

Package ‘BioSeqClass’

April 4, 2014

Version 1.20.0

Title Classification for Biological Sequences

Author Li Hong sysptm@gmail.com

Maintainer Li Hong sysptm@gmail.com

Imports Biostrings, ipred, e1071, klaR, randomForest, class, tree, nnet, rpart, party, foreign, Biobase, utils, stats, grDevices

Description Extracting Features from Biological Sequences and Building Classification Model

Keyword Classification

biocViews Classification

License LGPL (>= 2.0)

ZipData no

LazyLoad yes

Depends R (>= 2.10), scatterplot3d

Suggests scatterplot3d

R topics documented:

basic	2
classify	4
featureAAindex	6
featureBDNAVIDEO	8
featureBinary	8
featureCKSAAP	9
featureCTD	10
featureDIPRODB	11
featureDOMAIN	12
featureEvaluate	13

featureFragmentComposition	16
featureGapPairComposition	17
featureHydro	18
featurePseudoAAComp	19
featurePSSM	20
featureSSC	21
hr	22
model	24
performance	26
selectFFS	27
selectWeka	28
zzz	29

Index	31
--------------	-----------

basic	<i>Assistant Functions</i>
-------	----------------------------

Description

Assistant functions including read/write files, invoke perl programs, and so on.

Usage

```
## Elements and groups of base and amino acid
elements(ele.type)
aaClass(aa.type)

pwm(seq,class=elements("aminoacid"))

.pathPerl(perlName, os)
.callPerl(perlName, os)

data(dssp.ss)
data(aa.index)
data(PROPERTY)
data(DiProDB)
```

Arguments

ele.type	a string for the type of biological sequence. This must be one of the strings "rnaBase", "dnaBase", "aminoacid" or "aminoacid2".
aa.type	a string for the group of amino acids. This must be one of the strings "aaH", "aaV", "aaZ", "aaP", "aaF", "aaS" or "aaE".
seq	a string vector for the protein or gene sequences.
class	a list for the class of biological properties. It can be produced by elements and aaClass .

perlName a character string for the name of perl program.
 os character string, giving the Operating System (family) of the computer.

Details

`elements` returns a list of basic elements of biological sequence. Parameter "ele.type" supported following selection: "rnaBase" - basic elements of RNA (ATCG). "dnaBase" - basic elements of DNA (AUCG). "aminoacid" - 20 amino acids (RKEDQNWGASTPHYCVLIMF). "aminoacid2" - 20 amino acids and 1 pseudo amino acid "O" (RKEDQNWGASTPHYCVLIMFO). Unknown or uncomplete amino acids will be substituted by pseudo amino acid.

`aaClass` returns a list of amino acids groups depend on their physical-chemical properties. Parameter "aa.type" supports following selection: "aaH" (hydrophobicity): Polar(RKEDQN), Neutral(GASTPHY), Hydrophobic(CVLIMFW) "aaV" (normalized Van der Waals volume): Small(GASCTPD), Medium(NVEQIL), Large(MHKFRYW) "aaZ" (polarizability): Low polarizability (GASDT), Medium polarizability (CPNVEQIL), High polarizability (KMHFRYW) "aaP" (polarity): Low polarity (LIFWCMVY), Neutral polarity (PATGS), High polarity (HQRKNED) "aaF": Acidic (DE), Basic (HKR), Polar (CGNQSTY), Nonpolar (AFILMPVW) "aaS": Acidic (DE), Basic (HKR), Aromatic (FWY), Amide (NQ), Small hydroxyl (ST), Sulfur-containing (CM), Aliphatic (AGPILV) "aaE": Acidic (DE), Basic(HKR), Aromatic (FWY), Amide (NQ), Small hydroxyl (ST), Sulfur-containing (CM), Aliphatic 1 (AGP), Aliphatic 2 (ILV)

`pwm` returns a M*N position weight matrix (PWM) of input sequences. M is the number of elements given by parameter "class". N is the length of each sequence. Each row is a kind of element, and each column is a position. The input sequences must have equal length.

`.pathPerl` write the path of Perl to perl program file.

`.callPerl` invoke Perl program via R.

`dssp.ss` is a vector storing the secondary structure data from DSSP database (<http://swift.cmbi.ru.nl/gv/dssp/>).

`aa.index` is a list storing the properties of amino acids from AAIndex database (<http://www.genome.jp/aaindex>).

`PROPERTY` is a list storing the properties of dinucleotide from B-DNA-VIDEO PROPERTY database (<http://www.mgs.bionet.nsc.ru/mgs/systems/bdnvideo/>).

`DiProDB` is a list storing the conformational and thermodynamic dinucleotide properties from DiProDB database (<http://diprodb.fli-leibniz.de/>).

Author(s)

Hong Li

Examples

```
## amino acids groups depend on their hydrophobicity
aaClass("aaH")

## load data: dssp.ss
data(dssp.ss)
## see the data in dssp.ss
dssp.ss[1:5]
```

 classify

Classification with Specific Features and Cross-Validation

Description

Classification with selected features and cross-validation. It supports 10 classification algorithms, feature selection by Weka, cross-validation and leave-one-out test.

Usage

```
classify(data, classifyMethod="libsvm", cv=10,
         features, evaluator, search, n=200,
         svm.kernel="linear", svm.scale=FALSE,
         svm.path, svm.options="-t 0",
         knn.k=1,
         nnet.size=2, nnet.rang=0.7, nnet.decay=0, nnet.maxit=100)
```

Arguments

data	a data frame including the feature matrix and class label. The last column is a vector of class label comprising of "-1" or "+1"; Other columns are features.
classifyMethod	a string for the classification method. This must be one of the strings "libsvm", "svmlight", "NaiveBayes", "randomForest", "knn", "tree", "nnet", "rpart", "ctree", "ctreelibsvm", "bagging".
cv	an integer for the time of cross validation, or a string "leave_one_out" for the jackknife test.
features	an integer vector for the index of interested columns in data, which will be used as features for build classification model.
evaluator	a string for the feature selection method used by WEKA. This must be one of the strings "CfsSubsetEval", "ChiSquaredAttributeEval", "InfoGainAttributeEval", or "SVMAttributeEval".
search	a string for the search method used by WEKA. This must be one of the strings "BestFirst" or "Ranker".
n	an integer for the number of selected features.
svm.kernel	a string for kernel function of SVM.
svm.scale	a logical vector indicating the variables to be scaled.
svm.path	a character for path to SVMlight binaries (required, if path is unknown by the OS).
svm.options	Optional parameters to SVMlight. For further details see: "How to use" on http://svmlight.joachims.org/ . (e.g.: "-t 2 -g 0.1")
nnet.size	number of units in the hidden layer. Can be zero if there are skip-layer units.
nnet.rang	Initial random weights on [-rang, rang]. Value about 0.5 unless the inputs are large, in which case it should be chosen so that rang * max(x) is about 1.

nnet.decay	parameter for weight decay.
nnet.maxit	maximum number of iterations.
knn.k	number of neighbours considered in function <code>classifyModelKNN</code> .

Details

`classify` employ feature selection method in Weka and diverse classification model in other R packages to perform classification. "Cross Validation" is controlled by parameter "cv"; "Feature Selection" is controlled by parameter "features", "evaluator", "search", and "n"; "Classification Model Building" is controlled by parameter "classifyMethod".

Parameter "evaluator" supports three feature selection methods provided by WEKA: "CfsSubsetEval": Evaluate the worth of a subset of attributes by considering the individual predictive ability of each feature along with the degree of redundancy between them. "ChiSquaredAttributeEval": Evaluate the worth of an attribute by computing the value of the chi-squared statistic with respect to the class. "InfoGainAttributeEval": Evaluate attributes individually by measuring information gain with respect to the class. "SVMAttributeEval": Evaluate the worth of an attribute by using an SVM classifier. Attributes are ranked by the square of the weight assigned by the SVM. Attribute selection for multiclass problems is handled by ranking attributes for each class separately using a one-vs-all method and then "dealing" from the top of each pile to give a final ranking.

Parameter "search" supports three feature subset search methods provided by WEKA: "BestFirst": Searches the space of attribute subsets by greedy hillclimbing augmented with a backtracking facility. Setting the number of consecutive non-improving nodes allowed controls the level of backtracking done. Best first may start with the empty set of attributes and search forward, or start with the full set of attributes and search backward, or start at any point and search in both directions (by considering all possible single attribute additions and deletions at a given point). "Ranker": Ranks attributes by their individual evaluations.

Parameter "classifyMethod" supports multiple classification model: "libsvm": Employ `classifyModelLIBSVM` to perform Support Vector Machine by LibSVM. Package "e1071" is required. "svmLight": Employ `classifyModelSVMLIGHT` to Support Vector Machine by SVMLight. Package "klaR" is required. "NaiveBayes": Employ `classifyModelNB` to perform Naive Bayes classification. Package "klaR" is required. "randomForest": Employ `classifyModelRF` to perform random forest classification. Package "randomForest" is required. "knn": Employ `classifyModelKNN` to perform k Nearest Neighbor algorithm. Package "class" is required. "tree": Employ `classifyModelTree` to perform tree classification. Package "tree" is required. "nnet": Employ `classifyModelNNET` to perform neural net algorithm. Bundle "VR" is required. "rpart": Employ `classifyModelRPART` to perform Recursive Partitioning and Regression Trees. Package "rpart" is required. "ctree": Employ `classifyModelCTREE` to perform Conditional Inference Trees. Package "party" is required. "ctreelibsvm": Employ `classifyModelCTREELIBSVM` to combine Conditional Inference Trees and Support Vector Machine for classification. For each node in the tree, one SVM model will be constructed using train data in this node. Test data will be firstly classified to one node of the tree, and then use corresponding SVM to do classification. Package "party" and "e1071" is required. "bagging": Employ `classifyModelBAG` to perform bagging for classification trees. Package "ipred" is required.

Author(s)

Hong Li

Examples

```

## read positive/negative sequence from files.
tmpfile1 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
tmpfile2 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.neg40.pep")
posSeq = as.matrix(read.csv(tmpfile1,header=FALSE,sep="\t",row.names=1))[,1]
negSeq = as.matrix(read.csv(tmpfile2,header=FALSE,sep="\t",row.names=1))[,1]
seq=c(posSeq,negSeq)
classLable=c(rep("+1",length(posSeq)),rep("-1",length(negSeq)) )
data = data.frame(featureBinary(seq),classLable)

## Use LibSVM and 5-cross-validation to classify.
LIBSVM_CV5 = classify(data,classifyMethod="libsvm",cv=5,
                     svm.kernel="linear",svm.scale=FALSE)
## Features selection is done by invoking "CfsSubsetEval" method in WEKA.
FS_LIBSVM_CV5 = classify(data,classifyMethod="libsvm",cv=5,evaluator="CfsSubsetEval",
                        search="BestFirst",svm.kernel="linear",svm.scale=FALSE)

if(interactive()){

  KNN_CV5 = classify(data,classifyMethod="knn",cv=5,knn.k=1)

  RF_CV5 = classify(data,classifyMethod="randomForest",cv=5)

  TREE_CV5 = classify(data,classifyMethod="tree",cv=5)

  NNET_CV5 = classify(data,classifyMethod="nnet",cv=5)

  RPART_CV5 = classify(data,classifyMethod="rpart",cv=5,evaluator="")

  CTREE_CV5 = classify(data,classifyMethod="ctree",cv=5,evaluator="")

  BAG_CV5 = classify(data,classifyMethod="bagging",cv=5,evaluator="")

}

```

featureAAindex

Feature Coding by physicochemical/biochemical properties in AAindex

Description

Protein sequences are coded based on the physicochemical/biochemical properties of amino acids in AAindex database.

Usage

```

featureAAindex(seq,aaindex.name="all")
featureACI(seq,aaindex.name="all")
featureACF(seq,n,aaindex.name="all")

```

Arguments

seq	a string vector for the protein, DNA, or RNA sequences.
aaindex.name	a string for the name of physicochemical and biochemical properties in AAindex.
n	an integer used as parameter of <code>featureACF</code> ($1 \leq n \leq L-2$, L is the length of sequence). <code>featureACF</code> takes the auto-correlation between fragment $X(1) \dots X(L-m)$ and $X(m+1) \dots X(L)$ ($1 \leq m \leq n$) as features.

Details

`featureAAindex` returns a matrix measuring the physicochemical and biochemical properties of amino acids by AAindex (<http://www.genome.jp/aaindex>). If parameter `aaindex.name="all"`, all properties in AAindex will be considered, and each row represented the features of one sequence coding by a $531 * N$ dimension numeric vector. If parameter `aaindex.name` is a name of property in AAindex, each row represented the features of one sequence coding by a N dimension numeric vector.

`featureACI` returns a matrix with 531 columns, measuring the average cumulative value of AAindex. N is the length of input sequence, and N must be odd. Central residue of all windows are the central residue of input sequence. Each column is the average cumulative AAindex over a sliding window.

`featureACF` returns a matrix with $531 * n$ columns, measuring the Auto-Correlation Function (ACF) of AAindex. If parameter `aaindex.name` is a name of property in AAindex, each row represented the features of one sequence coding by a n dimension numeric vector.

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
  seq = as.matrix(read.csv(file,header=F,sep="\t",row.names=1))[,1]

  AI_all = featureAAindex(seq)
  AI_ANDN920101 = featureAAindex(seq,"ANDN920101")

  ACI_all = featureACI(seq)
  ACI_ANDN920101 = featureACI(seq,"ANDN920101")

  ACF_all_1 = featureACF(seq,1)
  ACF_ANDN920101_3 = featureACF(seq,3,"ANDN920101")
}
```

featureBDNAVIDEO	<i>Feature Coding by DNA/RNA property</i>
------------------	---

Description

DNA/RNA Sequences are coded with DNA or RNA property from B-DNA-VIDEO database.

Usage

```
featureBDNAVIDEO(seq)
```

Arguments

seq a string vector for the protein, DNA, or RNA sequences.

Details

`featureBDNAVIDEO` returns a matrix with 38 columns. Each column is the mean of DNA or RNA property from B-DNA-VIDEO database (<http://wwwmgs.bionet.nsc.ru/mgs/systems/bdnvideo/>).

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "test.rna")
  rna = as.matrix(read.csv(file,header=F,sep="\t"))[,1]

  BDNAVIDEO = featureBDNAVIDEO(rna)
}
```

featureBinary	<i>Feature Coding by Binary Vectors</i>
---------------	---

Description

Sequences are coded by binary vectors.

Usage

```
featureBinary(seq,class=elements("aminoacid"))
```


Arguments

- seq a string vector for the protein, DNA, or RNA sequences.
- class a list for the class of biological properties. It can be produced by [elements](#) and [aaClass](#).

Details

[featureBinary](#) returns a matrix with M*N columns. Each row represented features of one sequence coding by a M*N dimension 0-1 vector. Each base/amino acid is coded as a M dimension vector. For example: amino acid "A" is coded by "0000000000000000001"; base "T" is coded by "0010". The input sequences must have equal length.

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
  seq = as.matrix(read.csv(file,header=F,sep="\t",row.names=1))[,1]

  BIN1 = featureBinary(seq,elements("aminoacid"))
  BIN2 = featureBinary(seq,aaClass("aaE"))
}
```

featureCKSAAP

Feature Coding by k-spaced Aminoacids/Base Pairs

Description

Protein sequences are coded based on the frequency of k-spaced aminoacids/base pairs.

Usage

```
featureCKSAAP(seq,g,class=elements("aminoacid"))
```

Arguments

- seq a string vector for the protein, DNA, or RNA sequences.
- g an integer indicating the distance between two aminoacids/bases ($g \geq 0$).
- class a list for the class of biological properties. It can be produced by [elements](#) and [aaClass](#).

Details

`featureCKSAAP` returns a matrix with $(g+1)*M^2$ columns. Each row represented features of one sequence coding by a $(g+1)*M^2$ dimension numeric vector. Each column is the number of k-spaced aminoacids/base pair ($0 \leq k \leq g$).

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
  seq = as.matrix(read.csv(file,header=F,sep="\t",row.names=1))[,1]

  CKSAAP0 = featureCKSAAP(seq,0,elements("aminoacid"))
  CKSAAP2 = featureCKSAAP(seq,2,elements("aminoacid"))
}
```

featureCTD

Feature Coding by composition, transition and distribution

Description

Sequences are coded based on their composition, transition and distribution.

Usage

```
featureCTD(seq,class=elements("aminoacid"))
```

Arguments

`seq` a string vector for the protein, DNA, or RNA sequences.

`class` a list for the class of biological properties. It can be produced by `elements` and `aaClass`.

Details

`featureCTD` returns a matrix with $M+M*(M-1)/2+M*5$ columns. Each row represented features of one sequence coding by a $M+M*(M-1)/2+M*5$ dimension numeric vector. Three kinds of coding: composition (C), transition (T) and distribution (D) are used. C is the number of amino acids of a particular property (such as hydrophobicity) divided by the total number of amino acids. T characterizes the percent frequency with which amino acids of a particular property is followed by amino acids of a different property. D measures the chain length within which the first, 25, 50, 75 and 100 acids of a particular property is located respectively.

Author(s)

Hong Li

Examples

```

if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.fasta")
  library(Biostrings)
  tmp = readAAStringSet(file)

  proteinSeq = as.character(tmp)

  CTD1 = featureCTD(proteinSeq, class=elements("aminoacid") )
  CTD2 = featureCTD(proteinSeq, class=aaClass("aaV") )
}

```

featureDIPRODB

*Feature Coding by Dinucleotide Property***Description**

Sequences are coded by conformational or thermodynamic dinucleotide property from DiProDB database.

Usage

```
featureDIPRODB(seq, na.type="all", na.strand="all", diprodb.method="all",
  diprodb.type="all")
```

Arguments

seq	a string vector for the protein, DNA, or RNA sequences.
na.type	a string for nucleic acid type. It must be "DNA", "DNA/RNA", "RNA", or "all".
na.strand	a string for strand information. It must be "double", "single", or "all".
diprodb.method	a string for mode of property determination. It can be "experimental", "calculated", or "all".
diprodb.type	a string for property type. It can be "physicochemical", "conformational", "letter based", or "all".

Details

featureDIPRODB returns a matrix with 122 columns. Each column is the mean of conformational or thermodynamic dinucleotide property from DiProDB database (<http://diprodb.fli-leibniz.de>).

Author(s)

Hong Li

Examples

```

if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "test.rna")
  rna = as.matrix(read.csv(file,header=F,sep="\t"))[,1]

  DIPRODB1 = featureDIPRODB(rna)
  DIPRODB2 = featureDIPRODB(rna, na.type="RNA")
}

```

featureDOMAIN

*Feature Coding by domain organization***Description**

Protein sequences are coded based on their domains.

Usage

```

featureDOMAIN(domain)

# Protein Pfam domain prediction
predictPFAM(seq, hmmpfam.path, pfam.path, Evalue=10^-5)

```

Arguments

domain	a list of protein domains. It can be produced by function predictPFAM .
seq	a string vector for the protein, DNA, or RNA sequences.
hmmpfam.path	a string for the path of hmmpfam program in HMMER. hmmpfam will be employed to predict domains using models in Pfam database.
pfam.path	a string for the path of pfam domain database.
Evalue	a numeric value for the E-value cutoff of predicted Pfam domain.

Details

[featureDOMAIN](#) uses Pfam domains to code 0-1 feature vector.

[predictPFAM](#) predict Pfam domains by hmmpfam program. It returns a list, each element is a vector which denotes the domain composition of a protein.

Author(s)

Hong Li

Examples

```
if(interactive()){
}

```

featureEvaluate	<i>Evaluate Different Feature Coding Schemas</i>
-----------------	--

Description

Feature sets from different feature coding schemas are used as input of classification models, and the model performance are given in the result.

Usage

```
featureEvaluate(seq, classLable, fileName, ele.type, featureMethod,
               cv=10, classifyMethod="libsvm",
               group=c("aaH", "aaV", "aaZ", "aaP", "aaF", "aaS", "aaE"), k, g,
               hydro.methods=c("kpm", "SARAH1"), hydro.indexs=c("hydroE", "hydroF", "hydroC"),
               aaindex.name, n, d, w=0.05, start.pos, stop.pos, psiblast.path,
               database.path, hmmpfam.path, pfam.path, Evalue=10^-5,
               na.type="all", na.strand="all", diprodb.method="all", diprodb.type="all",
               svm.kernel="linear", svm.scale=FALSE, svm.path, svm.options="-t 0",
               knn.k=1, nnet.size=2, nnet.rang=0.7, nnet.decay=0, nnet.maxit=100)

```

Arguments

seq	a string vector for the protein, DNA, or RNA sequences.
classLable	a factor or vector for the class lable of sequences in seq.
fileName	a string for the output file name.
ele.type	a string for the type of biological sequence. This must be one of the strings "rnaBase", "dnaBase", "aminoacid" or "aminoacid2".
featureMethod	a string vector for the name of feature coding. The alternative names are "Binary", "CTD", "FragmentComposition", "GapPairComposition", "CKSAAP", "Hydro", "ACH", "AAindex", "ACI", "ACF", "PseudoAAComp", "PSSM", "DOMAIN", "BDNAVIDEO", and "DIPRODB".
classifyMethod	a string for the classification method. This must be one of the strings "libsvm", "svmlight", "NaiveBayes", "randomForest", "knn", "tree", "nnet", "rpart", "ctree", "ctreelibsvm", "bagging".
cv	an integer for the time of cross validation, or a string "leave_one_out" for the jackknife test.
group	a string vector for the group of amino acids. This alternative groups are: "aaH", "aaV", "aaZ", "aaP", "aaF", "aaS" or "aaE".
k	an integer indicating the length of sequence fragment (k>=1).

g	an integer indicating the distance between two aminoacids/bases ($g \geq 0$).
hydro.methods	a string vector for the methods of coding protein hydrophobic effect. This alternative groups are: "kpm" or "SARAH1".
hydro.indexs	a string vector for the methods of coding protein hydrophobic effect. This alternative groups are: "hydroE", "hydroF" or "hydroC".
aaindex.name	a string for the name of physicochemical and biochemical properties in AAindx.
n	an integer used as paramter of featureACF ($1 \leq n \leq L-2$, L is the the length of sequence). featureACF takes the auto-correlation between fragment $X(1) \dots X(L-m)$ and $X(m+1) \dots X(L)$ ($1 \leq m \leq n$) as features.
d	an integer used as paramter of featurePseudoAAComp ($d \geq 1$). Coupling between amino acids $X(i)$ and $X(i+d)$ are considered as features.
w	a numeric value for the weight factor of sequence order effect in featurePseudoAAComp .
start.pos	a integer vector denoting the start position of the fragment window. If it is missing, it is 1 by default.
stop.pos	a integer vector denoting the stop position of the fragment window. If it is missing, it is the length of sequence by default.
psiblast.path	a string for the path of PSI-BLAST program blastpgp. blastpgp will be employed to iteratively search database and generate position-specific scores for each position in the alignment.
database.path	a string for the path of formatted protein database. Database can be formatted by formatdb program.
hmmpfam.path	a string for the path of hmmpfam program in HMMER. hmmpfam will be employed to predict domains using models in Pfam database.
pfam.path	a string for the path of pfam domain database.
Evalue	a numeric value for the E-value cutoff of perdicted Pfam domain.
na.type	a string for nucleic acid type. It must be "DNA", "DNA/RNA", "RNA", or "all".
na.strand	a string for strand information. It must be "double", "single", or "all".
diprodb.method	a string for mode of property determination. It can be "experimental", "calculated", or "all".
diprodb.type	a string for property type. It can be "physicochemical", "conformational", "letter based", or "all".
svm.kernel	a string for kernel function of SVM.
svm.scale	a logical vector indicating the variables to be scaled.
svm.path	a character for path to SVMlight binaries (required, if path is unknown by the OS).
svm.options	Optional parameters to SVMlight. For further details see: "How to use" on http://svmlight.joachims.org/ . (e.g.: "-t 2 -g 0.1")
nnet.size	number of units in the hidden layer. Can be zero if there are skip-layer units.
nnet.rang	Initial random weights on [-rang, rang]. Value about 0.5 unless the inputs are large, in which case it should be chosen so that $\text{rang} * \max(x)$ is about 1.
nnet.decay	parameter for weight decay.
nnet.maxit	maximum number of iterations.
knn.k	number of neighbours considered in function classifyModelKNN .

Details

`featureEvaluate` can test feature coding methods for short peptide, protein, DNA or RNA. It returns a ranked list based on the accuracy of classification result. Each element in the list has three components: "data", "model", and "performance". "data" is a data.frame object, which stores feature matrix and its last column is the class label. "model" is a vector for feature coding method, which contains 6 elements: "Feature_Function", "Feature_Parameter", "Feature_Number", "Model", "Model_Parameter", and "Cross_Validataion". "performance" is a vector for the performance result of classification model, which contains 10 elements: "tp", "tn", "fp", "fn", "prcc", "sn", "sp", "acc", "mcc", "pc".

Author(s)

Hong Li

Examples

```
## read positive/negative sequence from files.
tmpfile1 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
tmpfile2 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.neg40.pep")
posSeq = as.matrix(read.csv(tmpfile1,header=FALSE,sep="\t",row.names=1))[,1]
negSeq = as.matrix(read.csv(tmpfile2,header=FALSE,sep="\t",row.names=1))[,1]
seq=c(posSeq,negSeq)
classLable=c(rep("+1",length(posSeq)),rep("-1",length(negSeq)) )
if(interactive()){
  ## test various feature coding methods.
  ## it may be time consuming.
  fileName = tempfile()
  testFeatureSet = featureEvaluate(seq, classLable, fileName, ele.type="aminoacid",
    featureMethod=c("Binary", "CTD", "FragmentComposition", "GapPairComposition",
    "Hydro"), cv=5, classifyMethod="libsvm",
    group=c("aaH", "aaV", "aaZ", "aaP", "aaF", "aaS", "aaE"), k=3, g=7,
    hydro.methods=c("kpm", "SARAH1"), hydro.indexs=c("hydroE", "hydroF", "hydroC") )
  summary = read.csv(fileName,sep="\t",header=T)
  fix(summary)

  ## Evaluate features from different feature coding functions
  feature.index = 1:5
  tmp <- testFeatureSet[[1]]$data
  colnames(tmp) <- paste(testFeatureSet[[feature.index[1]]]$model["Feature_Function"],testFeatureSet[[feature.index[1]]]$performance["acc"])
  data <- tmp[, -ncol(tmp)]
  for(i in 2:length(feature.index) ){
    tmp <- testFeatureSet[[feature.index[i]]]$data
    colnames(tmp) <- paste(testFeatureSet[[feature.index[i]]]$model["Feature_Function"],testFeatureSet[[feature.index[i]]]$performance["acc"])
    data <- data.frame(data, tmp[, -ncol(tmp)] )
  }
  name <- colnames(data)
  data <- data.frame(data, tmp[, ncol(tmp)] )
  ## feature forward selection by cv_FFS_classify
  ## it is very time consuming.
  combineFeatureResult = fsFFS(data,stop.n=50,classifyMethod="knn",cv=5)
  tmp = sapply(combineFeatureResult,function(x){c(length(x$features),x$performance["acc"])})
}
```

```

plot(tmp[1,],tmp[2,],xlab="featureNumber",ylab="Accuracy",main="result of FFS_KNN",pch=19)
lines(tmp[1,],tmp[2,])

## compare the prediction accuracy based on different feature coding methods and different classification models
## it is very time consuming.
testResult = lapply(c("libsvm", "randomForest", "knn", "tree"),
  function(x){
    tmp = featureEvaluate(seq, classLable, fileName = tempfile(),
      ele.type="aminoacid", featureMethod=c("Binary", "CTD", "FragmentComposition",
        "GapPairComposition", "Hydro"), cv=5, classifyMethod=x,
      group=c("aaH", "aaV", "aaZ", "aaP", "aaF", "aaS", "aaE"), k=3, g=7,
      hydro.methods=c("kpm", "SARAH1"), hydro.indexs=c("hydroE", "hydroF", "hydroC") );
    sapply(tmp,function(y){c(y$model[["Feature_Function"]], y$model[["Feature_Parameter"]], y$model[["Model_Type"]])})
  })
tmpFeature = as.factor(c(sapply(testResult,function(x){apply(x[1:2,],2,function(y){paste(y,collapse="; ")}))));
tmpModel = as.factor(c(sapply(testResult,function(x){x[3,]})))
tmp1 = data.frame(as.integer(tmpFeature), as.integer(tmpModel), as.numeric(c(sapply(testResult,function(x){x[4,]}))))
require(scatterplot3d)
s3d=scatterplot3d(tmp1,color=c("red","blue","green","yellow")[tmp1[,2]],pch=19,
  xlab="Feature Coding", ylab="Classification Model",
  zlab="Accuracy under 5-fold cross validation",lab=c(10,6,7),
  y.ticklabs=c("",as.character(sort(unique(tmpModel))),""))
}

```

featureFragmentComposition

Feature Coding by the composition of k-mer fragments

Description

Sequences are coded based on the frequency of k-mer sequence fragments.

Usage

```
featureFragmentComposition(seq,k,class=elements("aminoacid"))
```

Arguments

seq	a string vector for the protein, DNA, or RNA sequences.
k	an integer indicating the length of sequence fragment ($k \geq 1$).
class	a list for the class of biological properties. It can be produced by elements and aaClass .

Details

[featureFragmentComposition](#) returns a matrix with $M \times k$ columns. Each row represented features of one sequence coding by a $M \times k$ dimension numeric vector. Each column is the frequency of k-mer sequence fragment.

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
  seq = as.matrix(read.csv(file,header=F,sep="\t",row.names=1))[,1]

  FC2 = featureFragmentComposition(seq,2,aaClass("aaS"))
  FC3 = featureFragmentComposition(seq,3,aaClass("aaS"))
}
```

`featureGapPairComposition`*Feature Coding by g-spaced aminoacids/bases pairs*

Description

Sequences are coded based on the frequency of g-spaced aminoacids/bases pairs.

Usage

```
featureGapPairComposition(seq,g,class=elements("aminoacid"))
```

Arguments

<code>seq</code>	a string vector for the protein, DNA, or RNA sequences.
<code>g</code>	an integer indicating the distance between two aminoacids/bases ($g \geq 0$).
<code>class</code>	a list for the class of biological properties. It can be produced by <code>elements</code> and <code>aaClass</code> .

Details

`featureGapPairComposition` returns a matrix with M^2 columns. Each row represented features of one sequence coding by a M^2 dimension numeric vector. Each column is the frequency of g-spaced aminoacids/bases pair. `featureFragmentComposition(seq,2)` is same with `featureGapPairComposition(seq,0)`.

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
  seq = as.matrix(read.csv(file,header=F,sep="\t",row.names=1))[,1]

  GPC0 = featureGapPairComposition(seq,0,elements("aminoacid"))
  GPC2 = featureGapPairComposition(seq,2,elements("aminoacid"))
}
```

featureHydro

Feature Coding by hydrophobicity

Description

Protein sequences are coded based on their hydrophobicity.

Usage

```
featureHydro(seq,hydro.method="SARAH1")
featureACH(seq,hydro.index="hydroE")
```

Arguments

seq	a string vector for the protein, DNA, or RNA sequences.
hydro.method	a string for the method of coding protein hydrophobic effect. This must be one of the strings "kpm" or "SARAH1".
hydro.index	a string for the method of coding protein hydrophobic effect. This must be one of the strings "hydroE", "hydroF" or "hydroC".

Details

[featureHydro](#) returns a matrix measuring the hydrophobic effect. Parameter "hydro.method" supported following coding methods: "kpm": use a numeral to indicating the hydrophobic effect of amino acid. Each sequence is coded by a N dimension numeric vector. "SARAH1": use a 5 dimension 0-1 vector to indicating the hydrophobic effect of amino acid. Each sequence is coded by a 5*N dimension 0-1 vector.

[featureACH](#) returns a matrix with $(N-1)/2$ columns. N is the length of input sequence, and is N must be odd. Central residue of all windows are the central residue of input sequence. Each column is the average cumulative hydrophobicity over a sliding window.

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
  seq = as.matrix(read.csv(file,header=F,sep="\t",row.names=1))[,1]

  H1 = featureHydro(seq,"kpm")
  H2 = featureHydro(seq,"SARAH1")

  H3 = featureACH(seq,hydro.index="hydroE")
  H3 = featureACH(seq,hydro.index="hydroF")
  H3 = featureACH(seq,hydro.index="hydroC")
}
```

featurePseudoAAComp *Feature Coding by Pseudo Amino Acid Composition*

Description

Protein sequences are coded by pseudo amino acid composition.

Usage

```
featurePseudoAAComp(seq,d,w=0.05)
```

Arguments

seq	a string vector for the protein, DNA, or RNA sequences.
d	an integer used as parameter of featurePseudoAAComp ($d \geq 1$). Coupling between amino acids $X(i)$ and $X(i+d)$ are considered as features.
w	a numeric value for the weight factor of sequence order effect in featurePseudoAAComp .

Details

[featurePseudoAAComp](#) returns a matrix representing the pseudo amino acid composition. Each row represented features of one sequence coding by a $20+d$ dimension numeric vector. The first 20 features indicates the composition of 20 amino acids. The last d features indicates the coupling between amino acids $X(i)$ and $X(i+d)$. Coupling value is calculated by hydrophobicity, hydrophilicity and mass of amino acids.

Author(s)

Hong Li

Examples

```

if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
  seq = as.matrix(read.csv(file,header=F,sep="\t",row.names=1))[,1]

  PAC4 = featurePseudoAAComp(seq,4)
}

```

featurePSSM

*Feature Coding***Description**

A set of functions for extract features from biological sequences, and coding features by numeric vector.

Usage

```
featurePSSM(seq, start.pos, stop.pos, psiblast.path, database.path)
```

Arguments

seq	a string vector for the protein, DNA, or RNA sequences.
start.pos	a integer vector denoting the start position of the fragment window.
stop.pos	a integer vector denoting the stop position of the fragment window.
psiblast.path	a string for the path of blastpgp program. blastpgp will be employed to do PSI-BLAST and get Position-Specific Scoring Matrix.
database.path	a string for the path of a formatted reference database. Database can be formatted by "formatdb" program.

Details

[featurePSSM](#) returns a matrix with $20*N+N$ columns. Each row represented features of one sequence coding by a $20*N+N$ dimension numeric vector generated by PSI-BLAST. It contains two kinds of fatures: normalized position-specific score of PSSM (Position-Specific Scoring Matrix), Shannon entropy for each position of WOP (weighted observed percentages). Program PSI-BLAST and formatted NCBI non-redundant protein database are needed.

Author(s)

Hong Li

Examples

```

if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.fasta")
  tmp = readAAStringSet(file)
  proteinSeq = as.character(tmp)

  ## Need "blastpgp" program and a formatted database. Database can be formatted by "formatdb" program.
  PSSM1 = featurePSSM(proteinSeq[1:2], start.pos=rep(1,2), stop.pos=rep(10,2), psiblast.path="blastpgp", database
}

```

featureSSC

*Feature Coding by secondary structure***Description**

It is suitable for peptides with odd residues and the central residue has important role.

Usage

```

featureSSC(secondaryStructure, confidenceScore)

# secondary structure from DSSP database
getDSSP(pdb)
# Protein secondary structure prediction
predictPROTEUS(seq,proteus2.organism="euk")

```

Arguments

secondaryStructure
a string vector for the protein secondary structure. It is consisted of three kinds of secondary structures: H = Helix, E = Beta Strand, C = Coil.

confidenceScore
a string vector for the confidence score of secondary structure prediction (0-9, 0 = low, 9 = high).

pdb
a string vector for the name of pdb structure. (e.g. "43ca")

seq
a string vector for the protein, DNA, or RNA sequences.

proteus2.organism
a string for the organism of proteus2 program. This must be one of the strings "gram-", "gram+", "euk".

Details

`featureSSC` codes for the secondary structure of the central residue of peptides. It is suitable for peptides with odd residues and the central residue has important role.

`getDSSP` returns a vector of secondary structure extracted from DSSP database (<http://swift.cmbi.ru.nl/gv/dssp/>).

`predictPROTEUS` predicts secondary structure based on protein sequence using following methods : "PROTEUS2", "PSIPRED", "JNET", "TRANSSEC", "JURY-OF-EXPERTS PREDICTION". Parameter "proteus2.organism" can be "gram-" for "Gram negative prokaryote", "gram+" for "Gram positive prokaryote", "euk" for "Eukaryote". It returns.....

Author(s)

Hong Li

Examples

```
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.fasta")
  tmp = readAAStringSet(file)
  proteinSeq = as.character(tmp)

  DSSP1 = getDSSP(c("1081", "43ca"))
  DSSP2 = getDSSP(c("1081", "43ca", "aaaa"))

  ## Predict protein secondary structure
  PROTEUS = predictPROTEUS(proteinSeq[1:2], proteus2.organism="euk")

  ## Use general feature coding functions to codes protein secondary structure
  secondaryStructure = sapply(PROTEUS, function(x){paste(x[["PROTEUS2"]]$SecondaryStructure, collapse="")})
  confidenceScore = sapply(PROTEUS, function(x){paste(x[["PROTEUS2"]]$ConfidenceScore, collapse="")})
  SSCTD = featureCTD(secondaryStructure, class=list("H"="H", "E"="E", "C"="C"))
  # Codes for peptides which have equal length and their central residues are important
  secondaryStructure = sapply(PROTEUS, function(x){sub.seq(paste(x[["PROTEUS2"]]$SecondaryStructure, collapse=""))})
  confidenceScore = sapply(PROTEUS, function(x){sub.seq(paste(x[["PROTEUS2"]]$ConfidenceScore, collapse=""), 1, 11)})

  SS1 = featureSSC(secondaryStructure, confidenceScore)
}
```

hr

Homolog Reduction

Description

Filter homolog sequences by sequence similarity.

Usage

```
hr(seq, method, identity, cdhit.path)

cdhitHR(seq, identity=0.3, cdhit.path)
aligndisHR(seq, identity=0.6)
distance(seq1, seq2)

getTrain(seqfile, posfile, aa, w, identity, balance=T)
getNegSite(posSite, seq, aa)
```

Arguments

seq	a list with one element for each protein/gene sequence. The elements are in two parts, one the description ("desc") and the second is a character string of the biological sequence ("seq").
identity	a numeric value ranged from 0 to 1. It is used as a maximum identity cutoff among input sequences.
method	a string for the method of homolog reduction. This must be one of the strings "cdhit" or "aligndis".
cdhit.path	a string for the path of cdhit program directory. eg: "/people/hongli/cd-hit". It is necessary when method="cdhit".
seq1	a string for the protein or gene sequence.
seq2	a string for the protein or gene sequence. seq1 and seq2 must have same length.
seqfile	a string for the name of FASTA file.
posfile	a string for the name of file which contains the positive site dataset. It has two columns: 1st column is the protein name; 2st column is the positive site. Protein name should be consistent with the name used in seqfile.
aa	a character for the interested amino acid. eg: "C".
w	an integer for the window size of flanking peptide sequence. Window size is $2*w+1$, and the central residues are the positive sites in posfile.
balance	a logical value indicating whether negative sites will be random selected to have the same number with positive sites.
posSite	a string vector for the positive sites. It is consisted of protein description and positive site, eg: "P278168:952".

Details

hr employs [cdhitHR](#) and [aligndisHR](#) to filter homolog sequences. It supported following methods:

"cdhit": Use cd-hit program to quickly filter sequences by given identity. It is designed to filter full-length protein or gene sequences. "formatdb" and "blastall" are required for running cd-hit program. (<http://www.bioinformatics.org/download.php/cd-hit/cd-hit-2007-0131.tar.gz> or <http://www.bioinformatics.org/download.php/cd-hit/cd-hit-2007-0131-win32.tar.gz>)

"aligndis": Use the number of different residues to measure the identity between two sequences. It is designed to filter aligned sequences with equal length.

[getTrain](#) extract $2*w+1$ flanking peptides of positive sites and filter homolog sequences. Negative sites are non-positive sites in the same proteins.

[distance](#) calculate the number of positions with different residues between two sequences.

Value

hr return a list of reduced sequences.

Author(s)

Hong Li

Examples

```

distance("AABD", "ACBD")
distance("AABD", "ECBD")
if(interactive()){
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.fasta")
  library(Biostrings)
  seq = as.character(readAAStringSet(file))
  ## Homolog reduction of whole-length sequence by cd-hit
  # need cd-hit program;
  reducSeq50 = hr(seq, method="cdhit", identity=0.5, cdhit.path="/people/hongli/cd-hit")

  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.site")
  tmp = as.matrix(read.csv(file, sep="\t", header=F))
  logical = apply(tmp, 1, function(x){ l=nchar(seq[x[1]]); (l>=as.numeric(x[2])+7 & as.numeric(x[2])-7>0) })
  fragment = sub.seq(seq[tmp[logical,1]], as.numeric(tmp[logical,2])-7, as.numeric(tmp[logical,2])+7)
  ## Homolog reduction of short sequence fragment
  # It may be slow.
  reducSeq = hr(fragment, method="aligndis", identity=0.4)

  ## produce train set based on given positive sites and fasta sequences.
  file = file.path(path.package("BioSeqClass"), "example", "acetylation_K.fasta")
  posfile = file.path(path.package("BioSeqClass"), "example", "acetylation_K.site")
  ## "getTrain" integrate negative set construction and homolog reduction. It is designed for site level training d
  # It may be very slow.
  data = getTrain(file, posfile, aa="K", w=7, identity=0.4)
}

```

 model

Classification Models

Description

These functions build various classification models.

Usage

```

classifyModelLIBSVM(train, svm.kernel="linear", svm.scale=FALSE)
classifyModelSVMLIGHT(train, svm.path, svm.options="-t 0")
classifyModelNB(train)
classifyModelRF(train)
classifyModelKNN(train, test, knn.k=1)
classifyModelTree(train)
classifyModelNNET(train, nnet.size=2, nnet.rang=0.7, nnet.decay=0, nnet.maxit=100)
classifyModelRPART(train)
classifyModelCTREE(train)
classifyModelCTREELIBSVM(train, test, svm.kernel="linear", svm.scale=FALSE)
classifyModelBAG(train)

```


Arguments

<code>train</code>	a data frame including the feature matrix and class label. The last column is a vector of class label comprising of "-1" or "+1"; Other columns are features.
<code>svm.kernel</code>	a string for kernel function of SVM.
<code>svm.scale</code>	a logical vector indicating the variables to be scaled.
<code>svm.path</code>	a character for path to SVMlight binaries (required, if path is unknown by the OS).
<code>svm.options</code>	Optional parameters to SVMlight. For further details see: "How to use" on http://svmlight.joachims.org/ . (e.g.: "-t 2 -g 0.1")
<code>nnet.size</code>	number of units in the hidden layer. Can be zero if there are skip-layer units.
<code>nnet.rang</code>	Initial random weights on [-rang, rang]. Value about 0.5 unless the inputs are large, in which case it should be chosen so that rang * max(x) is about 1.
<code>nnet.decay</code>	parameter for weight decay.
<code>nnet.maxit</code>	maximum number of iterations.
<code>knn.k</code>	number of neighbours considered in function <code>classifyModelKNN</code> .
<code>test</code>	a data frame including the feature matrix and class label. The last column is a vector of class label comprising of "-1" or "+1"; Other columns are features.

Details

`classifyModelLIBSVM` builds support vector machine model by LibSVM. R package "e1071" is needed.

`classifyModelSVMLIGHT` builds support vector machine model by SVMlight. R package "klaR" is needed.

`classifyModelNB` builds naive bayes model. R package "klaR" is needed.

`classifyModelRF` builds random forest model. R package "randomForest" is needed.

`classifyModelKNN` builds k-nearest neighbor model. R package "class" is needed.

`classifyModelTree` builds tree model. R package "class" is needed.

`classifyModelRPART` builds recursive partitioning trees model. R package "rpart" is needed.

`classifyModelCTREE` builds conditional inference trees model. R package "party" is needed.

`classifyModelCTREELIBSVM` combines conditional inference trees and support vector machine. R package "party" and "e1071" is needed.

`classifyModelBAG` uses bagging method. R package "ipred" is needed.

Author(s)

Hong Li

Examples

```

## read positive/negative sequence from files.
tmpfile1 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
tmpfile2 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.neg40.pep")
posSeq = as.matrix(read.csv(tmpfile1,header=FALSE,sep="\t",row.names=1))[,1]
negSeq = as.matrix(read.csv(tmpfile2,header=FALSE,sep="\t",row.names=1))[,1]
data = data.frame(rbind(featureBinary(posSeq,elements("aminoacid")),
  featureBinary(negSeq,elements("aminoacid")) ),
  class=c(rep("+1",length(posSeq)),
  rep("-1",length(negSeq))) )

## sample train and test data
tmp = c(sample(1:length(posSeq),length(posSeq)*0.8),
  sample(length(posSeq)+(1:length(negSeq)),length(negSeq)*0.8))
train = data[tmp,]
test = data[-tmp,]

## Build classification model using training data
model1 = classifyModelLIBSVM(train,svm.kernel="linear",svm.scale=FALSE)
## Predict test data by classification model
testClass = predict(model1, test[,-ncol(test)])

```

performance

Performance Evaluation

Description

Evaluate the performance of classification model.

Usage

```
performance(predictClass, factClass)
```

Arguments

`predictClass` a factor of predicted classifications of training set, comprising of "-1" or "+1".
`factClass` a vector of true classifications of training set, comprising of "-1" or "+1".

Details

`performance` evaluates the performance of classification model. It cacluates: tp (true positive), tn(ture negative), fp(false positive), fn(false negative), prc(precision), sn(sensitivity), sp(specificity), acc(accuracy), mcc(Matthews Correlation Coefficient), pc(Performance Coefficient).

Author(s)

Hong Li

Examples

```

## read positive/negative sequence from files.
tmpfile1 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
tmpfile2 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.neg40.pep")
posSeq = as.matrix(read.csv(tmpfile1,header=FALSE,sep="\t",row.names=1))[,1]
negSeq = as.matrix(read.csv(tmpfile2,header=FALSE,sep="\t",row.names=1))[,1]
data = data.frame(rbind(featureBinary(posSeq,elements("aminoacid")),
  featureBinary(negSeq,elements("aminoacid")) ),
  class=c(rep("+1",length(posSeq)),
  rep("-1",length(negSeq))) )

## sample train and test data
tmp = c(sample(1:length(posSeq),length(posSeq)*0.8),
  sample(length(posSeq)+(1:length(negSeq)),length(negSeq)*0.8))
train = data[tmp,]
test = data[-tmp,]

## Build classification model using training data
model1 = classifyModelLIBSVM(train,svm.kernel="linear",svm.scale=FALSE)
## Predict test data by classification model
testClass = predict(model1, test[,-ncol(test)])
## Evaluate the performance of classification model
performance(testClass,test[,ncol(test)])

```

selectFFS

*feature forward selection***Description**

feature forward selection.

Usage

```
selectFFS(data, accCutoff, stop.n,
  classifyMethod="knn",cv=10)
```

Arguments

data	a data frame including the feature matrix and class label. The last column is a vector of class label comprising of "-1" or "+1"; Other columns are features.
accCutoff	a numeric indicating the minimum difference of accuracy between two models in selectFFS . Feature subsets will stop increasing when the difference of accuracy is smaller than accCutoff.
stop.n	number of selected features by selectFFS .
classifyMethod	a string for the classification method. This must be one of the strings "libsvm", "svmlight", "NaiveBayes", "randomForest", "knn", "tree", "nnet", "rpart", "ctree", "ctreelibsvm", "bagging".
cv	an integer for the time of cross validation, or a string "leave_one_out" for the jackknife test.

Details

`selectFFS` uses FFS (Feature Forward Selection) method to increase feature, and use NNA (Near-east Neighbor Analysis) to evaluate the performance of feature subset. Two conditions are used to stop feature increasing: control the difference of accuracy between two models; control the number of selected features by Parameter "stop.n".

Author(s)

Hong Li

Examples

```
## read positive/negative sequence from files.
tmpfile1 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.pos40.pep")
tmpfile2 = file.path(path.package("BioSeqClass"), "example", "acetylation_K.neg40.pep")
posSeq = as.matrix(read.csv(tmpfile1,header=FALSE,sep="\t",row.names=1))[,1]
negSeq = as.matrix(read.csv(tmpfile2,header=FALSE,sep="\t",row.names=1))[,1]
seq=c(posSeq,negSeq)
classLable=c(rep("+1",length(posSeq)),rep("-1",length(negSeq)) )
data = data.frame(featureBinary(seq),classLable)

if(interactive()){
  ## Use KNN to evaluate the performance of feature subset,
  ## and use Feature Forward Selection method to increase feature.
  # If the difference of accuracy between two models is less than 0.01, feature
  # selection will stop.
  FFS_NNA_CV5 = selectFFS(data,accCutoff=0.01,classifyMethod="knn",cv=5)
  # If 20 features have been selected, feature selection will stop.
  FFS_NNA_CV5 = selectFFS(data,stop.n=3,classifyMethod="knn",cv=5)
  # If any one condition is satisfied, feature selection will stop.
  FFS_NNA_CV5 = selectFFS(data,accCutoff=0.001,stop.n=100,classifyMethod="knn",cv=5)
}
```

selectWeka

Feature Selection by Weka

Description

feature selection by Weka.

Usage

```
selectWeka(train, evaluator="CfsSubsetEval", search="BestFirst", n)
```

Arguments

train	a data frame including the feature matrix and class label of training set.
evaluator	a string for the feature selection method used by WEKA. This must be one of the strings "CfsSubsetEval", "ChiSquaredAttributeEval", "InfoGainAttributeEval", or "SVMAttributeEval".
search	a string for the search method used by WEKA. This must be one of the strings "BestFirst" or "Ranker".
n	an integer for the number of selected features.

Details

Parameter "evaluator" supports three feature selection methods provided by WEKA: "CfsSubsetEval": Evaluate the worth of a subset of attributes by considering the individual predictive ability of each feature along with the degree of redundancy between them. "ChiSquaredAttributeEval": Evaluate the worth of an attribute by computing the value of the chi-squared statistic with respect to the class. "InfoGainAttributeEval": Evaluate attributes individually by measuring information gain with respect to the class. "SVMAttributeEval": Evaluate the worth of an attribute by using an SVM classifier. Attributes are ranked by the square of the weight assigned by the SVM. Attribute selection for multiclass problems is handled by ranking attributes for each class separately using a one-vs-all method and then "dealing" from the top of each pile to give a final ranking.

Parameter "search" supports three feature subset search methods provided by WEKA: "BestFirst": Searches the space of attribute subsets by greedy hillclimbing augmented with a backtracking facility. Setting the number of consecutive non-improving nodes allowed controls the level of backtracking done. Best first may start with the empty set of attributes and search forward, or start with the full set of attributes and search backward, or start at any point and search in both directions (by considering all possible single attribute additions and deletions at a given point). "Ranker": Ranks attributes by their individual evaluations.

Author(s)

Hong Li

 zzz

Load packages and data

Description

This functions load depended R packages and imports default data into global "options".

Usage

```
.onLoad(libname, pkgname)
```

Arguments

libname	a character string giving the library directory where the package defining the namespace was found.
pkgname	a character string giving the name of the package.

Details

After loading, loadNamespace looks for a hook function named .onLoad and runs it before sealing the namespace and processing exports.

Author(s)

Hong Li

Index

.callPerl, 3
.callPerl (basic), 2
.onLoad (zzz), 29
.pathPerl, 3
.pathPerl (basic), 2

aa.index, 3
aa.index (basic), 2
aaClass, 2, 3, 9, 10, 16, 17
aaClass (basic), 2
aligndisHR, 23
aligndisHR (hr), 22

basic, 2

cdhitHR, 23
cdhitHR (hr), 22
classify, 4, 5
classifyModelBAG, 5, 25
classifyModelBAG (model), 24
classifyModelCTREE, 5, 25
classifyModelCTREE (model), 24
classifyModelCTREELIBSVM, 5, 25
classifyModelCTREELIBSVM (model), 24
classifyModelKNN, 5, 14, 25
classifyModelKNN (model), 24
classifyModelLIBSVM, 5, 25
classifyModelLIBSVM (model), 24
classifyModelNB, 5, 25
classifyModelNB (model), 24
classifyModelNNET, 5
classifyModelNNET (model), 24
classifyModelRF, 5, 25
classifyModelRF (model), 24
classifyModelRPART, 5, 25
classifyModelRPART (model), 24
classifyModelSVMLIGHT, 5, 25
classifyModelSVMLIGHT (model), 24
classifyModelTree, 5, 25
classifyModelTree (model), 24

DiProDB, 3
DiProDB (basic), 2
distance, 23
distance (hr), 22
dssp.ss, 3
dssp.ss (basic), 2

elements, 2, 3, 9, 10, 16, 17
elements (basic), 2

featureAAindex, 6, 7
featureACF, 7, 14
featureACF (featureAAindex), 6
featureACH, 18
featureACH (featureHydro), 18
featureACI, 7
featureACI (featureAAindex), 6
featureBDNAVIDEO, 8, 8
featureBinary, 8, 9
featureCKSAAP, 9, 10
featureCTD, 10, 10
featureDIPRODB, 11, 11
featureDOMAIN, 12, 12
featureEvaluate, 13, 15
featureFragmentComposition, 16, 16
featureGapPairComposition, 17, 17
featureHydro, 18, 18
featurePseudoAAComp, 14, 19, 19
featurePSSM, 20, 20
featureSSC, 21, 21

getDSSP, 21
getDSSP (featureSSC), 21
getNegSite (hr), 22
getTrain, 23
getTrain (hr), 22

hr, 22, 23

model, 24

performance, [26](#), [26](#)
predictPFAM, [12](#)
predictPFAM (featureDOMAIN), [12](#)
predictPROTEUS, [22](#)
predictPROTEUS (featureSSC), [21](#)
PROPERTY, [3](#)
PROPERTY (basic), [2](#)
pwm, [3](#)
pwm (basic), [2](#)

selectFFS, [27](#), [27](#), [28](#)
selectWeka, [28](#)
sub.seq (basic), [2](#)

zzz, [29](#)