTR regions. "gene": SNPs in genes.

default:FALSE

default:FALSE, TRUE for some detailed statistics. Note: slows down calculations! detail

Fast computation. only works if there is no outgroup defined. **FAST**

do.R2 Ramos-Onsins' & Rozas' R2

show the results of each statistic, default:TRUE stats

show the theta values. default:FALSE theta

Value

The return value is a modified object of class "GENOME"

13. theta_Achaz.Watterson 14. theta_Achaz.Tajima 15. theta_Fay.Wu

The following slots will be modified in the "GENOME" object

	Slot	Reference	Description
1.	n.segregating.sites		Total number of segregating sites
2.	Tajima.D	[1]	Tajima's' D statistic 1989
3.	Fu.Li.F	[3]	Fu & Li's' F* statistic 1993
4.	Fu.Li.D	[3]	Fu & Li's D* statistic 1993
5.	Fay.Wu.H	[6]	Fay & Wu's H statistic 2000
6.	Zeng.E	[7]	Zeng's E statistic 2006
7.	Strobeck.S	[5]	Strobeck's S statistic 1987 (if detail==TRUE)
8.	Fu.F_S	[4]	Fu's F\$_S\$ statistic 1997 (if detail==TRUE)
9.	Rozas.R_2	[2]	Ramos-Onsins' & Rozas' \$R_2\$ statistic 2002
10.	theta_Tajima	[1]	
11.	theta_Watterson		
12.	theta_Fu.Li	[3]	

[6]

16. theta_Zeng [7]

References

- [1] Tajima, F.(1989) Statistical Method for Testing the Neutral Mutation Hypothesis by DNA Polymorphism. Genetics, 123(3): 585-595.
- [2] Ramos-Onsins, S.E. and J.Rozas (2002). *Statistical Properties of New Neutrality Tests Against Population Growth*. Mol.Biol.Evol.19(12),2092-2100
- [3] Fu, Y.X. and W.H.Li (1993). Statistical Tests of Neutrality of Mutations. Genetics 133(3),693-709
- [4] Fu, Y.-X.(1997). Statistical Tests of Neutrality of mutations against population growth, hitch-hiking and background selection. Genetics 147(2),915-925.
- [5] Strobeck, C. (1987). Average number of nucleotide differences in a sample from a single sub-population: a test for population subdivision. Genetics 117, 149-153
- [6] Fay, J.C. and C.-I. Wu (2000). *Hitchhiking under positive Darwinian selection*. Genetics 155 (3),1405-1413
- [7] Zeng, K., Y.-X. Fu, S. Shi, and C.-I. Wu (2006). Statistical tests for detecting positive selection by utilizing high-frequency variants. Genetics 174, 1431-1439

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class <- neutrality.stats(GENOME.class, FAST=TRUE)
# GENOME.class <- neutrality.stats(GENOME.class,list(1:4,5:10),subsites="syn")
# GENOME.class <- neutrality.stats(GENOME.class,list(c("seq1","seq5","seq3"),
# c("seq2","seq8")))
# GENOME.class <- neutrality.stats(GENOME.class,detail=TRUE)
# show the result:
# get.neutrality(GENOME.class)
# GENOME.class@Tajima.D --> population specific view
# detail = TRUE
# GENOME.class@region.stats
```

PG_plot.biallelic.matrix-methods

Plot the biallelic matrix

PopGenome 47

Description

This function plots the biallelic matrix of a specific region.

Usage

```
## S4 method for signature 'GENOME'
PG_plot.biallelic.matrix(object,region, ind.names = FALSE , cex.axis = 0.5,
title="")
```

Arguments

object of class "GENOME"

region the region ID

ind.names individual names/IDs. default:ALL

cex.axis size of text (y-axis) title Title of the plot

Examples

```
# GENOME.class <- readData("...\Alignments")
# PG_plot.biallelic.matrix(GENOME.class, region = 1)</pre>
```

PopGenome PopGenome

Description

R-package for Population genetic & genomic analyses

Details

Index:

F_ST.stats Fixation index diversity.stats Diversities

MKT McDonald & Kreitman test
MS Coalescent simulations
detail.stats Several misc. statistics
linkage.stats Linkage disequilibrium
neutrality.stats Neutrality statistics

readData Reading alignments and calculating summary data

readSNP Read data in .SNP format (e.g., from the 1001 Arabidopsis Genomes project)

48 PopGplot

```
readVCF Read data in VCF format (e.g., from the 1000 human Genomes project)
readHapMap Read data in HapMap format
sliding.window.transform Sliding window transformation
splitting.data Split data into subsites
test.params Set parameters for coalescent simulations.
```

Author(s)

Bastian Pfeifer Maintainer: Bastian Pfeifer <Bastian.Pfeifer@uni-duesseldorf.de>

See Also

?readData readData

Examples

```
# GENOME.class <- readData("...\Alignments")
# GENOME.class <- neutrality.stats(GENOME.class)
# values <- get.neutrality(GENOME.class)
# GENOME.class <- F_ST.stats(GENOME.class,list(1:5,6:10))
# values <- get.F_ST(GENOME.class)</pre>
```

PopGplot

Smoothed line-plot for multiple populations

Description

This function plots values with smoothed lines using spline interpolation.

Usage

```
PopGplot(values,colors=FALSE,span=0.1,ylab="",xlab="",
ylim=c(min(values,na.rm=TRUE),max(values,na.rm=TRUE)))
```

Arguments

values	the statistical values (matrix); columns=populations
colors	the colors for each population (character vector)
span	the degree of smoothing
ylab	a title for the y axis
xlab	a title for the x axis
ylim	ranges for the y axis

read.big.fasta 49

Examples

```
# GENOME.class <- readSNP("Arabidopsis",CHR=1)
# GENOME.class.slide <- sliding.window.transform(test,1000,1000)
# GENOME.class.slide <- diversity.stats(GENOME.class.slide)
# values <- GENOME.class.slide@nuc.divesity.within
# PopGplot(values)</pre>
```

read.big.fasta

Reading large FASTA alignments

Description

This function splits FASTA alignments that are too large to fit into the computer memory into chunks.

Usage

Arguments

filename the basepath of the FASTA alignment

outgroup vector of outgroup sequences

populations list of populations

window chunk size: number of columns/nucleotide sites

SNP. DATA should be switched to TRUE if you use SNP data in alignment format

include.unknown

include unknown positions in the biallelic.matrix

parallized Use parallel computations to speed up the reading - works only on UNIX sys-

ems!

FAST Fast computation. see readData()

big.data use the ff-package

Details

The algorithm reads the data for each individual and stores the information on disk. The data can be analyzed as regions of the defined window size, or can be concatenated in the PopGenome framework via the function concatenate.regions. This function should only be used when the FASTA file does not fit into the RAM; else, use the function readData.

50 readData

Value

The function creates an object of class "GENOME"

The following slots will be filled in the "GENOME" object

Slot Description 1. n.sites total number of sites 2. n.biallelic.sites number of biallelic sites region.names names of regions 4. region.data some detailed information about the data

Examples

```
# GENOME.class <- read.big.fasta("Alignment.fas", big.data=TRUE)</pre>
# GENOME.class
# GENOME.class@region.names
# CON <- concatenate.regions(GENOME.class)</pre>
# CON@region.data@biallelic.sites
# GENOME.class.slide <- sliding.window.transform(GENOME.class,100,100)</pre>
# GENOME.class <- neutrality.stats(GENOME.class,FAST=TRUE)</pre>
# show the result:
# get.sum.data(GENOME.class)
# GENOME.class@region.data
```

readData

Read alignments and calculate summary data

Description

This function reads alignments/SNP data in several formats and calculates some summary data.

Usage

```
readData(path,populations=FALSE,outgroup=FALSE,include.unknown=FALSE,
         gffpath=FALSE, format="fasta", parallized=FALSE,
         progress_bar_switch=TRUE, FAST=FALSE,big.data=FALSE,
         SNP.DATA=FALSE
        )
## S4 method for signature 'GENOME'
get.sum.data(object)
```

readData 51

Arguments

object of class "GENOME"

path the basepath (folder) of the alignments

outgroup vector of outgroup sequences

include.unknown

if positions with unknown nucleotides should be considered.

populations list of populations. default:FALSE

gffpath the basepath (folder) of the corresponding GFF-files. default:FALSE

format data formats. "fasta" is default. See details!

parallized parallel processing to accelerate the reading process. See details!

progress_bar_switch

progress_bar

FAST fast computation. See details!

big.data use the ff-package

SNP. DATA important for reference positions; should be TRUE if you use SNP-data in align-

ment format

Details

All data (alignments or SNP-files) have to be stored in one folder. The folder is the input of this function. If no GFF file (which also have to be stored in a folder) is specified, an alignment in the correct reading frame (starting at a first codon position) is expected.

Otherwise synonymous and non-synonymous positions are not identified correctly.

Note:

The GFF-files have to be EXACTLY the same names (without any extensions like .fas or .gff) as the files storing the nucleotide data to ensure correct matching

format:

```
"fasta", "nexus", "phylip",
```

"MAF", "MEGA"

"HapMap","VCF"

"RData"

Valid nucleotides are T,t,U,u,G,g,A,a,C,c,N,n,-

parallized:

- will speed up calculations if you use a very large amount of alignments

FAST:

- will not classify synonymous/non-synonymous SNPs directly
- fast computation (via compiled C code) of biallelic matrix, biallelic sites, transversions/transitions

52 readData

and biallelic substitutions

- can be switched to TRUE in case of SNP data without loss of information

big.data:

- use the ff-package
- ff mechanism is used for biallelic.matrix and GFF/GTF information
- is automatically activated for readVCF or readSNP
- Note! you should set this to TRUE if you use big chunks of data and you want to later concatenate them in the PopGenome framework (for example: sliding windows of the whole dataset).

SNP.DATA:

- should be switched to TRUE if you use SNP-data in alignment format.
- the corresponding SNP positions can be set via set.ref.positions

Value

The function creates an object of class "GENOME"

The following slots will be filled in the "GENOME" object

	Slot	Description
1.	n.sites	total number of sites
2.	n.biallelic.sites	number of biallelic sites
3.	n.gaps	number of sites with gaps
4.	n.unknowns	number of sites with unknown nucleotides
5.	n.valid.sites	number of valid sites
6.	n.polyallelic.sites	number of sites with >2 nucleotides
7.	trans.transv.ratio	transition/transversion ratio of biallelic sites
8.	region.names	names of regions
9.	region.data	some detailed information about the data read

```
# GENOME.class <- readData("...\Alignments", FAST=TRUE)</pre>
# GENOME.class <- readData("VCF", format="VCF")</pre>
# Note, "Alignments" and "VCF" are folders!
# GENOME.class@region.names
# GENOME.class <- readData("...\Alignments", big.data=TRUE)</pre>
# object.size(GENOME.class)
# GENOME.class <- readData("...\Alignments",gffpath="...\Alignments_GFF")</pre>
# GENOME.class
```

53 readHapMap

```
# show the result:
```

- # get.sum.data(GENOME.class)
- # GENOME.class@region.data

readHapMap

Read SNP data from the HapMap consortium

Description

This function reads HapMap data.

Usage

readHapMap(folder,hap_gffpath,populations=FALSE,outgroup=FALSE)

Arguments

folder the basepath of the variant_calls

hap_gffpath the basepath of the corresponding GFF files. Note! The HapMap GFF file does

not contain information about subsites. see details!

populations list of populations

outgroup vector of outgroup sequences

Details

PopGenome reads the GFF file distributed on the HapMap plattform only to verify the reference positions of the chromosomes. In the next release, this function will also handle GFF/GTF files to get information about subsites (exons, introns, ...). The input folder should include the files of different individuals for one chromosome. This facilitates FST calculations of the HapMap data. See also readData("...", format="HapMap") which can read the files of single populations directly.

Value

The function creates an object of class "GENOME"

The following slots will be filled in the "GENOME" object

Slot Description

total number of sites 1. n.sites 2. n.biallelic.sites number of biallelic sites

some detailed information about the data read region.data

54 readMS

Examples

```
# GENOME.class <- readHapMap("...\HapMapData")
# GENOME.class
# show the result:
# get.sum.data(GENOME.class)
# GENOME.class@region.data</pre>
```

readMS

Read output data from MS and MSMS

Description

This function reads data produced from the coalescent simulation programs MS (Hudson, 2002) and MSMS (Greg, 2010)

Usage

```
readMS(file,big.data=FALSE)
```

Arguments

file the basepath of the MS/MSMS output

big.data The ff package is used

Value

An object of class GENOME

References

Hudson, R. R. (2002). Generating samples under a Wright-Fisher neutral model of genetic variation. Bioinformatics 18: 337-338

Gregory Ewing and Joachim Hermisson, MSMS: A Coalescent Simulation Program Including Recombination, Demographic Structure, and Selection at a Single Locus. Bioinformatics 2010, doi: 10.1093/bioinformatics/btq322

Examples

```
# GENOME.class <- readMS("ms.output.txt")</pre>
```

GENOME.class@region.names

readSNP 55

readSNP	Read data in .SNP format	
---------	--------------------------	--

Description

This function reads data in .SNP (quality_variant) format, as distributed by the 1001 Genomes project (Arabidopsis).

Usage

```
readSNP(folder,populations=FALSE,outgroup=FALSE,gffpath=FALSE,
CHR=FALSE,ref.chr=FALSE,snp.window.size=FALSE,
parallized=FALSE,ffpackagebool=TRUE,
include.unknown=FALSE
)
```

Arguments

folder the basepath of the variant_calls outgroup vector of outgroup sequences populations list of populations gffpath the corresponding GFF file CHR which chromosome?, default: all chromosomes ref.chr reference chromosome (to classify synonymous/non-synonymous positions) snp.window.size scan SNP chunks parallized multicore computation ffpackagebool use the ff-package to save memory space. (slower) include.unknown include positions with unknown nucleotides

Details

The ff-package we use to store the SNP information limits the data size to individuals * (number of SNPs) <= .Machine\$integer.max

The text files containing the SNP information of each individual have to be stored in one folder. The slots transitions, biallelic.sites, and biallelic.substitutions of the class "regions.data" will be filled.

At this time, if a GFF/GTF is used the data should be organized in a way that

the "CHR" is a numerical value. The prefix "Chr" or "chr" is also supported.

56 readVCF

Value

The function creates an object of class "GENOME"

Following Slots will be filled in the "GENOME" object

Slot Description total number of sites 1. n.sites 2. n.biallelic.sites number of biallelic sites some detailed information about the data read 3. region.data 4. region.names names of regions

Examples

```
# GENOME.class <- readSNP("...\SNPData")</pre>
# GENOME.class <- readSNP("...\SNPData", CHR=1)</pre>
# GENOME.class <- readSNP("...\SNPData", CHR=1, gffpath="Gff_file.gff")
# GENOME.class
# GENOME.class <- neutrality.stats(GENOME.class,FAST=TRUE)</pre>
# show the result:
# get.sum.data(GENOME.class)
# GENOME.class@region.data
```

readVCF

Read SNP data in tabixed VCF format

Description

This function reads tabixed VCF-files, as distributed from the 1000 Genomes project (human).

Usage

```
readVCF(filename, numcols, tid, frompos, topos,
        samplenames=NA, gffpath = FALSE, include.unknown=FALSE, approx=FALSE,
out="", parallel=FALSE)
```

Arguments

the corresponding tabixed VCF-file filename

numcols number of SNPs that should be read in as a chunk readVCF 57

tid which chromosome ? (character)

frompos start of the region
topos end of the region
samplenames a vector of individuals
gffpath the corresponding GFF file

include.unknown

includ positions with unknown/missing nucleotides

approx see details!

out a folder suffix where the temporary files should be saved

parallel parallel computation using mclapply

Details

The readVCF function expects a tabixed VCF file with a diploid GT field. In case of haploid data, the GT field has to be transformed to a pseudo-diploid field (such as 0 -> 0|0). An alternative is to use readData(..., format="VCF"), which can read non-tabixed haploid and any kind of polyploid VCFs directly. When approx=TRUE, the algorithm will apply a logical OR to the GT-field: (0|0=0,1|0=1,0|1=1,1|1=1). Note, this is an approximation for diploid data, which will speed up calculations. In case of haploid data, approx should be switched to TRUE. If approx=FALSE, the full diploid information will be considered. The ff-package PopGenome uses to store the SNP information limits total data size to individuals * (number of SNPs) <= .Machine\$integer.max In case of very large data sets, the bigmemory package will be used; this will slow down calculations (e.g. this package have to be installed first !!!). Use the function vcf_handle <-.Call("VCF_open", filename) to open a VCF-file and .Call("VCF_getSampleNames",vcf_handle) to get and define the individuals which should be considered in the analysis. See also readData(..., format="VCF")!

Value

The function creates an object of class "GENOME"

The following slots will be filled in the "GENOME" object

The following slots will be filled in the GENORE Obje

Slot Description
1. n.sites total number of sites

1. n.sites total number of sites
2. n.biallelic.sites number of biallelic sites

3. region.data some detailed information about the data read

4. region.names names of regions

58 recomb.stats-methods

Examples

```
# GENOME.class <- readVCF("...\chr1.vcf.gz", 1000, "1", 1, 100000)
# GENOME.class
# GENOME.class@region.names
# GENOME.class <- neutrality.stats(GENOME.class,FAST=TRUE)
# show the result:
# get.sum.data(GENOME.class)
# GENOME.class@region.data</pre>
```

recomb.stats-methods Recombination statistics

Description

This generic function calculates the Four-Gamete test (Hudson 1985).

Usage

```
## S4 method for signature 'GENOME'
recomb.stats(object,new.populations=FALSE,subsites=FALSE)
## S4 method for signature 'GENOME'
get.recomb(object)
```

Arguments

```
object an object of class "GENOME"

new.populations
list of populations. default:FALSE

subsites "transitions": SNPs that are transitions.
    "transversions": SNPs that are transversions.
    "syn": synonymous sites.
    "nonsyn": nonsynonymous sites.
    "exon": SNPs in exon regions.
    "intron": SNPs in intron regions.
    "coding": SNPs in coding regions (CDS).
    "utr": SNPs in UTR regions.
    "gene": SNPs in genes.
    default:FALSE
```

region.as.fasta-methods 59

Value

```
The return value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object
```

Hudson.RM Four-gamete test

References

Hudson, R. K. (1985). Statistical Properties of the Number of Recombination Events in the History of a Sample of DNA Sequences Genetics 111 (1): 147-164.

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class <- recomb.stats(GENOME.class)
# GENOME.class <- recomb.stats(GENOME.class,list(1:7,8:12))
# show the result:
# recomb.values <- get.recomb(GENOME.class)
# recomb.values[[1]] # first population !
# GENOME.class@region.stats@Hudson.RM</pre>
```

```
region.as.fasta-methods
```

Extract a region and write it to a FASTA file

Description

This generic function writes a FASTA file of the observed biallelic positions to the current workspace.

Usage

```
## S4 method for signature 'GENOME'
region.as.fasta(object,region.id=FALSE,filename=FALSE,type=1,ref.chr=FALSE)
```

60 save.session

Arguments

object an object of class "GENOME"

region.id region of the genome filename name of the FASTA file

type 1: extract SNPs; 2: extract all nucleotides

ref.chr reference sequence

Details

In case of type=2 we recommend to use the function splitting.data(,positions=list(...), type=2) before and apply the region.as.fasta() to this splitted object afterwards. The type=1 method will write a FASTA file including only the biallelic.sites.

region. id is the the region number specified in the PopGenome class GENOME.

Examples

```
#GENOME.class <- readSNP("Arabidopsis",CHR=1)
# split the data into the genmic positions 100 to 2000
#GENOME.class.split <- splitting.data(GENOME.class, positions=list(100:2000),type=2)
#GENOME.class.split@region.names
#region.as.fasta(GENOME.class.split,1,"my_fasta_file.fas",type=2, ref.chr="chrom1.fas")</pre>
```

save.session

Save the "GENOME" object of a PopGenome session

Description

This function saves the "GENOME" object of a PopGenome session to the current workspace. The object can be loaded again with load.session().

Usage

```
save.session(object,folder)
```

Arguments

object of class "GENOME" folder name of the folder/object

Details

Saving R and ff-objects created by the ff-package in a folder.

set.filter-methods 61

Examples

```
# GENOME.class <- readData("...\Alignments")
# save.session(GENOME.class,"GENOME.class")
# load.session("GENOME.class")</pre>
```

set.filter-methods

Setting filter to the analysis

Description

A generic function to set filter regarding e.g missing data.

Usage

```
## S4 method for signature 'GENOME'
set.filter(object,
missing.freqs=TRUE,
minor.freqs=FALSE,
maf.lower.bound=0,
maf.upper.bound=1,
miss.lower.bound=0,
miss.upper.bound=1)
```

Arguments

```
object An object of class "GENOME"
missing.freqs Set filter for missing data
minor.freqs Set filter for the MAF
maf.lower.bound
frequency of the MAF
maf.upper.bound
...
miss.lower.bound
frequency of the missing freq.
miss.upper.bound
```

Details

This function sets the slot region.data@included.

62 set.outgroup-methods

Value

Returned value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

Slot Reference Description 1. region.data@included [x] ...

References

[x]

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class <- set.filter(GENOME.class, missing.freqs=TRUE,
# miss.lower.bound=0, miss.upper.bound=0.2)
# now apply any statistic to the filtered data set.
# GENOME.class <- calc.fixed.shared(GENOME.class, subsites="included")</pre>
```

Description

This generic function defines the outgroup by matching the specified vector against each region.

Usage

```
## S4 method for signature 'GENOME'
set.outgroup(object,new.outgroup=FALSE, diploid=FALSE)
```

Arguments

object an object of class "GENOME"

new.outgroup a vector of outgroup individuals
diploid if diploid data is present

set.populations-methods

Examples

```
# GENOME.class <- readData("\home\Alignments")
# outgroup <- c("seq1","seq2")
# GENOME.class <- set.outgroup(GENOME.class,new.outgroup=outgroup)
# GENOME.class <- neutrality.stats(GENOME.class)</pre>
```

```
set.populations-methods
```

Define populations

Description

This generic function defines the populations.

Using this function obviates the need to specify the populations for each calculation separately. The populations can be set differently for different PopGenome modules by applying the function between module calls.

Usage

```
## S4 method for signature 'GENOME'
set.populations(object,new.populations=FALSE, diploid=FALSE,
triploid=FALSE,tetraploid=FALSE)
```

Arguments

```
object an object of class "GENOME"

new.populations
list of populations. default:FALSE

diploid if diploid data is present

triploid if triploid data is present

tetraploid if tetraploid data is present
```

```
# GENOME.class <- readData("\home\Alignments")
# pop.1 <- c("seq1","seq2")
# pop.2 <- c("seq3","seq4","seq1")
# GENOME.class <- set.populations(GENOME.class,list(pop.1,pop.2))
# GENOME.class@region.data@populations2
# GENOME.class <- neutrality.stats(GENOME.class)</pre>
```

```
set.ref.positions-methods

Set reference positions for SNP data
```

Description

This generic function sets the positions of the SNP data. Should be used if you use alignment formats to store SNP data (i.e., data restricted to the polymorphic positions).

Usage

```
## S4 method for signature 'GENOME'
set.ref.positions(object, positions)
```

Arguments

object an object of class "GENOME" positions a list of reference positions

Value

returned value is a modified object of class "GENOME"

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class <- set.ref.positions(GENOME.class,list(c(1000,2001,3000),
# c(3200,12000)))</pre>
```

set.synnonsyn-methods Set synonymous positions for SNP data

Description

This generic function classifies the observed biallelic positions read from SNP data files into synonymous and non-synonymous SNPs.

show.slots-methods 65

Usage

```
## S4 method for signature 'GENOME'
set.synnonsyn(object,ref.chr,save.codons=FALSE)
```

Arguments

object an object of class "GENOME"

ref.chr the reference chromosome in FASTA format

save.codons save codon changes

Value

The return value is a modified object of class "GENOME" storing syn/nonsyn informations in the slot GENOME.class@region.data@synonymous for each SNP. (1=synonymous,0=non-synonymous)
When save.codons is TRUE the SNP related codon changes are saved in the corresponding slot GENOME.class@region.data@codons. (see also get.codons(), codontable() and codonise64())

Note

The data has to be read in with a corresponding GFF/GTF file (CDS fields must be specified); otherwise a correct classification is not possible. The set.synnonsyn() function does not work for splitted objects e.g produced via sliding.window.transform() or splitting.data(). Note, transcripts which are in the same CDS region but have different reading frames are are not specified correctly. PopGenome can also handle coding regions on reverse strands. We have used the program SNPeff to validate our results.

Examples

```
# GENOME.class <- readData("VCF",format="VCF",gffpath="GFF.Folder")
# GENOME.class <- set.synnonsyn(GENOME.class,ref.chr="ref.fas")
# GENOME.class@region.data@synonymous</pre>
```

show.slots-methods

Show Slots of class GENOME

Description

```
coming soon ...
```

Methods

```
object = "GENOME" coming soon ...
```

Examples

show.slots(GENOME.class)

```
sliding.window.transform-methods
```

Sliding Window Transformation

Description

This generic function transforms an existing object of class "GENOME" into another object of class "GENOME", in which each region corresponds to one window. This allows to apply the full spectrum of PopGenome methods to sliding window data.

Usage

```
## S4 method for signature 'GENOME'
sliding.window.transform(object,
width=7, jump=5,
type=1,
start.pos=FALSE,end.pos=FALSE,
whole.data=TRUE
)
```

Arguments

object an object of class "GENOME" width window size. default:7 jump jump size. default:5

type 1 scan only biallelic positions (SNPs), 2 scan the genome. default:1

start.pos start position end.pos end position

whole.data scan the complete data by concatenating the regions in "object". If FALSE, each

region is scanned seperately.

Value

The function creates a transformed object of class "GENOME".

Note

If you want to scan regions seperately (whole.data=FALSE), you may not use the big.data option in the readData function. PopGenome will scan the data from position 1 to the last observed SNP if start or end-positions are not specified.

snp_file 67

Examples

snp_file

.SNP file (variant call data from 1001 Arabidopsis Genomes project)

Description

A .SNP file stored in the directory "data" of the PopGenome package. The file contains variant calls for exactly one individual. Put all files (individuals of interest) into one folder (for example "SNP"). readSNP("SNP", CHR=1)

```
splitting.data-methods
```

Split data into subsites

Description

This generic function splits the data into subsites, if GFF/GTF information is present or if positions are defined accordingly.

Usage

Arguments

object an object of class "GENOME"

positions list of positions

subsites "exon": SNPs in exon regions.

"intron": SNPs in intron regions.

"coding": SNPs in coding regions (CDS).

"utr": SNPs in UTR regions. "gene": SNPs in genes.

type 1: SNP positions

2: Genome positions

whole.data Scan the whole data by concatenating the regions. If FALSE, the regions are

scanned seperately

Details

Note, if whole.data=FALSE data with n.biallelic.sites==0 should be removed.

Value

The return value is a modified object of class "GENOME".

Examples

```
# GENOME.class <- readData("\home\Alignments")
# GENOME.class
# GENOME.class.split <- splitting.data(GENOME.class,subsites="exon")
# GENOME.class.split@region.names
# GENOME.class.split <- splitting.data(GENOME.class,positions=list(1:7,8:12))
# GENOME.class.split <- splitting.data(GENOME.class,
# positions=list(2000:3000,12000:13000),type=2)
# GENOME.class.split</pre>
```

```
{\tt split\_data\_into\_GFF\_attributes}
```

Split the data into GFF attributes

Description

Splits the data into GFF attributes defined by the user.

Usage

```
split_data_into_GFF_attributes(object, gff.file, chr, attribute)
```

Arguments

object An object of class GENOME gff.file The corresponding GFF file

chr The chromosome/scaffold identifier attribute The attribute to use for splitting

Details

The algorithm splits the data into attributes. An attribute can be "gene_name", "Parent" or just a single gene name like "geneXYZ".

Value

The returned value is an object of class "GENOME" See GENOME.class.split@region.names and GENOME.class.split@region.names after splitting the data.

Examples

```
# GENOME.class <- readVCF("chr1.vcf.gz",1000,"1",1,100000)
# GENOME.class.split <- split_data_into_GFF_attributes(GENOME.class,"Homo_sapiens.GRCh37.73.gtf",
# "1", "gene_name")
# GENOME.class.split@region.names
# GENOME.class.split@feature.names</pre>
```

```
split_data_into_GFF_features

Split the data into GFF features
```

Description

Splits the data into GFF feautures defined by the user.

Usage

```
split_data_into_GFF_features(object, gff.file, chr, feature)
```

Arguments

object An object of class GENOME gff.file The corresponding GFF file

chr The chromosome/scaffold identifier

feature The feature used for splitting

70 sweeps.stats-methods

Details

```
The algorithm splits the data into features. A feature can be "gene", "exon" etc. depending on what is specified in the GFF3 file.
```

Value

```
The returned value is an object of class "GENOME" See GENOME.class.split@region.names and GENOME.class.split@region.names after splitting the data.
```

Examples

```
# GENOME.class <- readVCF("chr1.vcf.gz",1000,"1",1,100000)
# GENOME.class.split <- split_data_into_GFF_features(GENOME.class,"Homo_sapiens.GRCh37.73.gtf",
# "1", "gene")
# GENOME.class.split@region.names</pre>
sweeps.stats-methods Selective Sweeps
```

Description

This module calculates some statistics to detect selective sweeps.

Usage

```
## S4 method for signature 'GENOME'
sweeps.stats(object,new.populations=FALSE,subsites=FALSE,
freq.table=FALSE, FST=FALSE)
## S4 method for signature 'GENOME'
get.sweeps(object)
```

Arguments

```
object an object of class "GENOME"

new.populations

list of populations. default:FALSE

subsites "transitions": SNPs that are transitions.

"transversions": SNPs that are transversions.

"syn": synonymous sites.

"nonsyn": non-synonymous sites.

"exon": SNPs in exon regions.

"intron": SNPs in intron regions.

"coding": SNPs in coding regions (CDS).
```

71 sweeps.stats-methods

```
"utr": SNPs in UTR regions.
"gene": SNPs in genes.
default:FALSE
the frequency counts for the CLR test. "list"
```

FST use FST values instead of the minor allele frequencies

Details

freq.table

The freq. table contains the global sets of frequency counts. It can be produced with the module detail.stats. The values in the slot GENOME.class@region.stats@minor.allele.frequencies can be used to create this global set. (use the R function table) freq.table is a list of length n.pops.

Value

The return value is a modified object of class "GENOME"

The following slots will be modified in the "GENOME" object

CL Composite Likelihood of SNPs

CLR Nielsen's CLR test

References

Cai JJ (2008) PGEToolbox: A Matlab toolbox for population genetics and evolution Journal of Heredity Jul-Aug;99(4):438-40.doi:10.1093/jhered/esm127

Nielson, R. (2005). Genomic scans for selective sweeps using SNP data Genome Res. 2005 15: 1566-1575

```
# Reading one alignment stored in the folder Aln
# GENOME.class <- readData("\home\Aln")</pre>
# CI
# GENOME.class <- sweeps.stats(GENOME.class)</pre>
# GENOME.class@CL
# CLR
# create global set
# GENOME.class <- detail.stats(GENOME.class)</pre>
# freq <- GENOME.class@region.stats@minor.allele.freqs[[1]]</pre>
# freq.table <- list()</pre>
```

72 test.params-class

```
# freq.table[[1]] <- table(freq)
# define the region of interest
# GENOME.class.split <- splitting.data(GENOME.class, positions= ...)
# calculate CLR
# GENOME.class.split <- sweeps.stats(GENOME.class.split, freq.table=freq.table)
# GENOME.class@CLR</pre>
```

test.params-class

Set parameters for coalescent simulations with Hudson's MS and Ewing's MSMS.

Description

The object that contains the set parameter values can be passed to the function MS. This class simplifies the process of passing on all necessary values to the MS function.

Arguments

theta	mutation parameter theta (4Nmu), where N is the diplod effective population size and mu the mutation rate per locus. It needs to be provided as a vector of length n .regions
seeds	specify 3 random number seeds. a vector of length 3 with positive integer values is expected
fixedSegsites	usually the number of segregating sites varies in each iteration. Please provide a single numeric value if the number of segregating sites needs to be fixed.
recombination	provide a vector of format: $c(p, nsites)$, $p = cross$ -over parameter rate, nsites is the number of sites between which recombination occurs
geneConv	in addition to recombination, intra-locus non-cross-over exchange gene conversion can be included in the simulation; the expected format is c(f, gamma), where f denotes the ratio g/r (r is the probability per generation of crossing-over between adjacent sites (see Wiuf and Hein 2000), and gamma is the mean conversion tract length.
growth	population size is assumed to be $N(t) = N0 \exp^a h^*t$. Provide alpha as an integer value. Negative values indicate that population was larger in the past than present, positive values indicate that it was smaller.
migration	specify the migration rate between populations. Please provide a single numeric value.
demography	vector of length 3 or 4 with first value denoted as 'type' valid 'types' for vectors of length 3 are as follows: - 1 set a growth rate change alpha at a certain time t: c(1, t, alpha)

^{- 2} set all sub-populations to size \$x * N_0\$ and growth rate to zero:

vcf_file 73

```
c(2, t, x)
```

- 3 set all elements of the migration matrix to x/(npop-1): c(3, t, x)

valid 'types' for vectors of length 4 are as follows:
- 4 set growth rate of sub-population i to alpha at time z: c(4, t, i, alpha)

- 5 set sub-population i size to $x * N_0$ at time t and growth rate to zero: c(5, t, i, x)
- 6 split sub-population i into sub-population i and a new sub-population, labeled npop + 1. Each ancestral lineage in sub-population i is randomly assigned to sub-population i with probability p and sub-population npop + 1 with probability 1 p. The size of sub-population npop + 1 is set to \$N_0\$. Migration rates to and from the new sub-population are assumed to be zero and the growth rate of the new sub-population is set to zero: c(6, t, i, p)
- 7 move all lineages in sub-population i to sub-population j at time t. Migration rates from sub-population i are set to zero: c(7,t,i,j)

Author(s)

Bastian Pfeifer

See Also

MS

```
# params
# params@theta <- rep(5,n.regions)
# params@migration <- 3</pre>
```

Description

A VCF file stored in the directory "data" of the PopGenome package. The file (unpacked) has to be stored in a folder (for example "VCF"). Note that many VCF-files can be stored in this folder and are read consecutively. If the VCF file is too large to fit into the computer's main memory, split it into chunks (by position)! PopGenome is able to concatenate these chunks afterwards. readData("VCF", format="VCF", FAST=TRUE)

```
VCF_split_into_scaffolds
```

Split a VCF file into multiple scaffold-VCFs

Description

This function splits a VCF file into multiple VCFs including data for exactly one scaffold each.

Usage

```
VCF_split_into_scaffolds(VCF.file, output.folder)
```

Arguments

```
VCF.file the basepath of the VCF file
```

output.folder name of the folder where the VCFs should be stored

Details

The algorithm splits the VCF into multiple scaffold based VCFs and stores the files in a given folder. This folder can be used as an input for readData(,format="VCF")

Value

TRUE

```
# VCF_split_into_scaffolds("VCFfile.vcf","scaffoldVCFs")
# test <- readData("scaffoldVCFs", format="VCF")</pre>
```

weighted.jackknife 75

```
weighted.jackknife Weighted Jackknife
```

Description

Implements the weighted drop-one jackknife procedure.

Usage

```
## S4 method for signature 'GENOME'
weighted.jackknife(object,
do.D=TRUE,
do.BDF=TRUE,
per.region=FALSE,
block.size=1
)
```

Arguments

```
object an object of class "GENOME"

do.D default:TRUE

do.BDF default:TRUE

per.region FALSE drop a genomic region, TRUE drop single SNPs

block.size in case per.region=TRUE the number of SNPs to be dropped
```

Value

The function creates a transformed object of class "GENOME".\ The following slots are filled: BDF.z,BDF.pval,BDF.SE,D.z,D.p and D.SE.

Note

The introgression.stats module has to be performed prior to the analyses.

```
# GENOME.class <- readVCF("...", ...)
# GENOME.class <- set.populations()
# GENOME.class.slide <- sliding.window.transform(...)
# GENOME.class.slide <- introgression.stats(...)
# GENOME.class.slide <- weighted.jackknife(GENOME.class.slide, per.region=FALSE)
# GENOME.class.slide@BDF.z
# GENOME.class.slide@D.z</pre>
```

76 Whop_readVCF

Whop_readVCF Reading tabixed VCF files (an interface to WhopGenome)

Description

This function provides an interface to the WhopGenome package which is specialized to read tabix-indexed VCF files.

Usage

Arguments

v a vcf_handle returned from vcf_open()

numcols number of SNPs that should be read in as one chunk

tid which chromosome ? (character)

frompos start of the region topos end of the region

samplenames a vector of individual names/IDs gffpath the corresponding GFF file

include.unknown

including positions with unknown nucleotides

Details

WhopGenome is required! require(WhopGenome) WhopGenome provides some powerful filter meachanisms which can be applied to the VCF reading process. The filter rules can be set via WhopGenome functions. Whop_readVCF expects a vcf_handle returned from vcf_open. The Whop_readVCF function expects a tabixed VCF with a diploid GT-field.

In case of haploid data, the GT-field has to be transformed to a pseudo- diploid field (0 -> 010 etc.). An alternative is to use readData(..., format="VCFhap") which can read non-tabixed haploid VCFs directly.

The ff-package we use limits the data size to individuals * (number of SNPs) <= .Machine\$integer.max In case of very large data sets, the bigmemory package will be used.

This may slow down calculations.

See also readData(..., format="VCF")!

Whop_readVCF 77

Value

The function creates an object of class "GENOME"

The following slots will be filled in the "GENOME" object

Description Slot n.sites total number of sites 2. n.biallelic.sites number of biallelic sites region.data some detailed information on the data read 4. region.names names of regions

```
# require(WhopGenome)
# vcf_handle <- vcf_open("chr2.vcf.gz")</pre>
# GENOME.class <- Whop_readVCF(vcf_handle, 1000, "2", 1, 100000)</pre>
# GENOME.class
# GENOME.class@region.names
```

Index

*Topic classes	PG_plot.biallelic.matrix-methods,
GENOME-class, 22	46
test.params-class,72	PopGplot, 48
*Topic datasets	readData, 50
fasta_file, 17	readHapMap, 53
gff_file, 33	readMS, 54
<pre>snp_file, 67</pre>	readSNP, 55
vcf_file, 73	readVCF, 56
*Topic methods	${\sf recomb.stats-methods}, {\sf 58}$
Achaz.stats-methods, 3	region.as.fasta-methods,59
BayeScanR, 4	save.session, 60
calc.fixed.shared-methods, 6	set.filter-methods, 61
calc.R2-methods, 7	set.outgroup-methods, 62
codontable, 8	set.populations-methods, 63
concatenate.classes, 9	set.ref.positions-methods, 64
concatenate.regions, 10	set.synnonsyn-methods, 64
count.unknowns-methods, 10	show.slots-methods, 65
create.PopGenome.method, 11	sliding.window.transform-methods,
detail.stats-methods, 12	66
diversity.stats-methods, 14	splitting.data-methods,67
diversity.stats.between-methods,	sweeps.stats-methods, 70
16	weighted.jackknife,75
F_ST.stats-methods, 18	Whop_readVCF, 76
F_ST.stats.2-methods, 20	*Topic package
get.biallelic.matrix-methods, 27	PopGenome, 47
get.codons-methods, 28	
get.individuals-methods, 30	Achaz.stats (GENOME-class), 22
get.status-methods, 31	Achaz.stats,GENOME-method
get_gff_info, 32	(Achaz.stats-methods), 3
getBayes-methods, 31	Achaz.stats-methods, 3
introgression.stats-methods, 34	David Casar D. A
jack.knife.transform, 36	BayeScanR, 4
linkage.stats-methods, 37	calc.fixed.shared(GENOME-class), 22
load.session, 38	calc.fixed.shared,GENOME-method
MKT-methods, 39	(calc.fixed.shared-methods), 6
MS, 41	calc.fixed.shared-methods, 6
MS_getStats, 42	calc.R2 (GENOME-class), 22
mult.linkage.stats-methods, 43	calc.R2,GENOME-method
neutrality.stats-methods, 44	(calc.R2-methods), 7

INDEX 79

calc.R2-methods, 7	get.diversity,GENOME-method
codontable, 8	(F_ST.stats-methods), 18
concatenate.classes, 9	get.diversity-methods
concatenate.regions, 10	(F_ST.stats-methods), 18
count.unknowns (GENOME-class), 22	<pre>get.F_ST (GENOME-class), 22</pre>
count.unknowns,GENOME-method	get.F_ST,GENOME-method
(count.unknowns-methods), 10	(F_ST.stats-methods), 18
count.unknowns-methods, 10	<pre>get.F_ST-methods (F_ST.stats-methods),</pre>
create.PopGenome.method, 11	18
,	get.feature.names, 29
detail.stats(GENOME-class), 22	get.individuals (GENOME-class), 22
detail.stats,GENOME-method	get.individuals,GENOME-method
(detail.stats-methods), 12	(get.individuals-methods), 30
detail.stats-methods, 12	get.individuals-methods, 30
diversity.stats(GENOME-class), 22	get.linkage (GENOME-class), 22
diversity.stats,GENOME-method	get.linkage, GENOME-method
(diversity.stats-methods), 14	(linkage.stats-methods), 37
diversity.stats-methods, 14	, -
diversity.stats.between,GENOME-method	get.linkage-methods
(diversity.stats.between-methods),	(linkage.stats-methods), 37
16	get.MKT (GENOME-class), 22
diversity.stats.between-methods, 16	get.MKT, GENOME-method (MKT-methods), 39
	get.MKT-methods (MKT-methods), 39
F_ST.stats(GENOME-class), 22	get.neutrality(GENOME-class), 22
F_ST.stats,GENOME-method	<pre>get.neutrality,GENOME-method</pre>
(F_ST.stats-methods), 18	(neutrality.stats-methods), 44
F_ST.stats-methods, 18	get.neutrality-methods
F_ST.stats.2, 20	(neutrality.stats-methods), 44
F_ST.stats.2,GENOME-method	<pre>get.recomb (GENOME-class), 22</pre>
(F_ST.stats.2-methods), 20	get.recomb,GENOME-method
F_ST.stats.2-methods, 20	(recomb.stats-methods), 58
fasta_file, 17	get.recomb-methods
	(recomb.stats-methods), 58
GENOME-class, 22	get.status(GENOME-class), 22
get.biallelic.matrix(GENOME-class), 22	get.status,GENOME-method
get.biallelic.matrix,GENOME-method	(get.status-methods), 31
(get.biallelic.matrix-methods),	get.status-methods, 31
27	get.sum.data(GENOME-class), 22
get.biallelic.matrix-methods, 27	<pre>get.sum.data,GENOME-method(readData),</pre>
get.codons(GENOME-class), 22	50
get.codons,GENOME-method	<pre>get.sum.data-methods(readData),50</pre>
(get.codons-methods), 28	get.sweeps (GENOME-class), 22
get.codons-methods, 28	get.sweeps,GENOME-method
get.detail(GENOME-class), 22	(sweeps.stats-methods), 70
get.detail,GENOME-method	get.sweeps-methods
(detail.stats-methods), 12	(sweeps.stats-methods), 70
get.detail-methods	get_gff_info, 32
(detail.stats-methods), 12	getBayes (GENOME-class), 22
get.diversity (GENOME-class), 22	getBayes, GENOME-method

80 INDEX

(getBayes-methods), 31	read.big.fasta,49
getBayes-methods, 31	readData, 48, 50
<pre>getMS,GENOME-method(GENOME-class), 22</pre>	readHapMap, 53
gff_file, 33	readMS, 54
GFF_split_into_scaffolds, 33	readSNP, 55
	readVCF, 56
<pre>introgression.stats(GENOME-class), 22</pre>	recomb.stats(GENOME-class), 22
<pre>introgression.stats,GENOME-method</pre>	recomb.stats,GENOME-method
(introgression.stats-methods),	(recomb.stats-methods), 58
34	recomb.stats-methods, 58
introgression.stats-methods, 34	region.as.fasta(GENOME-class), 22
	region.as.fasta,GENOME-method
jack.knife.transform, 36	(region.as.fasta-methods), 59
<pre>jack.knife.transform(GENOME-class), 22</pre>	region.as.fasta-methods, 59
<pre>jack.knife.transform,GENOME-method</pre>	. 682011140114004 111041040, 09
(jack.knife.transform), 36	save.session, 60
jack.knife.transform-methods	set.filter(GENOME-class), 22
(jack.knife.transform), 36	set.filter,GENOME-method
	(set.filter-methods), 61
linkage.stats(GENOME-class), 22	set.filter-methods, 61
linkage.stats,GENOME-method	set.outgroup (GENOME-class), 22
(linkage.stats-methods), 37	set.outgroup,GENOME-method
linkage.stats-methods, 37	(set.outgroup-methods), 62
load.session, 38	set.outgroup-methods, 62
	set.populations (GENOME-class), 22
MKT (GENOME-class), 22	set.populations, GENOME-method
MKT, GENOME-method (MKT-methods), 39	(set.populations-methods), 63
MKT-methods, 39	set.populations-methods, 63
MS, 41, 73	set.ref.positions (GENOME-class), 22
MS_getStats, 42	set.ref.positions,GENOME-method
mult.linkage.stats(GENOME-class), 22	(set.ref.positions-methods), 64
mult.linkage.stats,GENOME-method	set.ref.positions-methods, 64
<pre>(mult.linkage.stats-methods),</pre>	set.synnonsyn (GENOME-class), 22
43	set.symnonsym, GENOME-method
mult.linkage.stats-methods, 43	(set.synnonsyn-methods), 64
. 1 (05)10)15 1	set.synnonsyn-methods, 64
neutrality.stats (GENOME-class), 22	show, GENOME-method (GENOME-class), 22
neutrality.stats,GENOME-method	show.slots (GENOME-class), 22
(neutrality.stats-methods), 44	show.slots, GENOME-method
neutrality.stats-methods, 44	(show.slots-methods), 65
DC mlot highlig mother	
PG_plot.biallelic.matrix	show.slots-methods, 65
(GENOME-class), 22	sliding.window.transform
PG_plot.biallelic.matrix,GENOME-method	(GENOME-class), 22
(PG_plot.biallelic.matrix-methods),	sliding.window.transform,GENOME-method
46	(sliding.window.transform-methods)
PG_plot.biallelic.matrix-methods, 46	66
popFSTN, GENOME-method (GENOME-class), 22	sliding.window.transform-methods,66
PopGenome, 47	snp_file, 67
PopGplot, 48	split_data_into_GFF_attributes,68

INDEX 81

```
split_data_into_GFF_features, 69
splitting.data(GENOME-class), 22
splitting.data,GENOME-method
        (splitting.data-methods), 67
splitting.data-methods, 67
sweeps.stats(GENOME-class), 22
sweeps.stats,GENOME-method
        (sweeps.stats-methods), 70
sweeps.stats-methods, 70
test.params(test.params-class), 72
test.params-class, 72
usage, GENOME-method (GENOME-class), 22
vcf_file, 73
VCF_split_into_scaffolds, 74
weighted.jackknife, 75
weighted.jackknife(GENOME-class), 22
weighted.jackknife,GENOME-method
        (weighted.jackknife), 75
weighted.jackknife-methods
        (weighted.jackknife), 75
Whop_readVCF, 76
```