Package ‘bigutilsr’

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as_model_matrix

Transform a data frame

Description

Transform a data frame into a matrix using one hot encoding.

Usage

as_model_matrix(df, intercept = FALSE)

Arguments

df A data frame.

intercept Whether to have a column with all 1s. Default is FALSE.

Value

A matrix.

Examples

mat <- as_model_matrix(iris)
str(mat)
Description

Deprecated

Usage

covRob(data, ...)

Arguments

data A matrix.
...
Not used.

See Also

bigutilsr::covrob_ogk() bigutilsr::dist_ogk()

covrob_ogk Robust Location and Scatter Estimation - Ortogonalized
Gnanadesikan-Kettenring (OGK)

Description

Computes a robust multivariate location and scatter estimate with a high breakdown point, using the
pairwise algorithm proposed by Marona and Zamar (2002) which in turn is based on the pairwise
robust estimator proposed by Gnanadesikan-Kettenring (1972).

Usage

covrob_ogk(U, niter = 2, beta = 0.9)
dist_ogk(U, niter = 2, beta = 0.9)

Arguments

U A matrix with no missing values and at least 2 columns.
niter Number of number of iterations for the first step of the algorithm, usually 1 or 2
since iterations beyond the second do not lead to improvement.
beta Coverage parameter for the final reweighted estimate. Default is 0.9.
Details

The method proposed by Maronna and Zamar (2002) allows to obtain positive-definite and almost affine equivariant robust scatter matrices starting from any pairwise robust scatter matrix. The default robust estimate of covariance between two random vectors used is the one proposed by Gnanadesikan and Kettenring (1972) but the user can choose any other method by redefining the function in slot vrob of the control object CovControlOgk. Similarly, the function for computing the robust univariate location and dispersion used is the tau scale defined in Yohai and Zamar (1998) but it can be redefined in the control object.

The estimates obtained by the OGK method, similarly as in CovMcd are returned as ‘raw’ estimates. To improve the estimates a reweighting step is performed using the coverage parameter beta and these reweighted estimates are returned as ‘final’ estimates.

Value
covrob_ogk(): list of robust estimates, $cov and $center.
dist_ogk(): vector of robust Mahalanobis (squared) distances.

References


See Also

rrcov::CovOgk()
stats::mahalanobis()

Examples

X <- readRDS(system.file("testdata", "three-pops.rds", package = "bigutilsr"))
svd <- svds(scale(X), k = 5)

U <- svd$u
dist <- dist_ogk(U)
str(dist)
Outlier detection (histogram)

Description

Outlier detection based on departure from histogram. Suitable for compact values (need a space between main values and outliers).

Usage

```r
hist_out(x, breaks = nclass.scottRob, pmax_out = 0.2, nboot = NULL)
```

Arguments

- **x**: Numeric vector (with compact values).
- **breaks**: Same parameter as for `hist()`. Default uses a robust version of Scott's rule. You can also use "FD" or `nclass.FD` for a bit more bins.
- **pmax_out**: Percentage at each side that can be considered outliers at each step. Default is 0.2.
- **nboot**: Number of bootstrap replicates to estimate limits more robustly. Default is NULL (no bootstrap, even if I would recommend to use it).

Value

A list with

- **x**: the initial vector, whose outliers have been removed,
- **lim**: lower and upper limits for outlier removal,
- **all_lim**: all bootstrap replicates for `lim` (if `nboot` not NULL).

Examples

```r
set.seed(1)
x <- rnorm(1000)
str(hist_out(x))

# Easy to separate
x2 <- c(x, rnorm(50, mean = 7))
hist(x2, breaks = nclass.scottRob)
str(hist_out(x2))

# More difficult to separate
x3 <- c(x, rnorm(50, mean = 6))
hist(x3, breaks = nclass.scottRob)
str(hist_out(x3))
str(hist_out(x3, nboot = 999))
```
knn_parallel

Find K nearest neighbours for multiple query points

Description

Find K nearest neighbours for multiple query points

Usage

knn_parallel(data, query = data, k, ..., ncores = bigparallelr::nb_cores())

Arguments

data Mxd matrix of M target points with dimension d
query Nxd matrix of N query points with dimension d (nb data and query must have same dimension). If missing defaults to data i.e. a self-query.
k an integer number of nearest neighbours to find
... Arguments passed on to nabor::knn
eps An approximate error bound. The default of 0 implies exact matching.
searchtype A character vector or integer indicating the search type. The default value of 1L is equivalent to "auto". See details.
radius Maximum radius search bound. The default of 0 implies no radius bound.
ncores Number of cores to use. Default uses bigparallelr::nb_cores().

Value

A list with elements nn.idx (1-indexed indices) and nn.dist (distances), both of which are N x k matrices. See details for the results obtained with 1 invalid inputs.

Examples

## Not run: knn_parallel(matrix(1:4, 2), k = 2, ncores = 2)
**Description**

LOF: Identifying Density-Based Local Outliers.

**Usage**

```r
LOF(
  U,
  seq_k = c(4, 10, 30),
  combine = max,
  robMaha = FALSE,
  log = TRUE,
  ncores = 1
)
```

**Arguments**

- **U** A matrix, from which to detect outliers (rows). E.g. PC scores.
- **seq_k** Sequence of numbers of nearest neighbors to use. If multiple k are provided, this returns the combination of statistics. Default is c(4, 10, 30) and use max to combine (see combine).
- **combine** How to combine results for multiple k? Default uses max.
- **robMaha** Whether to use a robust Mahalanobis distance instead of the normal euclidean distance? Default is FALSE, meaning using euclidean.
- **log** Whether to return the logarithm of LOFs? Default is TRUE.
- **ncores** Number of cores to use. Default is 1.

**References**


**See Also**

`prob_dist()`

**Examples**

```r
X <- readRDS(system.file("testdata", "three-pops.rds", package = "bigutilsr"))
svd <- svds(scale(X), k = 10)

llof <- LOF(svd$u)
hist(llof, breaks = nclass.scottRob)
```
maha_trans

Transform matrix

Description
Transform matrix to use Mahalanobis distance instead of Euclidean one.

Usage
maha_trans(U, estim = covrob_ogk(U))

Arguments

U
A matrix (e.g. PC scores).

estim
List of location and scatter estimates, $cov$ and $center$.

Value
U, transformed.

Examples

X <- readRDS(system.file("testdata", "three-pops.rds", package = "bigutilsr"))
svd <- svds(scale(X), k = 5)
U <- svd$s
dist1 <- dist_ogk(U)
U.maha <- maha_trans(U)
dist2 <- rowSums(U.maha^2)
all.equal(dist2, dist1)
nclass.scottRob

Compute the Number of Classes for a Histogram

Description
Compute the Number of Classes for a Histogram

Usage
nclass.scottRob(x)

Arguments
x a data vector.

Value
The suggested number of classes.

References

Examples
x <- rnorm(1000)
hist(x, breaks = nclass.scott)
hist(x, breaks = nclass.scottRob)

x2 <- c(x, rnorm(50, mean = 50))
hist(x2, breaks = nclass.scott)
hist(x2, breaks = nclass.scott, xlim = c(-5, 5))
hist(x2, breaks = nclass.scottRob, xlim = c(-5, 5))

pca_nspike
Number of spikes in PCA

Description
Estimate the number of distant spikes based on the histogram of eigenvalues.

Usage
pca_nspike(eigval, breaks = "FD", nboot = 100)
Arguments

- **eigval**: Eigenvalues (squared singular values).
- **breaks**: Same parameter as for `hist()`. Default uses a robust version of Scott’s rule. You can also use "FD" or `nclass.FD` for a bit more bins.
- **nboot**: Number of bootstrap replicates to estimate limits more robustly. Default is 100.

Value

The estimated number of distant spikes.

Examples

```r
N <- 400; M <- 2000; K <- 8
U <- matrix(0, N, K); U[] <- rnorm(length(U))
V <- matrix(0, M, K); V[] <- rnorm(length(V))
# X = U V^T + E
X <- tcrossprod(U, V) + 15 * rnorm(N * M)
pca <- prcomp(X)
eigval <- pca$sdev^2
plot(head(eigval, -1), log = "xy", pch = 20)
pca_nspike(eigval)
```

---

**pca_OADP_proj**  
**OADP projection**

Description

Online Augmentation, Decomposition, and Procrustes (OADP) projection of PC loadings onto some study data `X`.

Usage

```r
pca_OADP_proj(X, loadings, sval)
pca_OADP_proj2(XV, X_norm, sval)
```

Arguments

- **X**: Data to get PC loadings into.
- **loadings**: PC loadings of the reference PCA to project.
- **sval**: Singular values of the reference PCA (sqrt of the eigen values). Only the `ncol(loadings)` first ones will be used.
- **XV**: `X %*% loadings`
- **X_norm**: Vector of sums of squared rows (e.g. `rowSums(X^2)`).
Value

- `pca_OADP_proj()`: A list with the simple projection \( X \times \text{loadings} \) and the projection based on OADP.
- `pca_OADP_proj2()`: The projection based on OADP only (a matrix of same size of \( XV \)).

Examples

```r
X <- readRDS(system.file("testdata", "three-pops.rds", package = "bigutilsr"))
N <- 400; M <- ncol(X)
ind <- sample(nrow(X), N)

# Compute SVD using one part of samples
svd <- svds(X[ind, ], k = 5)
U <- sweep(svd$u, 2, svd$d, "/\text{Var}\)
col <- 2:3
plot(U[, col])
points(cbind(0, 0), pch = 8, col = "green", cex = 2)

# Projecting other samples
proj <- pca_OADP_proj(X = X[-ind, ], loadings = svd$v, sval = svd$d)
points(proj$simple_proj[, col], col = "red", pch = 20)  # shrunk towards 0
points(proj$OADP_proj[, col], col = "blue", pch = 20)  # unshrunk
```

predict.Procrustes  

**Predict method**

Description

Predict method for class Procrustes.

Usage

```r
## S3 method for class 'Procrustes'
predict(object, X, ...)
```

Arguments

- `object`  
  Object of class Procrustes.
- `X`  
  New matrix to transform.
- `...`  
  Not used.

Value

\( X \), transformed.

See Also

`procrustes()`.
prob_dist  

**Probabilistic set distance**

**Description**

Probabilistic set distance

**Usage**

```
prob_dist(U, kNN = 5, robMaha = FALSE, ncores = 1)
```

**Arguments**

- `U`  
  A matrix, from which to detect outliers (rows). E.g. PC scores.

- `kNN`  
  Number of nearest neighbors to use. Default is 5.

- `robMaha`  
  Whether to use a robust Mahalanobis distance instead of the normal euclidean distance? Default is FALSE, meaning using euclidean.

- `ncores`  
  Number of cores to use. Default is 1.

**References**


**See Also**

LOF()

**Examples**

```r
X <- readRDS(system.file("testdata", "three-pops.rds", package = "bigutilsr"))
svd <- svds(scale(X), k = 10)
U <- svd$u

test <- prob_dist(U)
plof <- test$dist.self / test$dist.nn
plof_ish <- test$dist.self / sqrt(test$dist.nn)
plot(U[, 1:2], col = (plof_ish > tukey_mc_up(plof_ish)) + 1, pch = 20)
plot(U[, 3:4], col = (plof_ish > tukey_mc_up(plof_ish)) + 1, pch = 20)
plot(U[, 5:6], col = (plof_ish > tukey_mc_up(plof_ish)) + 1, pch = 20)
```
Procrustes

Description

Procrustes transform \( Y = pXR \) (after centering), where \( p \) is a scaling coefficient and \( R \) is a rotation matrix that minimize \( \|Y - pXR\|_F \).

Usage

procrustes(Y, X, n_iter_max = 1000, epsilon_min = 1e-07)

Arguments

Y Reference matrix.
X Matrix to transform (\( ncol(X) \geq ncol(Y) \)).
n_iter_max Maximum number of iterations. Default is 1000.
epsilon_min Convergence criterion. Default is 1e-7.

Value

Object of class "procrustes", a list with the following elements:

- SR: the rotation matrix to apply to \( X \),
- Srho: the scaling coefficient to apply to \( X \),
- Sc: the column centering to apply to the resulting matrix,
- Sdiff: the average difference between \( Y \) and \( X \) transformed.

You can use method predict() to apply this transformation to other data.

Examples

A <- matrix(rnorm(200), ncol = 20)
B <- matrix(rnorm(length(A)), nrow = nrow(A))

proc <- procrustes(B, A)
str(proc)
plot(B, predict(proc, A)); abline(0, 1, col = "red")
### rollmean

**Gaussian smoothing**

**Description**

Gaussian smoothing

**Usage**

`rollmean(x, size)`

**Arguments**

- `x`: Numeric vector.
- `size`: Radius of the smoothing (smaller than half of the length of `x`). If using `size = 0`, it returns `x`.

**Value**

Numeric vector of the same length as `x`, smoothed.

**Examples**

```r
(x <- rnorm(10))
rollmean(x, 3)
```

---

### tukey_mc_up

**Outlier detection threshold (upper)**

**Description**

Outlier detection threshold (upper) based on Tukey’s rule, corrected for skewness using the ‘medcouple’, and possibly corrected for multiple testing.

**Usage**

`tukey_mc_up(x, coef = NULL, alpha = 0.05, a = -4, b = 3)`
Arguments

- x: Numeric vector. Should be somewhat normally distributed.
- coef: Number determining how far 'whiskers' extend out from the box. If NULL (default), this is computed to get an type-I error of alpha, after adjusting for multiple testing. A standard value to use is 1.5.
- alpha: See coef. Default is 0.05.
- a and b: Scaling factors multiplied by the medcouple \( \text{mc}() \) to determine outlier boundaries; see the references.

References


See Also

- `robustbase::adjbox()`

Examples

```r
hist(x <- c(rnorm(3, m = 6), rnorm(1e4, m = 0)))
(q <- tukey_mc_up(x))
abline(v = q, col = "red")
which(x > q)
```
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