

Package ‘fastreeR’

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Type Package

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Version 1.8.0

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Description Calculate distances, build phylogenetic trees or perform hierarchical clustering between the samples of a VCF or FASTA file. Functions are implemented in Java and called via rJava. Parallel implementation that operates directly on the VCF or FASTA file for fast execution.

License GPL-3

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Imports ape, data.table, dynamicTreeCut, methods, R.utils, rJava, stats, stringr, utils

SystemRequirements Java (>= 8)

RoxygenNote 7.3.1

URL <https://github.com/gkanogiannis/fastreeR>,
<https://github.com/gkanogiannis/BioInfoJava-Utills>

BugReports <https://github.com/gkanogiannis/fastreeR/issues>

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| | |
|------------------|---|
| fastreeR-package | <i>fastreeR: Phylogenetic, Distance and Other Calculations on VCF and Fasta Files</i> |
|------------------|---|

Description

Calculate distances, build phylogenetic trees or perform hierarchical clustering between the samples of a VCF or FASTA file. Functions are implemented in Java and called via rJava. Parallel implementation that operates directly on the VCF or FASTA file for fast execution.

Author(s)

Maintainer: Anestis Gkanogiannis <anestis@gkanogiannis.com> ([ORCID](https://orcid.org/0000-0002-6441-0688))

See Also

Useful links:

- <https://github.com/gkanogiannis/fastreeR>
- <https://github.com/gkanogiannis/BioInfoJava-Utils>
- Report bugs at <https://github.com/gkanogiannis/fastreeR/issues>

| | |
|---------------|--|
| dist2clusters | <i>Perform Hierarchical Clustering and tree pruning on a distance matrix</i> |
|---------------|--|

Description

Performs Hierarchical Clustering on a distance matrix (i.e. calculated with [vcf2dist](#) or [fasta2dist](#)) and generates a phylogenetic tree with agglomerative Neighbor Joining method (complete linkage) (as in [dist2tree](#)). The phylogenetic tree is then pruned with [cutreeDynamic](#) to get clusters (as in [tree2clusters](#)).

Usage

```
dist2clusters(inputDist, cutHeight = NULL, minClusterSize = 1, extra = TRUE)
```

Arguments

| | |
|----------------|--|
| inputDist | Input distances file location (generated with vcf2dist or fasta2dist). File can be gzip compressed. Or a dist distances object. |
| cutHeight | Define at which height to cut tree. Default automatically defined. |
| minClusterSize | Minimum size of clusters. Default 1. |
| extra | Boolean whether to use extra parameters for the cutreeDynamic . |

Value

A list of :

- [character](#) vector of the generated phylogenetic tree in Newick format
- [character](#) vector of the clusters. Each row contains data for a cluster, separated by space. The id of the cluster, the size of the cluster (number of elements) and the names of its elements, Cluster id 0 contains all the objects not assigned to a cluster (singletons). Example clusters output :

```
0 3 Sample1 Sample2 Sample3
1 3 Sample4 Sample5 Sample6
2 2 Sample7 Sample8
3 2 Sample9 Sample0
```

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utils>

Examples

```
my.clust <- dist2clusters(  
  inputDist =  
    system.file("extdata", "samples.vcf.dist.gz", package = "fastreeR")  
)
```

dist2tree

Generate phylogenetic tree from samples of a distance matrix

Description

Performs Hierarchical Clustering on a distance matrix (i.e. calculated with [vcf2dist](#) or [fasta2dist](#)) and generates a phylogenetic tree with agglomerative Neighbor Joining method (complete linkage).

Usage

```
dist2tree(inputDist)
```

Arguments

`inputDist` Input distances file location (generated with [vcf2dist](#) or [fasta2dist](#)). File can be gzip compressed. Or a [dist](#) distances object.

Value

A [character](#) vector of the generated phylogenetic tree in Newick format.

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utils>

Examples

```
my.tree <- dist2tree(  
  inputDist =  
    system.file("extdata", "samples.vcf.dist.gz", package = "fastreeR")  
)
```

| | |
|------------|--|
| fasta2dist | <i>Calculate distances between sequences of a FASTA file</i> |
|------------|--|

Description

This function calculates a d2_S type dissimilarity measurement between the n sequences (which can represent samples) of a FASTA file. See [doi:10.1186/s1285901611863](https://doi.org/10.1186/s1285901611863) for more details.

Usage

```
fasta2dist(  
  ...,  
  outputFile = NULL,  
  threads = 2,  
  kmer = 6,  
  normalize = FALSE,  
  compress = TRUE  
)
```

Arguments

| | |
|------------|--|
| ... | Input fasta files locations (uncompressed or gzip compressed). |
| outputFile | Output distances file location. |
| threads | Number of java threads to use. |
| kmer | Kmer length to use for analyzing fasta sequences. |
| normalize | Normalize on sequences length. |
| compress | Compress output (adds .gz extension). |

Value

A `dist` distances object of the calculation.

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utills>

Examples

```
my.dist <- fasta2dist(  
  inputfile = system.file("extdata", "samples.fasta.gz",  
    package = "fastreeR"  
  )  
)
```

| | |
|---------------|--|
| tree2clusters | <i>Perform Hierarchical Clustering and tree pruning on a phylogenetic tree</i> |
|---------------|--|

Description

The phylogenetic tree is pruned with `cutreeDynamic` to get clusters.

Usage

```
tree2clusters(
  treeStr,
  treeDistances = NULL,
  treeLabels = NULL,
  cutHeight = NULL,
  minClusterSize = 1,
  extra = TRUE
)
```

Arguments

| | |
|----------------|---|
| treeStr | A character vector of a phylogenetic tree in Newick format |
| treeDistances | numeric matrix of distances, that were used to generate the tree. If NULL, it will be inferred from tree branch lengths. |
| treeLabels | A character vector of tree leaf labels. |
| cutHeight | Define at which height to cut tree. Default automatically defined. |
| minClusterSize | Minimum size of clusters. Default 1. |
| extra | Boolean whether to use extra parameters for the <code>cutreeDynamic</code> . |

Value

- **character** vector of the clusters. Each row contains data for a cluster, separated by space. The id of the cluster, the size of the cluster (number of elements) and the names of its elements, Cluster id 0 contains all the objects not assigned to a cluster (singletons). Example clusters output :

```
0 3 Sample1 Sample2 Sample3
1 3 Sample4 Sample5 Sample6
2 2 Sample7 Sample8
3 2 Sample9 Sample0
```

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utils>

Examples

```
my.clust <- tree2clusters(
  treeStr = dist2tree(
    inputDist = system.file("extdata", "samples.vcf.dist.gz",
      package = "fastreeR"
    )
  )
)
```

| | |
|--------------|--|
| vcf2clusters | <i>Perform Hierarchical Clustering and tree pruning on samples of VCF file</i> |
|--------------|--|

Description

Performs Hierarchical Clustering on a distance matrix calculated as in [vcf2dist](#) and generates a phylogenetic tree with agglomerative Neighbor Joining method (complete linkage) (as in [dist2tree](#)). The phylogenetic tree is then pruned with [cutreeDynamic](#) to get clusters (as in [tree2clusters](#)).

Usage

```
vcf2clusters(
  inputFile,
  threads = 2,
  ignoreMissing = FALSE,
  onlyHets = FALSE,
  ignoreHets = FALSE,
  cutHeight = NULL,
  minClusterSize = 1,
  extra = TRUE
)
```

Arguments

| | |
|----------------|---|
| inputFile | Input vcf file location (uncompressed or gzip compressed). |
| threads | Number of java threads to use. |
| ignoreMissing | Ignore variants with missing data (./ or .) |
| onlyHets | Only calculate on variants with heterozygous calls. |
| ignoreHets | Only calculate on variants with homozygous calls. |
| cutHeight | Define at which height to cut tree. Default automatically defined. |
| minClusterSize | Minimum size of clusters. Default 1. |
| extra | Boolean whether to use extra parameters for the cutreeDynamic . |

Details

Biallelic or multiallelic (maximum 7 alternate alleles) SNP and/or INDEL variants are considered, phased or not. Some VCF encoding examples are:

- heterozygous variants : 1/0 or 0/1 or 0/2 or 1|0 or 0|1 or 0|2
- homozygous to the reference allele variants : 0/0 or 0|0
- homozygous to the first alternate allele variants : 1/1 or 1|1

If there are n samples and m variants, an $n \times n$ zero-diagonal symmetric distance matrix is calculated. The calculated cosine type distance $(1 - \text{cosine_similarity})/2$ is in the range $[0,1]$ where value 0 means completely identical samples (cosine is 1), value 0.5 means perpendicular samples (cosine is 0) and value 1 means completely opposite samples (cosine is -1).

The calculation is performed by a Java back-end implementation, that supports multi-core CPU utilization and can be demanding in terms of memory resources. By default a JVM is launched with a maximum memory allocation of 512 MB. When this amount is not sufficient, the user needs to reserve additional memory resources, before loading the package, by updating the value of the `java.parameters` option. For example in order to allocate 4GB of RAM, the user needs to issue options(`java.parameters="-Xmx4g"`) before `library(fastreeR)`.

Value

A list of :

- `dist` distances object.
- `character` vector of the generated phylogenetic tree in Newick format
- `character` vector of the clusters. Each row contains data for a cluster, separated by space. The id of the cluster, the size of the cluster (number of elements) and the names of its elements, Cluster id 0 contains all the objects not assigned to a cluster (singletons). Example clusters output :

```

0 3 Sample1 Sample2 Sample3
1 3 Sample4 Sample5 Sample6
2 2 Sample7 Sample8
3 2 Sample9 Sample0
```

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utils>

Examples

```
my.clust <- vcf2clusters(
  inputFile = system.file("extdata", "samples.vcf.gz",
    package = "fastreeR"
  )
)
```

vcf2dist

*Calculate distances between samples of a VCF file***Description**

This function calculates a cosine type dissimilarity measurement between the n samples of a VCF file.

Usage

```
vcf2dist(
  inputFile,
  outputFile = NULL,
  threads = 2,
  ignoreMissing = FALSE,
  onlyHets = FALSE,
  ignoreHets = FALSE,
  compress = FALSE
)
```

Arguments

| | |
|---------------|--|
| inputFile | Input vcf file location (uncompressed or gzip compressed). |
| outputFile | Output distances file location. |
| threads | Number of java threads to use. |
| ignoreMissing | Ignore variants with missing data (./. or . .) |
| onlyHets | Only calculate on variants with heterozygous calls. |
| ignoreHets | Only calculate on variants with homozygous calls. |
| compress | Compress output (adds .gz extension). |

Details

Biallelic or multiallelic (maximum 7 alternate alleles) SNP and/or INDEL variants are considered, phased or not. Some VCF encoding examples are:

- heterozygous variants : 1/0 or 0/1 or 0/2 or 1|0 or 0|1 or 0|2
- homozygous to the reference allele variants : 0/0 or 0|0
- homozygous to the first alternate allele variants : 1/1 or 1|1

If there are n samples and m variants, an $n \times n$ zero-diagonal symmetric distance matrix is calculated. The calculated cosine type distance $(1 - \text{cosine_similarity})/2$ is in the range $[0,1]$ where value 0 means completely identical samples (cosine is 1), value 0.5 means perpendicular samples (cosine is 0) and value 1 means completely opposite samples (cosine is -1).

The calculation is performed by a Java backend implementation, that supports multi-core CPU utilization and can be demanding in terms of memory resources. By default a JVM is launched with a maximum memory allocation of 512 MB. When this amount is not sufficient, the user needs to reserve additional memory resources, before loading the package, by updating the value of the `java.parameters` option. For example in order to allocate 4GB of RAM, the user needs to issue `options(java.parameters="-Xmx4g")` before `library(fastreeR)`.

Output file, if provided, will contain $n+1$ lines. The first line contains the number n of samples and number m of variants, separated by space. Each of the subsequent n lines contains $n+1$ values, separated by space. The first value of each line is a sample name and the rest n values are the calculated distances of this sample to all the samples. Example output file of the distances of 3 samples calculated from 1000 variants:

```
3 1000
Sample1 0.0 0.5 0.2
Sample2 0.5 0.0 0.9
Sample3 0.2 0.9 0.0
```

Value

A `dist` distances object of the calculation.

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utills>

Examples

```
my.dist <- vcf2dist(
  inputFile = system.file("extdata", "samples.vcf.gz",
    package = "fastreeR"
  )
)
```

vcf2istats *Calculate various per sample statistics from a VCF file*

Description

Only biallelic SNPs are considered. For each sample, the following statistics are calculated :

- INDIV : Sample name
- N_SITES : Total number of SNPs
- N_HET : Number of SNPs with heterozygous call (0/1 or 0|1 or 1/0 or 1|0)
- N_ALT : Number of SNPs with alternate homozygous call (1/1 or 1|1)
- N_REF : Number of SNPs with reference homozygous call (0/0 or 0|0)
- N_MISS : Number of SNPs with missing call (./. or .|.)
- P_HET : Percentage of heterozygous calls
- P_ALT : Percentage of alternate homozygous calls
- P_REF : Percentage of reference homozygous calls
- P_MISS : Percentage of missing calls (missing rate)

Usage

```
vcf2istats(inputFile, outputFile = NULL)
```

Arguments

| | |
|------------|--|
| inputFile | Input vcf file location (uncompressed or gzip compressed). |
| outputFile | Output samples statistics file location. |

Value

A [data.frame](#) of sample statistics.

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utills>

Examples

```
my.istats <- vcf2istats(  
  inputFile =  
    system.file("extdata", "samples.vcf.gz", package = "fastreeR")  
)
```

vcf2tree

*Generate phylogenetic tree from samples of a VCF file***Description**

This function calculates a distance matrix between the samples of a VCF file as in `vcf2dist` and performs Hierarchical Clustering on this distance matrix as in `dist2tree`. A phylogenetic tree is calculated with agglomerative Neighbor Joining method (complete linkage).

Usage

```
vcf2tree(
  inputFile,
  threads = 2,
  ignoreMissing = FALSE,
  onlyHets = FALSE,
  ignoreHets = FALSE
)
```

Arguments

| | |
|----------------------------|--|
| <code>inputFile</code> | Input vcf file location (uncompressed or gzip compressed). |
| <code>threads</code> | Number of java threads to use. |
| <code>ignoreMissing</code> | Ignore variants with missing data (./. or . .) |
| <code>onlyHets</code> | Only calculate on variants with heterozygous calls. |
| <code>ignoreHets</code> | Only calculate on variants with homozygous calls. |

Details

Biallelic or multiallelic (maximum 7 alternate alleles) SNP and/or INDEL variants are considered, phased or not. Some VCF encoding examples are:

- heterozygous variants : 1/0 or 0/1 or 0/2 or 1|0 or 0|1 or 0|2
- homozygous to the reference allele variants : 0/0 or 0|0
- homozygous to the first alternate allele variants : 1/1 or 1|1

If there are n samples and m variants, an $n \times n$ zero-diagonal symmetric distance matrix is calculated. The calculated cosine type distance $(1 - \text{cosine_similarity})/2$ is in the range $[0,1]$ where value 0 means completely identical samples (cosine is 1), value 0.5 means perpendicular samples (cosine is 0) and value 1 means completely opposite samples (cosine is -1).

The calculation is performed by a Java backend implementation, that supports multi-core CPU utilization and can be demanding in terms of memory resources. By default a JVM is launched with a maximum memory allocation of 512 MB. When this amount is not sufficient, the user needs to reserve additional memory resources, before loading the package, by updating the value of the `java.parameters` option. For example in order to allocate 4GB of RAM, the user needs to issue `options(java.parameters="-Xmx4g")` before `library(fastreeR)`.

Value

A **character** vector of the generated phylogenetic tree in Newick format.

Author(s)

Anestis Gkanogiannis, <anestis@gkanogiannis.com>

References

Java implementation: <https://github.com/gkanogiannis/BioInfoJava-Utills>

Examples

```
my.tree <- vcf2tree(  
  inputFile = system.file("extdata", "samples.vcf.gz",  
    package = "fastreeR"  
  )  
)
```

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