

Package ‘ipADMIXTURE’

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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

URL <https://github.com/DarkEyes/ipADMIXTURE>

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

Language en-US

License GPL-3

Encoding UTF-8

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Suggests knitr, rmarkdown

VignetteBuilder knitr

RoxygenNote 7.0.2

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biclustFunc	<i>biclustFunc function</i>
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Description

biclustFunc is a binary clustering function using hierarchical clustering.

Usage

```
biclustFunc(Qmat, admixRatioThs = 0.5, 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 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.
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 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)
```

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)
```

human27pop_labels	<i>Labels of 27 human populations</i>
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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	<i>A list of Q matrices of 27 human populations</i>
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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

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. ...

ipADMIXTURE	<i>Iterative Pruning Population Admixture Inference Framework (ipADMIXTURE)</i>
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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 hclust 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.
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)
```

plotAdmixClusters	<i>plotAdmixClusters</i>
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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	<i>plotClusterLeaves</i>
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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)
```

UD1labels	<i>Labels of 20 simulation populations</i>
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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. ...

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