Package 'ktspair'

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Title k-Top Scoring Pairs for Microarray Classification

Version 1.0

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Description These functions compute the k best pairs of genes used to
classify samples based on the relative rank of the genes
expression within each profile. A score based on the sensiblity
and the specificity is calculated for every possible pair. The
k pairs with the highest score will be selected with the
restriction that a gene can appear in at most one pair. The
value of k is either set as a parameter chosen by the user or
computed through crossvalidation. Other functions related to
the k-TSP are also available, for example the functions
prediction, summary, plot, etc. can be found in the package.

Maintainer Julien Damond <julien.damond@gmail.com>

Depends R (>= 2.2.1)

License GPL-2

Archs i386

R topics documented:

1

ktspair-package   *Computation of the k-TSP*

Description

The package computes the k-TSP. This method uses pairs of genes to perform a classification which compares the relative ordering of the gene expressions within each profile. It ranks pairs of genes with respect to a score based on the sensibility and the specificity achieved by each pair. It selects the k pairs that achieved the maximum score with the restriction that a gene can appear in at most one pair. The number of pairs of genes is computed through crossvalidation or can be chosen by the user. This package also contains function to display graphical properties of the k-TSP, to summarize the performance of the k-TSP, to predict new individual, etc. The functions deals also with "Expression Set" classes. The functions contained in this package are able to deal correctly with the presence of NAs in the dataset.

Details

Package:	ktspair
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Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

J. Damond, "Presentation and study of robustness for several methods to classify individuals based on their gene expressions"

Jeffrey T. Leek <jtleek@jhu.edu> (). tspair: Top Scoring Pairs for Microarray Classification. R package version 1.10.0.

See Also

kts.pair, ktspplot, predict.ktsp, summary.ktsp

Examples

```
    ## Not run:
    ## Load data
    data(ktspdata)
    ktsp <- ktspcalc(dat,grp,3)
    ktsp <- ktspcalc(eSet,1,3)
    ktsp <- ktspcalc(eSet,grp,3)
    ktsp
    plot(ktsp)
    summary(ktsp)
    predict(ktsp)

  ## End(Not run)
```

---

cv   *Crossvalidation for the parameter k*

Description

This function computes the value of k through crossvalidation.

Usage

```
    cv(dat, grp, cross = 5)
```

Arguments

dat
: Can either be (a) a matrix of m lines (the gene expressions) and n columns (the observations) or (b) an eSet object.

grp
: Can either be (a) a character (or numeric) vector indicating the group of each observations or (b) an integer indicating the column of pData(dat) that represents the group of the observations.

cross
: The number of fold that should be used in the crossvalidation.

Details

This function computes the value of k through crossvalidation. The number of fold is given by the variable cross and by default is 5. It also computes the percentage of correct prediction based on the same partition as for the crossvalidation for the possible values of k.

Value

k
: The selected value for k

accuracy_k
: The estimated percentage of correct prediction achieved by the k-TSP with the selected k.

accuracy
: A vector of the estimated percentage of correct prediction reached by the k-TSP with k = 1,3,5,7,9.

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

J. Damond, "Presentation and study of robustness for several methods to classify individuals based on their gene expressions"

Jeffrey T. Leek <jtleek@jhu.edu> (). tspair: Top Scoring Pairs for Microarray Classification. R package version 1.10.0.

See Also

ktspcalc, ktspplot, predict.ktsp, summary.ktsp

Examples

```
## Not run:
## Load data
data(ktspdata)
cv <- cv(dat, grp,cross =10)
ktsp <- ktspcalc(dat, grp, cv$k)
ktsp
cv

## End(Not run)
```

---

dat   *Simulated gene expressions of individuals.*

Description

This is a 1000 by 50 simulated gene expression matrix, where the lines represent the genes and the column the individuals.

Usage

```
dat
```

Format

matrix

---

eSet   *Simulated gene expressions of individuals.*

Description

This dataset is a simulated gene expression set under the form of an eSet, where exprs(eSet1) = dat and pData(eSet1) = grp.

Usage

```
eSet
```

Format

Expression Set

---

grp   *Group of the individuals.*

Description

This is a vector of the group of the simulated profiles contained in the matrix "dat" in the k-TSP package. The groups are "healthy" and "diseased".

Usage

```
grp
```

Format

vector

---

kts.pair   *Calculation of the k top scoring pairs.*

Description

This function computes the k pairs of genes that achieved the maximum difference between the sensitivity and the specificity (in absolute value) between two specific groups based on the comparison of the expressions of the two genes present in the pairs. The function ktspcalc() is the general function and uses the function kts.pair once the dataset has been prepared for this function. The function ktspcalc() is also able to deal with eSets.

Usage

```
kts.pair(dat, grp, k)
```

Arguments

`dat`	A matrix of m lines (the gene expressions) and n columns (the observations).
`grp`	A vector of 0 and 1 for the groups of the observations.
`k`	The number of pairs of genes that the function will select.

Details

This function only works with matrices and vector of group containing only 0 and 1. For a more general use (eSets and labels for the groups) see the function ktspcalc(). This classifier can only be used for classifications with two groups. The k-TSP was introduced in Tan et al. (2005) and is an extension of the TSP, which was presented in Geman et al. (2004).

Value

A ktsp object with the following elements:

`index`	A k by 2 matrix composed of genes where the ith row stands for the ith best pair of genes with the restriction that a gene can appear in only one pair. The pairs are seleceted with respect to the score Delta and Gamma (in case of ties), see Tan et al. (2005) for more details about the k-TSP.
`ktspcore`	A vector of size k containing the scores Delta achieved by each selected pair of genes. The score Delta is based on the sensitivity and the specificity of a pair, see Geman et al. (2004) for more details.
`grp`	The group for each observation in a binary form
`ktspdat`	The row i and the row i+k represents the expressions of the genes present in the ith pair.
`k`	The number of pairs of genes.
`labels`	The name of the two groups that were present in the original variable grp.
`rankscore`	The score Gamma achieved by each pair of genes, for more details on this score see Geman et al. (2004).
`accuracy`	A vector of the estimated percentage of correct prediction for the k-TSP with k=1,3,5,7,9.
`accuracy_k`	The estimated percentage of correct prediction of the k-TSP with the selected k.

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

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See Also

ktspcalc, ktspplot,predict.ktsp, summary.ktsp

Examples

```
    ## Not run:
    ## Load data
    data(ktspdata)
    ktsp <- kts.pair(dat,grp,3)
    ktsp$index
    ktsp$ktspscore

## End(Not run)
```

---

ktspcalc	*Compute the k top scoring pairs based on a gene expression matrix and a group indicator vector.*

Description

This function computes the k pairs of genes that achieved the maximum difference between the sensitivity and the specificity (in absolute value) between two specific groups based on the comparison of the expressions of the two genes present in the pairs.

Usage

```
ktspcalc(dat, grp, k=NULL, cross = 5, performance = FALSE, seed = NULL)
```

Arguments

dat   Can either be (a) a matrix of m lines (the gene expressions) and n columns (the observations) or (b) an eSet object.

grp   Can either be (a) a character (or numeric) vector indicating the group of each observations or (b) an integer indicating the column of pData(dat) that represents the group of the observations.

k   The number of pairs of genes used in the k-TSP (k). By default this parameter is computed through crossvalidation.

cross   The number of fold that should be used for the crossvalidation estimation of the parameter k. By default the number of fold is 5.

performance An indicator if the performance of the model should be computed or not.

seed   The crossvalidation and the computation of the performance of the model are based on a random partition of the dataset. The variable seed allows the user to fix a seed.

Details

The original version of the k-TSP only works for two groups classification. It is possible to deal with multiclass classification by using trees or multiple steps methods that reduce the problem to a combination of several two classes classifications, see Aik et al. (2005) for more details. The function computes the score Delta (see Geman et al. (2004) for more details about this score) for every possible pair of genes. This makes the required computational time to grow rapidly in the number of genes. A pre-filtering step can be useful in some cases. This function is able to deal with NA present in the dataset. It considers only the patients for which the gene expressions were measured and adapts the computation of the score Delta to the number of measures without NA. This function also deals with "Expression Set" dataset. The group indicator can be replaced by the number of the column of pData(eSet) that contains the indicatior vectors of the group. The user has the possibility to let the function compute a value for the parameter k. This value is computed through crossvalidation. The user can choose the number of fold. The special case of the Leave-One-Out crossvalidation is when the number of fold is equal to the number of observations. The user has the possibility to obtain the accuracy reached by the method via the variable performance. It will compute the accuracy using a partitioning of the dataset as in the crossvalidation. If the crossvalidation had to be computed, the performance will be computed at the same time and will be based on the same partition. The number of partition for the performance is also given by the variable cross. Finally the user can fix a seed via the variable seed.

Value

A ktsp object with the following elements:

`index`	A k by 2 matrix composed of genes where the ith row stands for the ith best pair of genes with the restriction that a gene can appear in only one pair. The pairs are seleceted with respect to the score Delta and Gamma (in case of ties), see Tan et al. (2005) for more details about the k-TSP.
`ktspcore`	A vector of size k containing the scores Delta achieved by each selected pair of genes. The score Delta is based on the sensitivity and the specificity of a pair, see Geman et al. (2004) for more details.
`grp`	The group for each observation in a binary form
`ktspdat`	The row i and the row i+k represents the expressions of the genes present in the ith pair.
`k`	The number of pairs of genes.
`labels`	The name of the two groups that were present in the original variable grp.
`rankscore`	The score Gamma achieved by each pair of genes, for more details on this score see Geman et al. (2004).
`accuracy`	A vector of the estimated percentage of correct prediction for the k-TSP with k=1,3,5,7,9.
`accuracy_k`	The estimated percentage of correct prediction of the k-TSP with the selected k.

Warning

If NAs are present in the dataset, the computation of the score Delta will be based only on observations for which the measures of the two genes of the current comparison are not NA. This will reduce the number of observations used to compute the score Delta and can produce lower accuracy of the estimation compared to the scores for others pairs.

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

Aik Choon Tan, Daniel Q. Naiman, Lei Xu, Raimond L. Winslow, and Donald Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21:3896NAK3904, October 2005.

J. Damond, "Presentation and study of robustness for several methods to classify individuals based on their gene expressions"

Jeffrey T. Leek <jtleek@jhu.edu> (). tspair: Top Scoring Pairs for Microarray Classification. R package version 1.10.0.

See Also

`kts.pair`, `ktspplot`,`predict.ktsp`, `summary.ktsp`

Examples

```
## Not run:
## Load data
data(ktspdata)
ktsp <- ktscalc(dat,grp,3)
ktsp <- ktspcalc(eSet,grp,3)
ktsp <- ktspcalc(eSet,1,3)
ktsp
ktsp$rankscore
ktsp$accuracy_k
ktsp$accuracy

## End(Not run)
```

---

ktspdata   *Simulated dataset of gene expressions in a matrix form.*

Description

This dataset can be used to illustrate the functions contained in the package "ktspair". The gene expressions are simulated from poisson random variables, where the means come from a normal distribution with different parameters for the group of healthy and diseased people. The first 25 measures are healthy people (represented by 0 in the group vector) and the 25 last measures are diseased people (represented by 1 in the group vector).

Usage

`dat`

| ktspplot | *Graphical representation of ktsp objects* |

Description

Show a graphical representation of ktsp objects based on the expressions of the genes present in the pairs constituting the k-TSP.

Usage

```
ktspplot(ktspobj, select = NULL)
```

Arguments

ktspobj	A ktsp object (computed through the functions ktspcalc or kts.pair).
select	If the number of TSPs in the k-TSP is greater than 1, one can choose the representation of a single TSP (select = 1,2,...,k). By default the graphical representation of every TSPs in succession is ploted.

Details

ktspplot() creates a two dimensional graph for a single TSP present in the k-TSP. The graph plots the expression of the first gene in the pair versus the expression of the second gene in the pair of interest. The group of the observations are ploted in red and blue, the score of the current pair is shown on the top of the graph. The black line of slope 1 and intercept 0 represents the decision rule of the current TSP. If not only one TSP is selected, hitting return will plot the next TSP in the k-TSP.

Value

No value is returned. Only a graph is ploted.

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

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See Also

ktspcalc, kts.pair, predict.ktsp, summary.ktsp

Examples

```
    ## Not run:
    ## Load data
    data(ktspdata)
    ktsp <- ktspcalc(dat,grp,3)
    ktspplot(ktsp,select=1)
    ktspplot(ktsp)

  ## End(Not run)
```

```
make.consecutive.int
```
Transform the group vector into a binary vector

Description

This function transforms the vector corresponding to the groups of the observations into a binary vector.

Usage

```
make.consecutive.int(y)
```

Arguments

y   A numeric or character vector.

Value

Return a vector containing only 0 and 1.

Note

This function is useful to link the functions kts.pair and ktspcalc (kts.pair accepts only a vector grp containing 0 and 1).

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

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See Also

ktspcalc, ktspplot,predict.ktsp, summary.ktsp

Examples

```
   ## Not run:
   ## Load data
   data(ktspdata)
   make.consecutive.int(grp)

## End(Not run)
```

---

plot.ktsp   *Graphical representation of ktsp objects*

Description

Show a graphical representation of ktsp objects based on the expressions of the genes present in the pairs constituting the k-TSP.

Usage

```
   ## S3 method for class 'ktsp'
plot(x,...)
```

Arguments

x   A ktsp object.

...   Plotting arguments, not used

Details

This is the generic function for ktspplot.

Value

No value is returned. Only a graph is ploted.

Author(s)

Julien Damond <julien.damond@gmail.com>

References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

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See Also

ktspcalc, kts.pair,predict.ktsp, summary.ktsp

Examples

```
  ## Not run:
  ## Load data
  data(ktspdata)
  ktsp <- kts.pair(dat,grp,3)
  plot(ktsp,select=1)
  plot(ktsp)

## End(Not run)
```

---

predict.ktsp   *Prediction using a ktsp object*

Description

This function is used to predict the group of an individual based on its gene expressions via a ktsp object.

Usage

```
predict.ktsp(object, dat = NULL, select = NULL)
```

Arguments

object	A ktsp object
dat	A dataset from which predictions should be computed. It can be either under the form of a matrix or under the form of an eSet.
select	An integer to perform the prediction based on a single TSP present in the k-TSP.

Details

By default, this function computes predictions of the orginal dataset (the one used to compute the k-TSP) based on the k-TSP. It is possible to predict new obsevations via the variable "dat". It can either be under the form of a matrix or of an eSet. The function searchs for the gene names of the ktsp and try to identify them in the rownames or featuresNames of the matrix of gene expressions "dat". If rownames or featureNames are not available, it uses the number of the row as name to perform the predictions. By default, the prediction is based on all the pairs present in the k-TSP and by using a voting system. It is also possible to have predictions based on a single pair by using the variable "select". In order to obtain a well defined predicton, the number of pairs of genes used has to be an odd number. If the number of pairs is even, the function will not consider the pair with the lowest score Delta in the calculation of the prediction.

Value

A vector containing the class predictions of each individual based on the k-TSP is returned.

warning

If rownames or featureNames of the gene expression matrix "dat" are not available, the number of the row will be used as name. To be correct the order of the genes in the matrix "dat" must be the same as in the ktsp object (or equivalently the same as in the original dataset).

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

J. Damond, "Presentation and study of robustness for several methods to classify individuals based on their gene expressions"

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See Also

ktspcalc, ktspplot,kts.pair, summary.ktsp

Examples

```
   ## Not run:
   ## Load data
   data(ktspdata)
   ktsp <- kts.pair(dat,grp,3)
   predict(ktsp)
   predict(ktsp, select=1)

## End(Not run)
```

---

 print.ktsp   *Print the results of the k-TSP*

Description

This function is used to print the results of a ktsp object.

Usage

```
   print.ktsp(x)
```

Arguments

x   A ktsp object.

Details

It prints the results of the k-TSP. More precisely, the number of pairs used in the k-TSP, the gene present in the pairs and the score of each pair.

Value

No value is returned. A table is ploted.

Note

Once the function ktsp.print is defined, writing "x" has the same effect as writing "print.ktsp(x)", where x is a ktsp object.

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

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See Also

`ktspcalc`, `kts.pair`,`predict.ktsp`, `summary.ktsp`

Examples

```
## Not run:
## Load data
data(ktspdata)
ktsp <- ktspcalc(dat, grp, 3)
ktsp.print(ktsp)
ktsp

## End(Not run)
```

---

rank_na   *Rank the gene expression and Replace NA*

Description

This function computes the ranks of the gene expression within each row (within one profile) and replaces the NAs present in the dataset by a given value.

Usage

```
rank_na(dat, na = -1e+05)
```

Arguments

dat   A gene expression dataset under the form of a matrix.

na   The value by which the NAs should be replaced, by default -1e+05.

Value

A matrix of the same size as the matrix dat. The columns of this matrix contain the ranks of the gene expressions within each profile. In other words the ith row of the new matrix contains the ranks of the gene expression of the ith column of the matrix dat. If NA are present in the matrix dat, they won't be take into account as computing the ranks and will be replaced by the value na, which is, by default, -1e+05.

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

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See Also

ktspcalc, kts.pair, predict.ktsp, summary.ktsp

Examples

```
## Not run:
## Load data
data(ktspdata)
rank_na(dat, 2000)

## End(Not run)
```

---

summary.ktsp *Summary of ktsp object*

Description

This function summarizes a ktsp object.

Usage

```
summary.ktsp(object, select = NULL, printall = FALSE)
```

Arguments

object   A ktsp object.

select   To obtain the summary for only a single TSP in the k-TSP.

printall   If the summary for the whole method k-TSP or if all the summary of the TSPs should be ploted in succession.

Details

It is possible to obtain the summary of one TSP present in the k-TSP via the variable select. To obtain the summary of all the TSPs in succession one should use the variable printall with the value TRUE. By default, a summary of the whole method k-TSP will be ploted.

Value

No value is returned. Only a table is ploted.

Note

It has the same effect to write "summary.ktsp(x)" or "summary(x)" for a ktsp object x.

Author(s)

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References

D. Geman, C. d'Avignon, D. Naiman and R. Winslow, "Classifying gene expression profiles from pairwise mRNA comparisons," Statist. Appl. in Genetics and Molecular Biology, 3, 2004.

A.C. Tan, D.Q. Naiman, L. Xu, R.L. Winslow, D. Geman, "Simple decision rules for classifying human cancers from gene expression profiles," Bioinformatics, 21: 3896-3904, 2005.

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See Also

ktspcalc, ktspplot, predict.ktsp, summary.ktsp

Examples

```
## Not run:
## Load data
data(ktspdata)
ktsp <- kts.pair(dat,grp,3)
summary.ktsp(ktsp, select=1)
summary(ktsp, select=1)
summary(ktsp, printall=FALSE)
summary(ktsp, printall=TRUE)

## End(Not run)
```

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