

Package ‘hddplot’

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Type Package

Title Use known groups in high-dimensional data to derive scores for plots

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Depends MASS

Description Cross-validated linear discriminant calculations determine the optimum number of features. Test and training scores from successive cross-validation steps determine, via a principal components calculation, a low-dimensional global space onto which test scores are projected, in order to plot them. Further functions are included that serve didactic purposes.

License GPL (>= 2)

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Description

Cross-validated linear discriminant calculations determine the optimum number of features. Test and training scores from successive cross-validation steps determine, via a principal components calculation, a low-dimensional global space onto which test scores are projected, in order to plot them. Further functions are included for didactic purposes.

Details

Package: hddplot
 Type: Package
 Version: 1.0
 Date: 2006-01-09
 License: GPL Version 2 or later.

The most important functions are

`cvdisc`: Determine variation in cross-validated accuracy with number of features

`cvscores`: For a specific choice of number of features, determine scores that can be used for plotting

Note also `scoreplot` (plot scores), `qqthin` (qqplots, designed to avoid generating large files when there are many points), and functions that are intended to illustrate issues that arise in the plotting of expression array and other high-dimensional data

Author(s)

John Maindonald

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References

Maindonald, J.H. and Burden, C.J., 2005. Selection bias in plots of microarray or other data that have been sampled from a high-dimensional space. In R. May and A.J. Roberts, eds., *Proceedings of 12th Computational Techniques and Applications Conference CTAC-2004*, volume 46, pp. C59–C74.

<http://anziamj.austms.org.au/V46/CTAC2004/Main> [March 15, 2005].

See Also

[cvscores](#), [scoreplot](#)

Examples

```
## Use first 500 rows (expression values) of Golub, for demonstration.
data(Golub)
data(golubInfo)
attach(golubInfo)
miniG.BM <- Golub[1:500, BM.PB=="BM"] # 1st 500 rows only
cancer.BM <- cancer[BM.PB=="BM"]
miniG.cv <- cvdisc(miniG.BM, cl=cancer.BM, nfeatures=1:10,
                  nfold=c(10,4))
miniG.scores <- cvscores(cvlist=miniG.cv, nfeatures=4, cl.other=NULL)
subsetB <- (cancer=="allB") & (tissue.mf %in% c("BM:f", "BM:m", "PB:m"))
tissue.mfB <- tissue.mf[subsetB, drop=TRUE]
scoreplot(scorelist=miniG.scores, cl.circle=tissue.mfB,
          circle=tissue.mfB%in%c("BM:f", "BM:m"),
          params=list(circle=list(col=c("cyan", "gray"))),
          prefix="BM samples -")
detach(golubInfo)
## Not run: demo(biasedPlots)
## Not run: demo(CVscoreplot)
```

accTrainTest

Two subsets of data each take in turn the role of test set

Description

A division of data is specified, for use of linear discriminant analysis, into a training and test set. Feature selection and model fitting is formed, first with I/II as training/test, then with II/I as training/test

Usage

```
accTrainTest(x = Golub.BM, cl = cancer.BM, traintest = gp.id, nfeatures = NULL, print.acc = FALSE)
```

Arguments

x	Matrix; rows are features, and columns are observations ('samples')
cl	Factor that classifies columns into groups that will classify the data for purposes of discriminant calculations
traintest	Values that specify a division of observations into two groups. In the first pass (fold), one to be training and the other test, with the roles then reversed in a second pass or fold.
nfeatures	integer: numbers of features for which calculations are required
print.acc	logical: should accuracies be printed?

Value

sub1.2	row numbers of features, by order of values of the group separation measure, for the first subset (I) of the x
acc1.2	accuracies, with I as training set and II as test
sub2.1	row numbers of features, by order of values of the group separation measure, for the second subset (II) of the x
acc2.1	accuracies, with II as training set and I as test

Author(s)

John Maindonald

Examples

```

mat <- matrix(rnorm(1000), ncol=20)
cl <- factor(rep(1:3, c(7,9,4)))
gp.id <- divideUp(cl, nset=2)
accTrainTest(x=mat, cl=cl, traintest=gp.id,
             nfeatures=1:16, print.acc=TRUE)

## The function is currently defined as
function(x=Golub.BM, cl=cancer.BM, traintest=gp.id,
        nfeatures=NULL, print.acc=FALSE){
  traintest <- factor(traintest)
  train <- traintest==levels(traintest)[1]
  testset <- traintest==levels(traintest)[2]
  cl1 <- cl[train]
  cl2 <- cl[testset]
  ng1 <- length(cl1)
  ng2 <- length(cl2)
  maxg <- max(c(ng1-length(unique(cl1))-2,
               ng2-length(unique(cl2))-2))
  if(is.null(nfeatures)){
    max.features <- maxg
    nfeatures <- 1:max.features
  } else
  {
    if(max(nfeatures)>maxg)nfeatures <- nfeatures[nfeatures<=maxg]
    max.features <- max(nfeatures)
  }
  ord1 <- orderFeatures(x, cl, subset=train)[1:max.features]
  ord2 <- orderFeatures(x, cl, subset=testset)[1:max.features]
  ord <- unique(c(ord1, ord2))
  sub1 <- match(ord1, ord)
  sub2 <- match(ord2, ord)
  df1 <- data.frame(t(x[ord, train]))
  df2 <- data.frame(t(x[ord, testset]))
  acc1 <- acc2 <- numeric(max(nfeatures))
  for(i in nfeatures){
    cat(paste(i, ":", sep=""))
    df1.llda <- lda(df1[, sub1[1:i], drop=FALSE], cl1)
  }
}

```

```

    hat2 <- predict(df1.lda, newdata=df2[, sub1[1:i], drop=FALSE])$class
    tab <- table(hat2, cl2)
    acc1[i] <- sum(tab[row(tab)==col(tab)])/sum(tab)
    df2.lda <- lda(df2[, sub2[1:i], drop=FALSE], cl2)
    hat1 <- predict(df2.lda, newdata=df1[, sub2[1:i], drop=FALSE])$class
    tab <- table(hat1, cl1)
    acc2[i] <- sum(tab[row(tab)==col(tab)])/sum(tab)
  }
  cat("\n")
  if(print.acc){
    print(round(acc1,2))
    print(round(acc2,2))
  }
  maxacc1 <- max(acc1)
  maxacc2 <- max(acc2)
  sub1 <- match(maxacc1, acc1)
  sub2 <- match(maxacc2, acc2)
  nextacc1 <- max(acc1[acc1<1])
  nextacc2 <- max(acc1[acc1<2])
  lower1 <- maxacc1-sqrt(nextacc1*(1-nextacc1)/ng1)
  lower2 <- maxacc2-sqrt(nextacc2*(1-nextacc2)/ng2)
  lsub1 <- min((1:ng1)[acc1>lower1])
  lsub2 <- min((1:ng2)[acc2>lower2])
  lower <- c("Best accuracy, less 1SD ",
            paste(paste(round(c(lower1, lower2),2), c(lsub1, lsub2),
                    sep=" (", " features) ", sep=")"))
  best <- c("Best accuracy",
           paste(paste(round(c(maxacc1, maxacc2),2), c(sub1, sub2),
                    sep=" (", " features)", sep=")"))
  acc.df <- cbind(lower, best)
  dimnames(acc.df) <- list(c("Training/test split",
                            "I (training) / II (test) ",
                            "II (training) / I (test)  "),c("", ""))
  print(acc.df, quote=FALSE)
  invisible(list(sub1.2=ord1, acc1.2=acc1, sub2.1=ord2, acc2.1=acc2))
}

```

aovFbyrow

calculate aov F-statistic for each row of a matrix

Description

Returns on aov F-statistic for each row of x

Usage

```
aovFbyrow(x = Golub, cl = golub.info$cancer)
```

Arguments

x	features by observations matrix
c1	fact that classifies the values in each row

Details

This uses the functions `qr()` and `qr.qty()` for the main part of the calculation, for handling the calculations efficiently

Value

one F-statistic for each row of x

Author(s)

John Maindonald

See Also

See also [orderFeatures](#)

Examples

```
mat <- matrix(rnorm(1000), ncol=20)
c1 <- factor(rep(1:3, c(7,9,4)))
Fstats <- aovFbyrow(x = mat, c1 = c1)

## The function is currently defined as
aovFbyrow <-
function(x=matrix(rnorm(1000), ncol=20),
         cl=factor(rep(1:3, c(7,9,4)))){
  y <- t(x)
  qr.obj <- qr(model.matrix(~c1))
  qty.obj <- qr.qty(qr.obj,y)
  tab <- table(factor(c1))
  dfb <- length(tab)-1
  dfw <- sum(tab)-dfb-1
  ms.between <- apply(qty.obj[2:(dfb+1)], , drop=FALSE]^2, 2, sum)/dfb
  ms.within <- apply(qty.obj[-(1:(dfb+1))], , drop=FALSE]^2, 2, sum)/dfw
  Fstat <- ms.between/ms.within
}
```

cvdisc *Cross-validated accuracy, in linear discriminant calculations*

Description

Determine cross-validated accuracy, for each of a number of features in a specified range, with feature selection repeated at each step of the cross-validation.

Usage

```
cvdisc(x = GolubB, cl = tissue.mfB, nfold = c(10,1), test = "f", nfeatures = 2, seed = 31, funda = lda, pr
```

Arguments

x	Matrix; rows are features, and columns are observations ('samples')
cl	Factor that classifies columns into groups
nfold	Number of folds for the cross-validation. Optionally, a second number specifies the number of repeats of the cross-validation.
test	What statistic will be used to measure separation between groups? Currently "f" is the only possibility.
nfeatures	Specifies the different numbers of features (e.g., 1:10) that will be tried, to determine cross-validation accuracy in each instance
seed	This can be used to specify a starting value for the random number generator, in order to make calculations repeatable
funda	Function that will be used for discrimination. Currently lda is the only option
print.progress	Set to TRUE (default) for printing out, as calculations proceed, the number of the current fold
subset	Allows the use of a subset of the samples (observations)

Value

fold	Each column gives, for one run of the cross-validation, numbers that identify the nfold distinct folds of the cross-validation
xUsed	returns the rows of x that were used, in at least one fold
cl	Factor that classifies columns into groups
acc.cv	Cross-validated accuracy
genelist	Array: max(nfeatures) by number of folds by number of repeats, identifying the features chosen at each repeat of each fold. (for k < max(nfeatures) features, take the initial k rows)
Fmatrix	Array, with the same dimensions as genelist, that gives the anova F-statistic when that feature is used on its own to separate groups
nfeatures	Specifies the different numbers of features that were tried, to determine cross-validation accuracy in each instance

Author(s)

John Maindonald

See Also

See also [cvscores](#), [scoreplot](#)

Examples

```
## Use first 500 rows (expression values) of Golub, for demonstration.
data(Golub)
data(golubInfo)
attach(golubInfo)
miniG.BM <- Golub[1:500, BM.PB=="BM"] # 1st 500 rows only
cancer.BM <- cancer[BM.PB=="BM"]
miniG.cv <- cvdisc(miniG.BM, cl=cancer.BM, nfeatures=1:10,
                  nfold=c(3,1))
## Plot cross-validated accuracy, as a function of number of features
plot(miniG.cv$acc.cv, type="l")

## The function is currently defined as
function(x=GolubB, cl=tissue.mfB, nfold=NULL, test="f",
        nfeatures=2, seed=31, funda=lda, print.progress=TRUE,
        subset=NULL){
  ## If nfold is not specified, use leave-one-out CV
  if(is.null(nfold))nfold <- sum(!is.na(cl))
  ## Option to omit one or more points
  if(!is.null(subset)){cl[!is.na(cl)][!subset] <- NA
    nfold[1] <- min(nfold[1], sum(!is.na(cl)))
  }
  if(any(is.na(cl))){x <- x[,!is.na(cl)]
    cl <- cl[!is.na(cl)]
  }
  if(length(nfold)==1)nfold <- c(nfold,1)
  cl <- factor(cl)
  ngp <- length(levels(cl))
  genes <- rownames(x)
  nobs <- dim(x)[2]
  if(is.null(genes)){
    genes <- paste(1:dim(x)[1])
    print("Input rows (features) are not named. Names")
    print(paste(1,":", dim(x)[1], " will be assigned.", sep=""))
    rownames(x) <- genes
  }
  require(MASS)
  if(!is.null(seed))set.seed(seed)
  Fcut <- NULL
  maxgenes <- max(nfeatures)
  ## Cross-validation calculations
  if(nfold[1]==nobs)foldids <- matrix(sample(1:nfold[1]),ncol=1) else
  foldids <- sapply(1:nfold[2], function(x)
```

```

        divideUp(cl, nset=nfold[1]))
genelist <- array("", dim=c(nrow=maxgenes, ncol=nfold[1], nleaf=nfold[2]))
Fmatrix <- array(0, dim=c(nrow=maxgenes, ncol=nfold[1], nleaf=nfold[2]))
testscores <- NULL
acc.cv <- numeric(maxgenes)
if(print.progress)
  cat("\n", "Preliminary per fold calculations","\n")
for(k in 1:nfold[2])
  {
    foldk <- foldids[,k]
    ufold <- sort(unique(foldk))
    for(i in ufold){
      if(print.progress) cat(paste(i,":",sep=""))
      trainset <- (1:nobs)[foldk!=i]
      cli <- factor(cl[trainset])

      stat <- aovFbyrow(x=x[, trainset], cl=cli)
      ordi <- order(-abs(stat))[1:maxgenes]
      genelist[,i, k] <- genes[ordi]
      Fmatrix[, i, k] <- stat[ordi]
    }
  }
ulist <- unique(as.vector(genelist))
df <- data.frame(t(x[ulist, , drop=FALSE]))
names(df) <- ulist
#####
if(print.progress)cat("\n", "Show each choice of number of features:", "\n")
for(ng in nfeatures){
  hat <- cl
  if(print.progress)cat(paste(ng,":",sep=""))
  for(k in 1:nfold[2])
    {
      foldk <- foldids[,k]
      ufold <- sort(unique(foldk))
      for(i in ufold){
        testset <- (1:nobs)[foldk==i]
        trainset <- (1:nobs)[foldk!=i]
        ntest <- length(testset)
        ntrain <- nobs-ntest
        genes.i <- genelist[1:ng, i, k]
        dfi <- df[-testset, genes.i, drop=FALSE]
        newdfi <- df[testset, genes.i, drop=FALSE]
        cli <- cl[-testset]
        xy.xda <- funda(cli~., data=dfi)
        subs <- match(colnames(dfi), rownames(df))
        newpred.xda <- predict(xy.xda, newdata=newdfi, method="debiased")
        hat[testset] <- newpred.xda$class
      }
      tabk <- table(hat,cl)
      if(k==1)tab <- tabk else tab <- tab+tabk
    }
  acc.cv[ng] <- sum(tab[row(tab)==col(tab)])/sum(tab)
}

```

```

cat("\n")
if(length(nfeatures)>1&all(diff(nfeatures)==1)){
  nobs <- length(cl)
  ng1 <- length(acc.cv)
  maxacc1 <- max(acc.cv)
  sub1 <- match(maxacc1, acc.cv)
  nextacc1 <- max(acc.cv[acc.cv<1])
  lower1 <- maxacc1-sqrt(nextacc1*(1-nextacc1)/nobs)
  lsub1 <- min((1:ng1)[acc.cv>lower1])
  lower <- c("Best accuracy, less 1SD ",
            paste(paste(round(c(lower1),2), c(lsub1),
                        sep=" (", " features) ", sep=")"))
  best <- c("Best accuracy",
            paste(paste(round(c(maxacc1),2), c(sub1),
                        sep=" (", " features)", sep=")"))
  acc.df <- cbind(lower, best)
  dimnames(acc.df) <- list(c("Accuracy",
                            "(Cross-validation)"),c("", ""))
  print(acc.df, quote=FALSE)
}
invisible(list(foldids=foldids, xUsed=df, cl=cl, acc.cv=acc.cv,
              genelist=genelist, Fmatrix=Fmatrix, nfeatures=nfeatures))
}

```

cvscores

For high-dimensional data with known groups, derive scores for plotting

Description

This is designed to be used with the output from `cvdisc`. Test and training scores from successive cross-validation steps determine, via a principal components calculation, a low-dimensional global space onto which test scores are projected, in order to plot them.

Usage

```
cvscores(cvlist = BMonly.cv, nfeatures = 3, ndisc = NULL, cl.other = factor("PB:f"), x.other = Golub.PBf)
```

Arguments

<code>cvlist</code>	Output object from <code>cvdisc</code>
<code>nfeatures</code>	Number of features to use
<code>ndisc</code>	Dimension of space in which scores will be formed, at most one less than the number of groups
<code>cl.other</code>	Classifies additional observations that are to be projected onto the same low-dimensional space
<code>x.other</code>	Matrix from which additional observations will be taken

keepcols	Number of sets of principal component scores to use in discriminant calculations and consequent evaluation of scores that will determine the low-dimensional global space
print.progress	Set to TRUE (default) for printing out, as calculations proceed, the number of the current fold

Value

scores	Scores that can be plotted
cl	Factor that was used to classify observations into groups
other.scores	Other scores, if any, for plotting
cl.other	Factor that was used to classify the 'other' data into groups
nfeatures	Number of features used

Note

The methodology used here has developed beyond that described in Maindonald and Burden (2005)

Author(s)

John Maindonald

References

Maindonald, J.H. and Burden, C.J., 2005. Selection bias in plots of microarray or other data that have been sampled from a high-dimensional space. In R. May and A.J. Roberts, eds., *Proceedings of 12th Computational Techniques and Applications Conference CTAC-2004*, volume 46, pp. C59–C74.

<http://anziamj.austms.org.au/V46/CTAC2004/Main> [March 15, 2005]

See Also

See also [cvdisc](#), [scoreplot](#)

Examples

```
## Use first 500 rows (expression values) of Golub, for demonstration.
data(Golub)
data(golubInfo)
attach(golubInfo)
miniG.BM <- Golub[1:500, BM.PB=="BM"] # 1st 500 rows only
cancer.BM <- cancer[BM.PB=="BM"]
miniG.cv <- cvdisc(miniG.BM, cl=cancer.BM, nfeatures=1:10,
                  nfold=c(3,1))
miniG.scores <- cvscores(cvlist=miniG.cv, nfeatures=4,
                        cl.other=NULL)
detach(golubInfo)

## The function is currently defined as
```

```

function(cvlist=BOnly.cv, nfeatures=3, ndisc=NULL,
        cl.other=factor("PB:f"), x.other=Golub.PBf,
        keepcols=NULL, print.progress=TRUE
        ){
  library(MASS)
  foldids <- cvlist$foldids
  nfold <- c(length(unique(foldids)), dim(foldids)[2])

  ugenes <- unique(as.vector(cvlist$genelist[1:nfeatures, ]))
  df <- cvlist$xUsed[, ugenes]
  cl <- cvlist$cl
  if(!length(cl)==dim(df)[1])
    stop(paste("length(cl) =", length(cl),"does not equal",
              "dim(cvlist$df)[1] =", dim(df)[1]))
  levnames <- levels(cl)
  if(is.null(ndisc))ndisc <- length(levnames)-1
  ngp <- length(levnames)
  nobs <- dim(df)[1]
  allscores <- array(0, dim=c(nrow=nobs, ncol=ndisc*nfold[1], nleaf=nfold[2]))
  if(!is.null(cl.other)){
    cl.other <- factor(cl.other)
    if(is.null(dim(x.other)))stop("x.other must have dimension 2")
    if(!length(cl.other)==dim(x.other)[2])
      stop(paste("length(cl.other) =", length(cl.other),"does not equal",
                "dim(x.other)[2] =", dim(x.other)[2]))
    df.other <- data.frame(t(x.other[ugenes, ],drop=FALSE))
    colnames(df.other) <- ugenes
  }
  else other.scores <- NULL
  for(k in 1:nfold[2]){
    foldk <- foldids[,k]
    ufold <- sort(unique(foldk))
    j <- 0
    for(i in ufold){
      j <- j+1
      if(print.progress)cat(paste(if(j>1) ":" else "", i,sep=""))
      testi <- (1:nobs)[foldk==i]
      traini <- (1:nobs)[foldk!=i]
      ntest <- length(testi)
      ntrain <- nobs-ntest
      genes.i <- cvlist$genelist[1:nfeatures, i, k]
      dfi <- as.data.frame(df[-testi, genes.i, drop=FALSE])
      newdfi <- as.data.frame(df[testi, genes.i, drop=FALSE])
      cli <- cl[-testi]
      xy.xda <- lda(cli~., data=dfi)
      allscores[, ((i-1)*ndisc)+(1:ndisc), k] <-
        predict(xy.xda, newdata=df, dimen=ndisc)$x
    }
  }
  cat("\n")
  dim(allscores) <- c(nobs, ndisc*prod(nfold))
  if(is.null(keepcols))keepcols <- min(nfeatures, dim(allscores)[2])
  allscores.pcp <- data.frame(pcp(allscores, varscores=FALSE)$g[, 1:keepcols])

```

```

globals <- predict(lda(cl ~ ., data=allscores.pcp))$x[,1:ndisc]
fitscores <- array(0, dim=c(nrow=nobs, ncol=ndisc, nleaf=nfold[2]))
for(k in 1:nfold[2]){
  foldk <- foldids[,k]
  ufold <- sort(unique(foldk))
  ##   ntimes.genes <- table(cvlist$genelist[1:nfeatures,,k])
  av <- colMeans(df)
  j <- 0
  for(i in ufold){
    j <- j+1
    cat(paste(if (j>1) ":" else "", i,sep=""))
    testi <- (1:nobs)[foldk==i]
    traini <- (1:nobs)[foldk!=i]
    genes.i <- cvlist$genelist[1:nfeatures, i, k]
    dfi <- data.frame(df[-testi, genes.i, drop=FALSE])
    newdfi <- data.frame(df[testi, genes.i, drop=FALSE])
    cli <- cl[-testi]
    traini.xda <- lda(cli~., data=dfi)
    scorei <- predict(traini.xda)$x[,1:ndisc]
    newpred.xda <- predict(traini.xda, newdata=newdfi)
    scorei.out <- newpred.xda$x[, 1:ndisc, drop=FALSE]
    scorei.all <- globals[-testi, 1:ndisc]
    avcol <- colMeans(scorei.all)
    scorei.all <- sweep(scorei.all, 2, avcol, "-")
    avi <- colMeans(scorei)
    scorei <- sweep(scorei, 2, avi, "-")
    trans <- qr.solve(scorei, scorei.all)
    scorei.out <- sweep(scorei.out, 2, avi, "-")
    fitscores[testi, , k] <- sweep(scorei.out%%trans, 2, avcol, "+")
  }
}
fitscores <- apply(fitscores, 1:2, mean)

if(!is.null(cl.other)){
  Fmatrix <- cvlist$Fmatrix
  ord <- order(Fmatrix)[1:nfeatures]
  rowcol <- cbind(as.vector(row(Fmatrix))[ord],as.vector(col(Fmatrix))[ord])
  ugenes <- unique(as.vector(cvlist$genelist[rowcol]))
  df <- cvlist$xUsed[, ugenes]
  xy.xda <- lda(cl~., data=df)
  train.scores <- predict(xy.xda, dimen=ndisc)$x
  other.scores <- predict(xy.xda, newdata=df.other,
                        dimen=ndisc)$x
  avcol <- colMeans(globals)
  all.scores <- sweep(globals, 2, avcol, "-")
  av.train <- colMeans(train.scores)
  train.scores <- sweep(train.scores, 2, av.train, "-")
  trans <- qr.solve(train.scores, all.scores)
  other.scores <- sweep(other.scores%%trans, 2, avcol, "+")
}
if(print.progress)cat("\n")
invisible(list(scores=fitscores, cl=cl, other=other.scores,
              cl.other=cl.other, nfeatures=nfeatures))

```

}

 defectiveCVdisc *defective accuracy assessments from linear discriminant calculations*

Description

Determine cross-validated accuracy, for each of a number of features in a specified range, in each case with a set of features that have been selected using the total data. The "accuracy" assessment are provided only for comparative purposes

Usage

```
defectiveCVdisc(x = GolubB, c1 = tissue.mfB, nfold = NULL, FUN = aovFbyrow, nfeatures = 2, seed = 31, fun
```

Arguments

x	Matrix; rows are features, and columns are observations ('samples')
c1	Factor that classifies columns into groups
nfold	Number of folds for the cross-validation. Optionally, a second number specifies the number of repeats of the cross-validation
FUN	function used to calculate a measure, for each row, of separation into groups
nfeatures	Specifies the different numbers of features (e.g., 1:10) that will be tried, to determine cross-validation accuracy in each instance
seed	This can be used to specify a starting value for the random number generator, in order to make calculations repeatable
funda	Function that will be used for discrimination. Currently lda is the only option
foldids	Fold information, as output from cvdisc()
subset	Allows the use of a subset of the samples (observations)
print.progress	Set to TRUE (default) for printing out, as calculations proceed, the number of the current fold

Value

acc.resub	resubstitution measure of 'accuracy'
acc.sel1	'accuracy' from cross-validation, with the initially selected features

Author(s)

John Maindonald

See Also

[cvdisc](#)

Examples

```

mat <- matrix(rnorm(1000), ncol=20)
cl <- factor(rep(1:3, c(7,9,4)))
badaccs <- defectiveCVdisc(mat, cl, nfold=c(3,1), nfeatures=1:5)
## Note the list elements acc.resub and acc.sel1

## The function is currently defined as
function(x=GolubB, cl=tissue.mfB, nfold=NULL, FUN=aovFbyrow,
        nfeatures=2, seed=31, funda=lda, foldids=NULL,
        subset=NULL, print.progress=TRUE){
  ## Option to omit one or more points
  if(!is.null(subset)) cl[!is.na(cl)][!subset] <- NA
  if(any(is.na(cl))){x <- x[,!is.na(cl)]
                    cl <- cl[!is.na(cl)]
                    }
  nobs <- dim(x)[2]
  ## Get fold information from foldids, if specified,
  ## else if nfold is not specified, use leave-one-out CV
  if(!is.null(foldids))
    nfold <- c(length(unique(foldids)), dim(foldids)[2])
  if(is.null(nfold)&is.null(foldids))nfold <- sum(!is.na(cl))
  else if(nfold[1]==nobs)foldids <- sample(1:nfold[1])
  else foldids <- sapply(1:nfold[2], function(x)
                        divideUp(cl, nset=nfold[1]))
  if(length(nfold)==1)nfold <- c(nfold,1)
  cl <- factor(cl)
  ngp <- length(levels(cl))
  genes <- rownames(x)
  if(is.null(genes)){
    genes <- paste(1:dim(x)[1])
    print("Input rows (features) are not named. Names")
    print(paste(1,":", dim(x)[1], " will be assigned.", sep=""))
    rownames(x) <- genes
  }
  require(MASS)
  if(!is.null(seed))set.seed(seed)
  Fcut <- NULL
  maxgenes <- max(nfeatures)

  stat <- FUN(x=x, cl)
  Fcut <- list(F=sort(stat, decreasing=TRUE)[nfeatures],
              df=c(ngp-1, nobs-ngp))
  ord <- order(-abs(stat))[1:maxgenes]
  genes.ord <- genes[ord]
  selectonce.df <- data.frame(t(x[ord, , drop=FALSE]))
  acc.resub <- acc.sel1 <- numeric(maxgenes)
  if(nfold[1]==0)acc.sel1 <- NULL

  for(ng in nfeatures){
    resub.xda <- funda(cl~., data=selectonce.df[,1:ng,drop=FALSE])
    hat.rsb <- predict(resub.xda)$class
  }
}

```

```

tab.rsb <- table(hat.rsb, cl)
acc.resub[ng] <- sum(tab.rsb[row(tab.rsb)==col(tab.rsb)]/sum(tab.rsb)
if(nfold[1]==0)next
if(nfold[1]==nobs){
  hat.sel1 <- funda(cl~., data=selectonce.df[,1:ng,drop=FALSE],
                   CV=TRUE)$class
  tab.one <- table(hat.sel1, cl)
  acc.sel1[ng] <- sum(tab.one[row(tab.one)==col(tab.one)]/sum(tab.one)
} else
{
  hat <- cl
  if(print.progress)cat(paste(ng,":",sep=""))
  for(k in 1:nfold[2])
  {
    foldk <- foldids[,k]
    ufold <- sort(unique(foldk))
    for(i in ufold){
      testset <- (1:nobs)[foldk==i]
      trainset <- (1:nobs)[foldk!=i]
      dfi <- selectonce.df[-testset, 1:ng, drop=FALSE]
      newdfi <- selectonce.df[testset, 1:ng, drop=FALSE]
      cli <- cl[-testset]
      xy.xda <- funda(cli~., data=dfi)
      subs <- match(colnames(dfi), rownames(df))
      newpred.xda <- predict(xy.xda, newdata=newdfi, method="debiased")
      hat[testset] <- newpred.xda$class
    }
    tabk <- table(hat,cl)
    if(k==1)tab <- tabk else tab <- tab+tabk
  }
  acc.sel1[ng] <- sum(tab[row(tab)==col(tab)]/sum(tab)
}
}
if(print.progress)cat("\n")
invisible(list(acc.resub=acc.resub, acc.sel1=acc.sel1, genes=genes.ord))
}

```

divideUp
Partition data into multiple nearly equal subsets

Description

Randomly partition data into nearly equal subsets. If `balanced=TRUE` the requirement is imposed that the subsets should as far as possible be balanced with respect to a classifying factor. The multiple sets are suitable for use for determining the folds in a cross-validation.

Usage

```
divideUp(cl, nset = 2, seed = NULL, balanced=TRUE)
```

Arguments

<code>cl</code>	classifying factor
<code>nset</code>	number of subsets into which to partition data
<code>seed</code>	set the seed, if required, in order to obtain reproducible results
<code>balanced</code>	logical: should subsets be as far as possible balanced with respect to the classifying factor?

Value

a set of indices that identify the `nset` subsets

Author(s)

John Maindonald

Examples

```
foldid <- divideUp(cl=rep(1:3, c(17,14,8)), nset=10)
table(rep(1:3, c(17,14,8)), foldid)
foldid <- divideUp(cl=rep(1:3, c(17,14,8)), nset=10,
  balanced=FALSE)
table(rep(1:3, c(17,14,8)), foldid)

## The function is currently defined as
function(cl = rep(1:3, c(7, 4, 8)), nset=2, seed=NULL, balanced=TRUE){
  if(!is.null(seed))set.seed(seed)
  if(balanced){
    ord <- order(cl)
    ordcl <- cl[ord]
    gp0 <- rep(sample(1:nset), length.out=length(cl))
    gp <- unlist(split(gp0,ordcl), function(x)sample(x))
    gp[ord] <- gp
  } else
    gp <- sample(rep(1:nset, length.out=length(cl)))
  as.vector(gp)
}
```

Golub

Golub data (7129 rows by 72 columns), after normalization

Description

These are a normalized version of the Golub leukemia data from the `golubEsets` package, available from:

<http://www.bioconductor.org/download/experiments/>

Usage

```
data(Golub)
```

Format

Numeric matrix: 7129 rows by 72 columns.

Details

Data have been normalized and are supplied, here, as a matrix.

Source

See the help page for the dataset `golubMerge`, in the `golubEsets` package, for details of the source of the original data.

References

Molecular Classification of Cancer: Class Discovery and Class Prediction by Gene Expression Monitoring, *Science*, 531-537, 1999, T. R. Golub and D. K. Slonim and P. Tamayo and C. Huard and M. Gaasenbeek and J. P. Mesirov and H. Coller and M.L. Loh and J. R. Downing and M. A. Caligiuri and C. D. Bloomfield and E. S. Lander

Examples

```
data(Golub)
## Select 20 rows from the data; show boxplots of variation across chips
boxplot(data.frame(t(Golub[sample(1:7129, 20), ])))
```

golubInfo

Classifying factors for the 72 columns of the Golub data set

Description

Details are given of the classifying factors for the 72 columns of the Golub data set.

Usage

```
data(golubInfo)
```

Format

A data frame with 72 observations on the following 6 variables, that identifies the samples (observations) in the data set `Golub`

`Samples` a numeric vector: sample number

`BM.PB` a factor with levels BM (from bone marrow) PB (from peripheral blood)

`Gender` a factor with levels F M

Source a factor with levels CALGB CCG DFCI St-Jude. These are the hospitals from which the sample came

tissue.mf a factor with levels BM:NA BM:f BM:m PB:NA PB:f PB:m. This factor identifies the several combinations of source and Gender

cancer a factor with levels allB allT aml There are two types of Acute Lymphoblastic Leukemia (allB and allT), plus Acute Myoblastic Leukemia (aml)

Source

See the help page for the dataset golubMerge, in the golubEsets package, for details of the source of the original data.

References

Molecular Classification of Cancer: Class Discovery and Class Prediction by Gene Expression Monitoring, Science, 531-537, 1999, T. R. Golub and D. K. Slonim and P. Tamayo and C. Huard and M. Gaasenbeek and J. P. Mesirov and H. Coller and M.L. Loh and J. R. Downing and M. A. Caligiuri and C. D. Bloomfield and E. S. Lander

Examples

```
data(golubInfo)
str(golubInfo)
```

orderFeatures	<i>Order features, based on their ability to discriminate</i>
---------------	---

Description

For each row of data, an F or (potentially) other statistic is calculated, using the function FUN, that measures the extent to which this variable separates the data into groups. This statistic is then used to order the rows.

Usage

```
orderFeatures(x, cl, subset = NULL, FUN = aovFbyrow, values = FALSE)
```

Arguments

x	Matrix; rows are features, and columns are observations ('samples')
cl	Factor that classifies columns into groups
subset	allows specification of a subset of the columns of data
FUN	specifies the function used to measure separation between groups
values	if TRUE, F-values as well as the ordering are returned

Value

Either (values=FALSE) a vector that orders the rows, or (values=TRUE)

ord a vector that orders the rows
 stat ordered values of the statistic

Author(s)

John Maindonald

Examples

```
mat <- matrix(rnorm(1000), ncol=20)
cl <- factor(rep(1:3, c(7,9,4)))
ord <- orderFeatures(mat, cl)

## The function is currently defined as
function(x, cl, subset=NULL, FUN=aovFbyrow, values=FALSE){
  if(dim(x)[2]!=length(cl))stop(paste("Dimension 2 of x is",
    dim(x)[2], "differs from the length of cl (=)",
    length(cl)))
  ## Ensure that cl is a factor & has no redundant levels
  if(is.null(subset))
    cl <- factor(cl)
  else
    cl <- factor(cl[subset])
  if(is.null(subset))
    stat <- FUN(x, cl)
  else
    stat <- FUN(x[, subset], cl)
  ord <- order(-abs(stat))
  if(!values)ord else(list(ord=ord, stat=stat[ord]))
}
```

pcp

convenience version of the singular value decomposition

Description

Packages results from an SVD on what can be either a cases by variables (features) or variables by cases layout, for use in principal component and related calculations

Usage

```
pcp(x = USArrests, varscores = TRUE, cases = "rows", center = "vars", standardize = FALSE, scale.cases =
```

Arguments

x	matrix on which SVD is to be performed
varscores	logical; should scores be returned?
cases	specify either "rows" or "columns"
center	logical: if set to "vars", then values of variables will be centered
standardize	logical: should values of variables be standardized to zero mean and unit deviance. Takes precedence over the setting of center
scale.cases	set to a value in [0,1]. scale.cases=0 gives a pure rotation of the variables. scale.cases=1 weights a/c the singular values
log	logical: should logarithms be taken, prior to the calculation?
sc	the variable scores are divided by $\sqrt{sc - 1}$. By default, sc = number of cases
reflect	a vector of two elements, by default c(1,1). Use of -1 in one or both positions can be useful in reconciling results with output from other software

Value

g	case scores
h	variable scores
avv	variable means
sdev	singular values, divides by the square root of one less than the number of cases

Author(s)

John Maindonald

See Also

[La.svd](#)

Examples

```
USArrests.svd <- pcp(x = USArrests)

## The function is currently defined as
function(x=USArrests,
        varscores=TRUE,
        cases="rows",
        center="vars",
        standardize=FALSE,
        scale.cases=1,
        log=FALSE,
        sc=1,
        reflect=c(1,1))
{
  x <- as.matrix(x)
  avv <- 0
  sdv <- 1
}
```

```

casedim <- 2-as.logical(cases=="rows")
vardim <- 3-casedim
## casedim=1 if rows are cases; otherwise casedim=2
## scale.cases=0 gives a pure rotation of the variables
## scale.cases=1 weights a/c the singular values
ncases <- dim(x)[casedim]
nvar <- dim(x)[vardim]
if(is.null(sc))sc <- dim(x)[casedim]-1
if(log)x <- log(x, base=2)
if(standardize){
  avv <- apply(x, vardim, mean)
  sdv <- apply(x, vardim, sd)
  x <- sweep(x, vardim, avv,"-")
  x <- sweep(x, vardim, sdv,"/")
}
else if(as.logical(match("vars", center, nomatch=0))){
  avv <- apply(x,vardim, mean)
  x <- sweep(x, vardim, avv,"-")}

svdx <- La.svd(x, method = c("dgesdd"))
h <- NULL
if(cases=="rows"){
  g <- sweep(svdx$u, 2, svdx$d^scale.cases, "*")*sqrt(sc)
  if(varscores)
    h <- t((svdx$d^(1-scale.cases)* svdx$vt )/sqrt(sc)
}
else if(cases=="columns"){
  g <- sweep(t(svdx$vt), 2, svdx$d^scale.cases, "*")*sqrt(sc)
  if(varscores)
    h <- sweep(svdx$u, 2, svdx$d^(1-scale.cases),"*")/sqrt(sc)
}
invisible(list(g=g, rotation=h, av=avv, sdev=svdx$d/sqrt(ncases-1)))
}

```

plotTrainTest

Plot predictions for both a I/II train/test split, and the reverse

Description

A division of data is specified, for use of linear discriminant analysis, into a training and test set. Feature selection and model fitting is formed, first with I/II as training/test, then with II/I as training/test. Two graphs are plotted – for the I (training) /II (test) scores, and for the II/I scores.

Usage

```
plotTrainTest(x = Golub.BM, nfeatures = c(11, 11), cl = cancer.BM, traintest = divideUp(cancer.BM), titl
```

Arguments

x	Matrix; rows are features, and columns are observations ('samples')
nfeatures	integer: numbers of features for which calculations are required
cl	Factor that classifies columns into groups that will classify the data for purposes of discriminant calculations
traintest	Values that specify a division of observations into two groups. In the first pass (fold), one to be training and the other test, with the roles then reversed in a second pass or fold.
titles	A character vector of length 2 giving titles for the two graphs

Value

Two graphs are plotted.

Author(s)

John Maindonald

Examples

```
mat <- matrix(rnorm(1000), ncol=20)
cl <- factor(rep(1:3, c(7,9,4)))
gp.id <- divideUp(cl, nset=2)
plotTrainTest(x=mat, cl=cl, traintest=gp.id, nfeatures=c(2,3))
```

```
## The function is currently defined as
function(x=Golub.BM, nfeatures=c(11,11), cl=cancer.BM,
        traintest=divideUp(cancer.BM),
        titles=c("A: I/II (train with I, scores are for II)",
                 "B: II/I (train with II, scores are for I)")){
  oldpar <- par(mfrow=c(1,2), pty="s")
  on.exit(par(oldpar))
  if(length(nfeatures)==1)nfeatures <- rep(nfeatures,2)
  traintest <- factor(traintest)
  train <- traintest==levels(traintest)[1]
  testset <- traintest==levels(traintest)[2]
  cl1 <- cl[train]
  cl2 <- cl[testset]
  nf1 <- nfeatures[1]
  ord1 <- orderFeatures(x, cl, subset=train)
  df1 <- data.frame(t(x[ord1[1:nf1], train]))
  df2 <- data.frame(t(x[ord1[1:nf1], testset]))
  df1.lda <- lda(df1, cl1)
  scores <- predict(df1.lda, newdata=df2)$x
  scoreplot(scorelist=list(scores=scores, cl=c12,
                           nfeatures=nfeatures[1], other=NULL, cl.other=NULL),
            prefix.title="")
  mtext(side=3, line=2, titles[1], adj=0)
```

```

nf2 <- nfeatures[2]
ord2 <- orderFeatures(x, c1, subset=testset)
df2 <- data.frame(t(x[ord2[1:nf2], testset]))
df1 <- data.frame(t(x[ord2[1:nf2], train]))
df2.lda <- lda(df2, c12)
scores <- predict(df2.lda, newdata=df1)$x
scoreplot(scorelist=list(scores=scores, c1=c1,
                        nfeatures=nfeatures[2], other=NULL, c1.other=NULL),
          prefix.title="")
mtext(side=3, line=2, titles[2], adj=0)
}

```

qqthin

a version of qqplot() that thins out points that overplot

Description

QQ-plots with large numbers of points typically generate graphics files that are unhelpfully large. This function handles the problem by removing points that are, for all practical purposes, redundant

Usage

```
qqthin(x, y, ends = c(0.01, 0.99), eps = 0.001, xlab = deparse(substitute(x)), adj.xlab = NULL, ylab = de
```

Arguments

x	ordered values of x will be plotted on the x-axis
y	ordered values of y will be plotted on the y-axis
ends	outside these cumulative proportions of numbers of points, all points will be included in the graph
eps	controls the extent of overplotting
xlab	label for x-axis
adj.xlab	positioning of x-label
ylab	label for y-axis
show.line	logical; show the line y=x?
centerline	logical; draw a line though the part of the graph where some points have been omitted?
...	additional graphics parameters

Value

Gives a qqplot

Author(s)

John Maindonald

References

~put references to the literature/web site here ~

Examples

```

mat <- matrix(rnorm(1000), ncol=20)
cl <- factor(rep(1:3, c(7,9,4)))
Fstats <- aovFbyrow(x = mat, cl = cl)
qqthin(qf(ppoints(length(Fstats)), 2, 17), Fstats, eps=0.01)

## The function is currently defined as
function(x, y, ends=c(.01,.99), eps=0.001,
        xlab = deparse(substitute(x)), adj.xlab=NULL,
        ylab = deparse(substitute(y)), show.line=TRUE,
        centerline=TRUE, ...){
  ## qqthin() is a substitute for qqplot(), that thins
  ## out plotted points from the region where they are
  ## dense. Apart from the overlaid curve that shows
  ## the region where points have been thinned, it may
  ## be hard to distinguish the result of qqthin()
  ## from that of qqplot()
  xlab <- xlab
  ylab <- ylab
  x <- sort(x)
  y <- sort(y)
  dx<-diff(x)
  epsdist <- sqrt(diff(range(x))^2+diff(range(y))^2)*eps
  dx<-0.5*(c(dx[1],dx)+c(dx,dx[length(dx)]))
  dy<-diff(y)
  dy<-0.5*(c(dy[1],dy)+c(dy,dy[length(dy)]))
  dpoints <- epsdist/sqrt(dx^2+dy^2)
  ## dpoints is a local measure of the number of points
  ## per unit distance along the diagonal, with the unit
  ## set to approximately eps*(length of diagonal)
  dig<-floor(dpoints)+1
  ## dig is, roughly, the number of points per unit distance.
  ## We wish to retain one point per unit distance. For this
  ## retain points where cdig rounds to an integer. For such
  ## points, cdig has increased by approx 1, relative to the
  ## previous point that is retained.
  cdig<-round(cumsum(1/dig))
  subs<-match(unique(cdig), cdig)
  if(is.null(adj.xlab))
  plot(x[sub], y[sub], xlab=xlab, ylab=ylab)
  else {
    plot(x[sub], y[sub], xlab="", ylab=ylab)
    mtext(side=1, xlab, adj=adj.xlab, line=par()$mgp[1])
  }
}

```

```

}
if(any(diff(subs)>1)){
n1 <- min(subs[c(diff(subs),0)>1])
n2 <- max(subs[c(0,diff(subs))>1])
ns1 <- match(n1, subs)
ns2 <- match(n2, subs)
print(paste("Graph retains", length(subs), "points."))
if(centerline)
  lines(smooth.spline(x[subns1:ns2], y[subns1:ns2]),
        col="grey", lwd=2)
}
if(show.line)abline(0, 1, col="red")
}

```

scoreplot

Plot discriminant function scores, with various identification

Description

There is provision for the plotting of two sets of scores on the same graph, possibly with different classifying factors. The function is designed for use with output from `cvscores()` or from `simulateScores()`. This is an alpha version! Suggestions for code changes and/or enhancements that will improve the graphs will be welcomed.

Usage

```
scoreplot(scorelist = miniG.scores, plot.disc = 1:2, xlab = NULL, ylab = NULL, params = NULL, circle = NU
```

Arguments

scorelist	list, with elements scores (a matrix of scores) c1 (a classifying factor), other (optional, a further sets of scores), c1.other (a a classifying factor for other, optional) and nfeatures (optional, used to label the graph)
plot.disc	choice of columns of scorelist to plot
xlab	label for x-axis
ylab	label for y-axis
params	List, with optional elements (lists) points, other, circle and legend. Allowed list elements for points and other are cex, lwd, pch and col. For circle they are cex, lwd and col. For legend, they are cex and cex.other
circle	identifies points that are to be circled
c1.circle	different colors may be used for different points, according to levels of c1.circle
circle.pos	This is a vector of length 2, that specifies where to place the legend information for the circling of points. Possibilities are c(0,0) (left, below), c(1,1) (right, above), etc.
adj.circle	controls positioning of circle legend

adj.title	controls positioning of title
join.legends	logical; should legends for points and other be combined?
prefix.title	prefix, to place before title
cex.title	cex for title
ratio	y-scale to x-scale ratio for graph
plot.folds	Plot individual fold information, comparing projected training scores with their projections onto the global space. This is not at present implemented

Value

A graph is plotted.

Author(s)

John Maindonald

See Also

See also [cvdisc](#), [cvscores](#)

Examples

```
## Use first 500 rows (expression values) of Golub, for demonstration.
data(Golub)
data(golubInfo)
attach(golubInfo)
miniG.BM <- Golub[1:500, BM.PB=="BM"] # 1st 500 rows only
cancer.BM <- cancer[BM.PB=="BM"]
miniG.cv <- cvdisc(miniG.BM, cl=cancer.BM, nfeatures=1:10,
                  nfold=c(3,1))
miniG.scores <- cvscores(cvlist=miniG.cv, nfeatures=4,
                       cl.other=NULL)
subsetB <- (cancer=="allB") & (tissue.mf %in% c("BM:f", "BM:m", "PB:m"))
tissue.mfB <- tissue.mf[subsetB, drop=TRUE]
scoreplot(scorelist=miniG.scores, cl.circle=tissue.mfB,
          circle=tissue.mfB%in%c("BM:f", "BM:m"),
          params=list(circle=list(col=c("cyan", "gray"))),
          prefix="BM samples -")
detach(golubInfo)

## The function is currently defined as
function(scorelist=BMonly.scores, plot.disc=1:2,
        xlab=NULL, ylab=NULL, params=NULL,
        circle=NULL, cl.circle=NULL, circle.pos=c(1,1),
        adj.circle=1,
        adj.title=0.5, join.legends=T, prefix.title="Golub data - ",
        cex.title=1.0, ratio=1, plot.folds=FALSE ){
  library(MASS)
  combine.params <-
    function(params=list(circle=list(col=c("cyan", "gray")))){
```

```

default.params=list(points=list(cex=1, lwd=1.25, pch=1:8, col=1:8),
  other=list(cex=0.65, lwd=1.25, pch=13:9, col=c(6:8,5:1)),
  circle=list(cex=2, lwd=1, pch=1.75, col="gray40"),
  legend=list(cex=1, cex.other=1))
nam <- names(params)
if(!is.null(nam))
  for(a in nam){
    nam2 <- names(params[[a]])
    for(b in nam2)default.params[[a]][[b]] <- params[[a]][[b]]
  }
default.params
}
params <- combine.params(params=params)
cl <- scorelist$cl
cl.other <- scorelist$cl.other
if(!is.null(cl.other)) cl.other <- factor(cl.other)
nfeatures <- scorelist$nfeatures
if(length(plot.disc)==2){
  n1 <- plot.disc[1]
  n2 <- plot.disc[2]
  if(is.null(xlab))xlab <- paste("Discriminant function", n1)
  if(is.null(ylab))ylab <- paste("Discriminant function", n2)
} else stop("plot.disc must be a vector of length 2")
if(!is.factor(cl))cl <- factor(cl)
levnames <- levels(cl)
fitscores <- scorelist$scores
other.scores <- scorelist$other
ngp <- length(levnames)
n1lim <- range(fitscores[,n1])
n2lim <- range(fitscores[,n2])
if(!is.null(cl.other)){
  n1lim <- range(c(n1lim, other.scores[,n1]))
  n2lim <- range(c(n2lim, other.scores[,n2]))
  levnum <- unclass(cl.other)
  levnames.other <- levels(cl.other)
  intlev.other <- unclass(cl.other)
  ngp.other <- length(levels(cl.other))
}
n1 <- plot.disc[1]; n2 <- plot.disc[2]
intlev <- unclass(cl)
oldpar <- par(lwd=1)
on.exit(par(oldpar))
eqscplot(n1lim, n2lim, type="n",
  xlab=xlab, ylab=ylab, ratio=ratio)
with(params$points,
  points(fitscores[,n1], fitscores[,n2], col=col[intlev],
    pch=pch[intlev], cex=cex, lwd=lwd))
if(!is.null(cl.other))
  with(params$other,
    points(other.scores[,n1], other.scores[,n2],
      pch=pch[intlev.other],
      col=col[intlev.other],
      cex=cex, lwd=lwd))

```

```

if(!is.null(cl.circle)){
  cl.circle <- factor(cl.circle[circle])
  lev.circle <- levels(cl.circle)
  with(params$circle,
        points(fitscores[circle, n1], fitscores[circle,n2], pch=pch,
              cex=cex, col=col[unclass(cl.circle)], lwd=lwd))
}
par(xpd=TRUE)
chw <- par()$cxy[1]
chh <- par()$cxy[2]
par(lwd=1.5)
ypos <- par()$usr[4]
xmid <- mean(par()$usr[1:2])
top.pos <- 0
mtext(side=3, line=(top.pos+1), paste(prefix.title,
  nfeatures, "features"), cex=cex.title, adj=adj.title)
ypos.legend <- ypos+(top.pos-0.45)*chh*0.8

if(join.legends&!is.null(cl.other)){
  leg.info <- legend(xmid, ypos.legend, xjust=0.5, yjust=0, plot=FALSE,
    x.intersp=0.5, ncol=ngp, legend=levnames,
    pt.lwd=params$points$lwd,
    pt.cex=params$points$cex,
    cex=params$legend$cex,
    pch=params$points$pch)
  legother.info <- legend(xmid, ypos.legend, xjust=0.5, yjust=0,
    plot=FALSE, x.intersp=0.5,
    ncol=ngp.other, legend=levnames.other,
    pt.lwd=params$other$lwd,
    pt.cex=params$other$cex,
    cex=params$legend$cex.other,
    pch=params$other$pch)
  leftoff <- 0.5*legother.info$rect$w-0.5*chw
  rightoff <- 0.5*leg.info$rect$w+0.5*chw
  ypos.other <- ypos.legend
}
else {
  leftoff <- 0
  rightoff <- 0
  ypos.other <- ypos+(top.pos-1.5)*chh*0.8
}
legend(xmid-leftoff, ypos.legend, xjust=0.5, yjust=0,
  bty="n", pch=params$points$pch,
  x.intersp=0.5, col=params$points$col, ncol=ngp,
  legend=levnames,
  pt.lwd=params$points$lwd,
  pt.cex=params$points$cex,
  cex=params$legend$cex)
par(lwd=1)
if(!is.null(cl.other))
  lego.info <- legend(xmid+rightoff, ypos.other, xjust=0.5, yjust=0,
    pch=params$other$pch, x.intersp=0.5,
    col=params$other$col, ncol=ngp.other,

```

```

        pt.lwd=params$other$lwd,
        pt.cex=params$other$cex,
        legend=levnames.other,
        cex=params$legend$cex.other,
        bty="n")
if(!is.null(c1.other)&join.legends)
  text(lego.info$rect$left+c(0.4*chw,lego.info$rect$w-0.25*chw),
       rep(ypos.other,2)+0.8*chh, labels=c(",",""),
       cex=params$legend$cex,
       lwd=params$legend$lwd, bty="n")
par(lwd=params$circle$lwd)
if(!is.null(c1.circle))if(lev.circle[1]!=""){
  pch.circle <- params$circle$pch
  xy <- par()$usr[circle.pos+c(1,3)]
  legend(xy[1], xy[2],
         xjust=adj.circle[1], yjust=circle.pos[2], bty="n", x.intersp=0.5,
         pch=rep(pch.circle,length(lev.circle)), col=params$circle$col,
         ncol=1, legend=lev.circle, cex=0.85, pt.cex=1.5)
}
par(lwd=1, xpd=FALSE)
if(plot.folds){
  mtext(side=1, line=1.25, "Discriminant function 1", outer=T)
  mtext(side=2, line=1.25, "Discriminant function 2", outer=T)
}
}

```

simulateScores

Generate linear discriminant scores from random data, after selection

Description

Simulates the effect of generating scores from random data, possibly with predicted scores calculates also for additional 'observations'

Usage

```
simulateScores(nrows = 7129, c1 = rep(1:3, c(19, 10, 2)), x = NULL, c1.other = NULL, x.other = NULL, nfea
```

Arguments

nrows	number of rows of random data matrix
c1	classifying factor
x	data matrix, by default randomly generated
c1.other	classifying factor for additional observations
x.other	additional observations
nfeatures	number of features to select (by default uses aov F-statistic)
dimen	number of sets of discriminant scores to retain (at most one less than number of levels of c1)
seed	set, if required, so that calculations can be reproduced

Value

scores	matrix of scores
cl	classifying factor
other	matrix of 'other' scores
cl.other	classifying factor for scores.other
nfeatures	number of features used in generating the scores

Note

NB: Prior to 0.53, this function made (wrongly) a random selection of features.

Author(s)

John Maindonald

Examples

```
scorelist <- simulateScores(nrows=500, cl=rep(1:3, c(19,10,2)))
plot(scorelist$scores, col=unclass(scorelist$cl), pch=16)

## The function is currently defined as
simulateScores <-
  function (nrows = 7129, cl = rep(1:3, c(19, 10, 2)), x = NULL,
           cl.other = NULL, x.other = NULL, nfeatures = 15, dimen = 2,
           seed = NULL)
{
  if (!is.null(seed))
    set.seed(seed)
  m <- length(cl)
  m.other <- length(cl.other)
  if (is.null(x)) {
    x <- matrix(rnorm(nrows * m), nrow = nrows)
    rownames(x) <- paste(1:nrows)
  }
  else nrows <- dim(x)[1]
  if (is.null(x.other)) {
    x.other <- matrix(rnorm(nrows * m.other), nrow = nrows)
    rownames(x.other) <- paste(1:nrows)
  }
  if (is.numeric(cl))
    cl <- paste("Gp", cl, sep = "")
  if(!is.null(cl.other)){
    if (is.numeric(cl.other))
      cl.other <- paste("Gp", cl.other, sep = "")
    cl.other <- factor(cl.other)
  }
  cl <- factor(cl)
  if (dimen > length(levels(cl)) - 1)
    dimen <- length(levels(cl)) - 1
}
```

```
ordfeatures <- orderFeatures(x, cl = cl, values = TRUE)
stat <- ordfeatures$stat[1:nfeatures]
ord.use <- ordfeatures$ord[1:nfeatures]
xUse.ord <- data.frame(t(x[ord.use, ]))
xUseOther.ord <- data.frame(t(x.other[ord.use, ]))
ordUse.lda <- lda(xUse.ord, grouping = cl)
scores <- predict(ordUse.lda, dimen = dimen)$x
if(!is.null(cl.other))
  scores.other <- predict(ordUse.lda, newdata = xUseOther.ord,
                        dimen = dimen)$x else
scores.other <- NULL
invisible(list(scores = scores, cl = cl, other = scores.other,
              cl.other = cl.other, nfeatures = nfeatures))
}
```

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