## Package 'ipADMIXTURE'

March 26, 2020

Title Iterative Pruning Population Admixture Inference Framework

Version 0.1.0

Description A data clustering package based on admixture ratios (Q matrix) of population structure. The framework is based on iterative Pruning procedure that performs data clustering by splitting a given population into subclusters until meeting the condition of stopping criteria the same as ipPCA, iNJclust, and IPCAPS frameworks. The package also provides a function to retrieve phylogeny tree that construct a neighbor-joining tree based on a similar matrix between clusters. By given multiple Q matrices with varying a number of ancestors (K), the framework define a similar value between clusters i,j as a minimum number K\* that makes majority of members of two clusters are in the different clusters. This K\* reflexes a minimum number of ancestors we need to splitting cluster i,j into different clusters if we assign K\* clusters based on maximum admixture ratio of individuals. The publication of this package is at Chainarong Amornbunchornvej, Pongsakorn Wangkumhang, and Sissades Tongsima (2020) <doi:10.1101/2020.03.21.001206>.

**Depends** R (>= 3.5.0) **Imports** stats,treemap,ape

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BugReports https://github.com/DarkEyes/ipADMIXTURE/issues

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2 biclustFunc

## **R** topics documented:

bicl	stFunc biclustFunc function	
Index		9
	UD1_Qmat	8
	UD1labels	
	printClustersFromLabels	
	plotClusterLeaves	
	plotAdmixClusters	
	ipADMIXTURE	
	human27pop_Qmat	4
	human27pop_labels	
	getPhyloTree	3
	biclustFunc	2

## Description

biclustFunc is a binary clustering function using hierarchical clustering.

### Usage

```
biclustFunc(Qmat, admixRatioThs = 0.5, method = "average")
```

#### Arguments

Qmat	represents the admixture ratio of ancestor j for individual i.
admixRatioThs	is a threshold to determine that if a cluster has maxDiffAdmixRatio lower than

threshold, then the cluster is a homogeneous cluster.

method is a method parameter of hclust object for hierarchical clustering analysis. The

default is "average".

#### Value

This function returns binary clustering results.

heteroFlag is a flag that represents a status whether a given cluster is heterogeneous (having

sub-clusters). It is TRUE if maxDiffAdmixRatio >= admixRatioThs.

clusterInx is a vector of clustering assignment where indexClsVec[i] is a cluster number

of individual i.

meanDiffAdmixRatio

is a vector of magnitude-difference of admixture ratios. It is calculated by splitting a given cluster into two sub-clusters. Then, we take the absolute on the

difference between mean admixture ratios of sub-clusters.

getPhyloTree 3

Qmat1 is a Q matrix of sub-cluster #1 after splitting a given cluster into two sub-clusters

that contains admixture ratios of all individuals where the  ${\tt Qmat[i,j]}$  represents

the admixture ratio of ancestor j for individual i.

Qmat2 is a Q matrix of sub-cluster #2 after splitting a given cluster into two sub-clusters

that contains admixture ratios of all individuals where the Qmat[i,j] represents

the admixture ratio of ancestor j for individual i.

maxDiffAdmixRatio

is a maximum of magnitude-difference of admixture ratios for a given cluster

before splitting into two sub-clusters.

## **Examples**

```
# Running biclustFunc on Q matrix of 27 human population dataset where K = 12
obj<-biclustFunc(Qmat=ipADMIXTURE::human27pop_Qmat[[11]], admixRatioThs =0.15)</pre>
```

getPhyloTree

getPhyloTree

## **Description**

getPhyloTree is function that reports a phylogenetic tree of clusters based on admixture analysis. The phylogeny tree that construct a neighbor-joining tree based on a similar matrix between clusters. By given multiple Q matrices with varying a number of ancestors (K), the framework define a similar value between clusters i,j as a minimum number K that makes majority of members of two clusters are in the different clusters. This K reflexes a minimum number of ancestors we need to splitting cluster i,j into different clusters if we assign K clusters based on maximum admixture ratio of individuals.

## Usage

```
getPhyloTree(QmatList, indexClsVec)
```

#### **Arguments**

QmatList is list of Q matrix where QmatList[[k]] is a Q matrix with k+1 ancestors.

indexClsVec is a vector of clustering assignment where indexClsVec[i] is a cluster number

of individual i.

#### Value

This function returns an object of nj tree as well as a matrix minDiffAncestorClsMat that is used as a similarity matrix.

tree is an object of nj tree calculated by ape::nj() function on a dissimilarity version

of minDiffAncestorClsMat.

minDiffAncestorClsMat

is a minimum-ancestor-number matrix where minDiffAncestorClsMat[i,j] is a minimum number of ancestors that make i and j to be different clusters while minDiffAncestorClsMat[i,j]-1 makes majority of members from i and j belong to the same cluster.

#### **Examples**

# Running ipADMIXTURE on Q matrices (K=2-12) of 27 human population dataset.
h27pop\_obj<-ipADMIXTURE(Qmat=ipADMIXTURE::human27pop\_Qmat[[11]], admixRatioThs =0.15)
out<-ipADMIXTURE::getPhyloTree(ipADMIXTURE::human27pop\_Qmat,h27pop\_obj\$indexClsVec)
plot(out\$tree)</pre>

human27pop\_labels

Labels of 27 human populations

## **Description**

Labels of 27 human populations

### Usage

human27pop\_labels

#### Format

Labels of 27 human populations. :

human27pop\_labels It is a vector of labels of 544 individuals. There are 27 populations. ...

human27pop\_Qmat

A list of Q matrices of 27 human populations

## Description

A dataset containing admixture ratios of 544 individuals from 27 human populations where the number of ancestors ranges from 2 to 12. This dataset was the result of running ADMIXTURE software developed by Zhou, H., et al. (2011). A quasi-Newton acceleration for high-dimensional optimization algorithms. Statistics and computing, 21(2), 261-273. on the 27-human-population dataset published by Xing, J., Watkins, W. S. et al. (2009). Fine-scaled human genetic structure revealed by SNP microarrays. Genome research, 19(5), 815-825.

### Usage

human27pop\_Qmat

ipADMIXTURE 5

#### **Format**

A list of Q matrices of 544 individuals from 27 human populations. There are 2-12 ancestors in the list

**human27pop\_Qmat** It is list of Q matrices that contains admixture ratios of 544 individuals from the 27 population human dataset. human27pop\_Qmat[[k]][i,j] is the admixture ratio of jth ancestor for ith individual in the (k+1)-ancestor Q matrix. ...

 $\begin{tabular}{ll} {\it ipADMIXTURE} & {\it Iterative Pruning Population Admixture Inference Framework (ipAD-MIXTURE)} \\ \end{tabular}$ 

## Description

A data clustering package based on admixture ratios (Q matrix) of population structure.

The framework is based on iterative Pruning procedure that performs data clustering by splitting a given population into subclusters until meeting the condition of stopping criteria the same as ipPCA, iNJclust, and IPCAPS frameworks. The package also provides a function to retrieve phylogeny tree that construct a neighbor-joining tree based on a similar matrix between clusters. By given multiple Q matrices with varying a number of ancestors (K), the framework define a similar value between clusters i,j as a minimum number K that makes majority of members of two clusters are in the different clusters. This K reflexes a minimum number of ancestors we need to splitting cluster i,j into different clusters if we assign K clusters based on maximum admixture ratio of individuals.

## Usage

```
ipADMIXTURE(Qmat, admixRatioThs, method = "average")
```

#### **Arguments**

Qmat is a Q matrix that contains admixture ratios of all individuals where the Qmat[i,j]

represents the admixture ratio of ancestor j for individual i.

admixRatioThs is a threshold to determine that if a cluster has maxDiffAdmixRatio lower than

threshold, then the cluster is a homogeneous cluster.

method is a method parameter of holust object for hierarchical clustering analysis. The

default is "average".

#### Value

This function returns clustering results in a form of an object of ipADMIXTURE class. The object contains the following items.

indexClsVec is a vector of clustering assignment where indexClsVec[i] is a cluster number

of individual i.

homoClusters is a list of cluster objects where each object contains member indices, cluster's

maxDiffAdmixRatio, ID, etc.

6 plotAdmixClusters

maxDiffAdmixRatioVec

is a vector of maxDiffAdmixRatios for all clusters.

Qmat is a Q matrix that contains admixture ratios of all individuals where the Qmat[i,j]

represents the admixture ratio of ancestor j for individual i.

admixRatioThs is a threshold to determine that if a cluster has maxDiffAdmixRatio lower than

threshold, then the cluster is a homogeneous cluster.

## Author(s)

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## **Examples**

```
# Running ipADMIXTURE on Q matrix of 27 human population dataset where K = 12
h27pop_obj<-ipADMIXTURE(Qmat=ipADMIXTURE::human27pop_Qmat[[11]], admixRatioThs =0.15)</pre>
```

plotAdmixClusters

plotAdmixClusters

#### **Description**

plotAdmixClusters is function that plots admixture ratios where the x axis represents individuals with cluster labels and y axis represents admixture ratios.

## Usage

```
plotAdmixClusters(obj)
```

## **Arguments**

obj

is an object of ipADMIXTURE class.

## Examples

```
h27pop_obj<-ipADMIXTURE(Qmat=ipADMIXTURE::human27pop_Qmat[[11]], admixRatioThs =0.15) ipADMIXTURE::plotAdmixClusters(h27pop_obj)
```

plotClusterLeaves 7

plotClusterLeaves

plotClusterLeaves

## **Description**

plotClusterLeaves is function that plots clusters in a form of treemap plot. Subsquares represent clusters. Each subsquare contains cluster label (ID), number of members (N), and a maximum of manitude-difference of admixture ratios (md). A size of each subsquare represents a ratio of member numbers compared to other clusters. A color represents an md value of cluster.

## Usage

```
plotClusterLeaves(obj)
```

## Arguments

obj

is an object of ipADMIXTURE class.

## **Examples**

```
h27pop_obj<-ipADMIXTURE(Qmat=ipADMIXTURE::human27pop_Qmat[[11]], admixRatioThs =0.15) ipADMIXTURE::plotClusterLeaves(h27pop_obj)
```

```
printClustersFromLabels
```

printClustersFromLabels

## Description

printClustersFromLabels is function that reports that clustering results in text mode.

#### Usage

```
printClustersFromLabels(obj, labels)
```

## Arguments

obj is an object of ipADMIXTURE class.

labels is a vector of labels of all individuals.

#### **Examples**

```
h27pop_obj<-ipADMIXTURE(Qmat=ipADMIXTURE::human27pop_Qmat[[11]], admixRatioThs =0.15) ipADMIXTURE::printClustersFromLabels(h27pop_obj,ipADMIXTURE::human27pop_labels)
```

8 UD1\_Qmat

UD1labels

Labels of 20 simulation populations

### Description

Labels of 20 simulation populations

## Usage

UD1labels

#### **Format**

Labels of 20 populations. :

**UD1labels** It is a vector of labels of 1200 individuals. There are 20 populations. ...

UD1\_Qmat

A list of Q matrices of simulation of 20 populations

## **Description**

A dataset containing admixture ratios of 1200 individuals from 20 simulation populations where the number of ancestors ranges from 2 to 18. This dataset was the result of running LEA library developed by Frichot, E., & François, O. (2015). LEA: An R package for landscape and ecological association studies. Methods in Ecology and Evolution, 6(8), 925-929. on the 20-simulation-population dataset published by Limpiti, T., et al. (2014). iNJclust: iterative neighbor-joining tree clustering framework for inferring population structure. IEEE/ACM transactions on computational biology and bioinformatics, 11(5), 903-914.

#### Usage

UD1\_Qmat

#### **Format**

A list of Q matrices of 1200 individuals from 20 populations. There are Q matrices that have the number of ancestors ranges from from 2 to 18.

**UD1\_Qmat** It is list of Q matrices that contains admixture ratios of 1200 individuals from the 20-population dataset. UD1\_Qmat[[k]][i,j] is the admixture ratio of jth ancestor for ith individual in the (k+1)-ancestor Q matrix. ...

# **Index**

```
*Topic datasets
human27pop_labels, 4
human27pop_Qmat, 4
UD1_Qmat, 8
UD1labels, 8
biclustFunc, 2
getPhyloTree, 3
human27pop_labels, 4
human27pop_Qmat, 4
ipADMIXTURE, 5
plotAdmixClusters, 6
plotClusterLeaves, 7
printClustersFromLabels, 7
UD1_Qmat, 8
UD1labels, 8
```