Package ‘orclus’

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Title Subspace Clustering Based on Arbitrarily Oriented Projected Cluster Generation
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Description Functions to perform subspace clustering and classification.
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R topics documented:

<table>
<thead>
<tr>
<th>Function</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>orclass</td>
<td>1</td>
</tr>
<tr>
<td>orclus</td>
<td>4</td>
</tr>
<tr>
<td>predict.orclass</td>
<td>7</td>
</tr>
<tr>
<td>predict.orclus</td>
<td>9</td>
</tr>
</tbody>
</table>

Index 11

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>orclass</td>
<td>Subspace clustering based local classification using ORCLUS.</td>
</tr>
</tbody>
</table>

Description

Function to perform local classification where the subclasses are concentrated in different subspaces of the data.
orclass

Usage

orclass(x, ...)

## Default S3 method:
orclass(x, grouping, k, l, k0, a = 0.5, prior = NULL, inner.loops = 1,
predict.train = "nearest", verbose = TRUE, ...)

## S3 method for class 'formula'
orclass(formula, data = NULL, ...)

Arguments

x
A matrix or data frame containing the explanatory variables. The method is
restricted to numerical data.

grouping
A factor specifying the class for each observation.

formula
A formula of the form grouping ~ x1 + x2 + ... That is, the response is the
grouping factor and the right hand side specifies the (non-factor) discriminators.

data
Data frame from which variables specified in formula are to be taken.

k
Prespecifies the final number of clusters.

l
Prespecifies the dimension of the final cluster-specific subspaces (equal for all
clusters).

k0
Initial number of clusters (that are computed in the entire data space). Must be
greater than k. The number of clusters is iteratively decreased by factor a until
the final number of k clusters is reached.

a
Prespecified factor for the cluster number reduction in each iteration step of the
algorithm.

prior
Argument for optional specification of class prior probabilities if different from
the relative class frequencies.

inner.loops
Number of repetitive iterations (i.e. recomputation of clustering and cluster-
specific subspaces) while the number of clusters and the subspace dimension
are kept constant.

predict.train
Character pecifying whether prediction of training data should be pursued. If
"nearest" the class distribution in orclus cluster assignment is used for clas-
sification.

verbose
Logical indicating whether the iteration process sould be displayed.

... Currently not used.

Details

For each cluster the class distribution is computed.

Value

Returns an object of class orclass.

orclus.res Object of class orclus containing the resulting clusters.
orclass

cluster.posteriors
Matrix of clusterwise class posterior probabilities where clusters are rows and classes are columns.

cluster.priors
Vector of relative cluster frequencies weighted by class priors.
purity
Statistics indicating the discriminability of the identified clusters.
prior
Vector of class prior probabilities.
predict.train
Prediction of training data if specified.
orclass.call
(Matched) function call.

Author(s)
Gero Szepannek

References

See Also
predict.orclass, orclus, predict.orclus

Examples
# definition of a function for parameterized data simulation
sim.orclus <- function(k = 3, nk = 100, d = 10, l = 4, sd.cl = 0.05, sd.rest = 1, locshift = 1){
  ### input parameters for data generation
  # k number of clusters
  # nk observations per cluster
  # d original dimension of the data
  # l subspace dimension where the clusters are concentrated
  # sd.cl (within cluster subspace) standard deviations for data generation
  # sd.rest standard deviations in the remaining space
  # locshift parameter of a uniform distribution to sample different cluster means
  x <- NULL
  for(i in 1:k){
    # cluster centers
    apts <- locshift*matrix(rnorm(l*k), ncol = l)
    # sample points in original space
    xi.original <- cbind(matrix(rnorm(nk * l, sd = sd.cl), ncol=l),
                        matrix(rnorm(nk * (d-l), sd = sd.rest), ncol = (d-l)))
    # subspace generation
    sym.mat <- matrix(rnorm(nk * (d-l), sd = sd.rest), ncol = (d-l)))
    for(m in 1:d){
      for(n in 1:m){
        sym.mat[m,n] <- sym.mat[n,m] <- runif(1)
      }
    }
  }
  return(x)
}
subspace <- eigen(sym.mat)$vectors
# transformation
xi.transformed <- xi.original %*% subspace
x <- rbind(x, xi.transformed)
}
coids <- rep(1:k, each = nk)
result <- list(x = x, cluster = clids)
return(result)

# simulate data of 2 classes where class 1 consists of 2 subclasses
simdata <- sim.orclus(k = 3, nk = 200, d = 15, l = 4,
                      sd.cl = 0.05, sd.rest = 1, locshift = 1)

x <- simdata$x
y <- c(rep(1,400), rep(2,200))
res <- orclass(x, y, k = 3, l = 4, k0 = 15, a = 0.75)
res
# compare results
table(res$predict.train$class, y)

orclus

Arbitrarily ORiented projected CLUSter generation

Description

Function to perform subspace clustering where the clusters are concentrated in different cluster specific subspaces of the data.

Usage

orclus(x, ...)
  ## Default S3 method:
  orclus(x, k, l, k0, a = 0.5, inner.loops = 1, verbose = TRUE, ...)

Arguments

- **x**: A matrix or data frame containing the explanatory variables. The method is restricted to numerical data.
- **k**: Prespecifies the final number of clusters.
- **l**: Prespecifies the dimension of the final cluster-specific subspaces (equal for all clusters).
- **k0**: Initial number of clusters (that are computed in the entire data space). Must be greater than k. The number of clusters is iteratively decreased by factor a until the final number of k clusters is reached.
The function performs ORCLUS subspace clustering (Aggarwal and Yu, 2000). Simultaneously both cluster assignments as well as cluster specific subspaces are computed. Cluster assignments have minimal euclidean distance from the cluster centers in the corresponding subspaces. As an extension to the originally proposed algorithm initialization in the full data space is done by calling \texttt{kmeans} for \( k_0 \) clusters. Further, by \texttt{inner.loops} a number of repetitions during the iteration process for each number of clusters and subspace dimension can be specified. An outlier option has not been implemented. Even though increasing the initialization parameter \( k_0 \) most strongly effects the computation time it should be chosen as large as possible (at least several times greater then \( k \)).

### Value

Returns an object of class \texttt{orclus}. Its structure is similar to objects resulting from calling \texttt{kmeans}.

- \texttt{cluster} Returns the final cluster labels.
- \texttt{centers} A matrix where each row corresponds to a cluster center (in the original space).
- \texttt{size} The final number of observations in each cluster.
- \texttt{subspaces} List of matrices for projection of the data onto the cluster-specific subspaces by post-multiplication.
- \texttt{subspace.dimension} Dimension of the final subspaces.
- \texttt{within.projensus} Corresponds to \texttt{withinss} of \texttt{kmeans} objects: projected within cluster energies for each cluster.
- \texttt{sparsity.coefficient} Sparsity coefficient of the clustering result. If its value is close to 1 the subspace dimension may have been chosen too large. A small value close to 0 can be interpreted as a hint that a strong cluster structure has been found.

### Author(s)

Gero Szepannek

### References

See Also

predict.orclus

Examples

# generate simple artificial example of two clusters
clus1.v1 <- runif(100)
clus2.v1 <- runif(100)
xample <- rbind(cbind(clus1.v1, 0.5 - clus1.v1), cbind(clus2.v1, -0.5 + clus2.v1))
plot(xample, col=rep(1:2, each=100))

# try standard kmeans clustering
kmeans.res <- kmeans(xample, 2)
plot(xample, col = kmeans.res$cluster)

# use orclus instead
orclus.res <- orclus(x = xample, k = 2, l = 1, k0 = 8, a = 0.5)
plot(xample, col = orclus.res$cluster)

# show data in cluster-specific subspaces
par(mfrow=c(1,2))
for(i in 1:length(orclus.res$size)) plot(xample %*% orclus.res$subspaces[[i]],
     col = orclus.res$cluster, ylab = paste("Identified subspace for cluster",i))

### second 'more multivariate' example to play with...

# definition of a function for parameterized data simulation
sim.orclus <- function(k = 3, nk = 100, d = 10, l = 4,
                        sd.cl = 0.05, sd.rest = 1, locshift = 1){
    ### input parameters for data generation
    # k number of clusters
    # nk observations per cluster
    # d original dimension of the data
    # l subspace dimension where the clusters are concentrated
    # sd.cl (within cluster subspace) standard deviations for data generation
    # sd.rest standard deviations in the remaining space
    # locshift parameter of a uniform distribution to sample different cluster means
    x <- NULL
    for(i in 1:k){
        # cluster centers
        apts <- locshift*matrix(runif(l*k), ncol = l)
        # sample points in original space
        xi.original <- cbind(matrix(rnorm(nk * l, sd = sd.cl), ncol=l) + matrix(rep(apts[i,], nk),
                                           ncol = l, byrow = TRUE),
                           matrix(rnorm(nk * (d-l), sd = sd.rest), ncol = (d-l)))
        # subspace generation
        sym.mat <- matrix(rnorm(nk * (d-l), sd = sd.rest), ncol = (d-l)))
        for(m in 1:d){
            for(n in 1:m){
                sym.mat[m,n] <- sym.mat[n,m] <- runif(1)
predict.orclass

The function `predict.orclass` is used to assign clusters and distances and classes for new data according to the intrinsic subspace clusters of an `orclass` classification model.

### Description

Assigns clusters and distances and classes for new data according to the intrinsic subspace clusters of an `orclass` classification model.

### Usage

```r
## S3 method for class 'orclass'
predict(object, newdata, type = "nearest", ...)  
```

### Arguments

- **object**: Model resulting from a call of `orclass`.
- **newdata**: A matrix or data frame to be clustered by the given model.
- **type**: Default "nearest" computes relative class frequencies of nearest cluster as class posterior probabilities.
- **...**: Currently not used.
Details

For prediction the class distribution of the "nearest" cluster is used. If type = "fuzzywts" cluster memberships (see e.g. Bezdek, 1981) are computed based on the cluster distances of cluster assignment by predict.orclus. For orclass prediction the class distributions of the clusters are weighted using the cluster memberships of an observation.

Value

class Vector of predicted class levels.
posterior Matrix where columns contain class posterior probabilities.
distances A matrix where columns are the distances to all cluster centers in the corresponding subspaces for the new data.
cluster The resulting cluster labels for the new data.

Author(s)

Gero Szepannek

References


See Also

orclass, orclus, predict.orclus

Examples

# definition of a function for parameterized data simulation
sim.orclus <- function(k = 3, nk = 100, d = 10, l = 4,
                        sd.cl = 0.05, sd.rest = 1, locshift = 1){
    ### input parameters for data generation
    # k number of clusters
    # nk observations per cluster
    # d original dimension of the data
    # l subspace dimension where the clusters are concentrated
    # sd.cl (within cluster subspace) standard deviations for data generation
    # sd.rest standard deviations in the remaining space
    # locshift parameter of a uniform distribution to sample different cluster means
    x <- NULL
    for(i in 1:k){
        # cluster centers
        apts <- locshift*matrix(runif(l*k), ncol = l)
        # sample points in original space
        xi.original <- cbind(matrix(rnorm(nk * l, sd = sd.cl), ncol = l) + matrix(rep(apts[1,], nk),
predict.orclus

ncol = l, byrow = TRUE),
    matrix(rnorm(nk * (d-l), sd = sd.rest), ncol = (d-l)))

# subspace generation
sym.mat <- matrix(nrow=d, ncol=d)
for(m in 1:d){
  for(n in 1:m){
    sym.mat[m,n] <- sym.mat[n,m] <- runif(1)
  }
}
subspace <- eigen(sym.mat)$vectors
# transformation
xi.transformed <- xi.original %*% subspace
x <- rbind(x, xi.transformed)
clids <- rep(1:k, each = nk)
result <- list(x = x, cluster = clids)
return(result)

# simulate data of 2 classes where class 1 consists of 2 subclasses
simdata <- sim.orclus(k = 3, nk = 200, d = 15, l = 4,
    sd.cl = 0.05, sd.rest = 1, locshift = 1)
x <- simdata$x
y <- c(rep(1,400), rep(2,200))
res <- orclass(x, y, k = 3, l = 4, k0 = 15, a = 0.75)
prediction <- predict(res, x)

# compare results
table(prediction$class, y)

predict.orclus

Arbitrarily ORiented projected CLUSter generation

Description

Assigns clusters and distances to cluster centers in the corresponding subspaces for new data according to a subspace clustering model of class orclus.

Usage

## S3 method for class 'orclus'
predict(object, newdata, ...)

Arguments

object       Model resulting from a call of orclus.
newdata     A matrix or data frame to be clustered by the given model.
...          Currently not used.
Value

- **distances**: A matrix where columns are the distances to all cluster centers in the corresponding subspaces for the new data.

- **cluster**: The resulting cluster labels for the new data.

Author(s)

Gero Szepannek

References


See Also

orclus

Examples

```r
# generate simple artificial example of two clusters
clus1.v1 <- runif(100)
clus2.v1 <- runif(100)
xample <- rbind(cbind(clus1.v1, 0.5 - clus1.v1), cbind(clus2.v1, -0.5 + clus2.v1))

orclus.res <- orclus(x = xample, k = 2, l = 1, k0 = 8, a = 0.5)

# generate new data and predict it using the
newclus1.v1 <- runif(100)
newclus2.v1 <- runif(100)
true.clusterids <- rep(1:2, each = 100)
xample2 <- rbind(cbind(newclus1.v1, 0.5 - newclus1.v1),
                 cbind(newclus2.v1, -0.5 + newclus2.v1))

orclus.prediction <- predict(orclus.res, xample2)
table(orclus.prediction$cluster, true.clusterids)
```
Index

* classif
  orclass, 1
  orclus, 4
  predict.orclass, 7
  predict.orclus, 9
* cluster
  orclass, 1
  orclus, 4
  predict.orclass, 7
  predict.orclus, 9
* multivariate
  orclass, 1
  orclus, 4
  predict.orclass, 7
  predict.orclus, 9

kmeans, 5

orclass, 1, 7, 8
orclus, 3, 4, 8–10

predict.orclass, 3, 7
predict.orclus, 3, 6, 8, 9
print.orclass (orclass), 1
print.orclus (orclus), 4