Package 'shapes'

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Title Statistical Shape Analysis

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Author Ian L. Dryden

Description Routines for the statistical analysis of landmark
shapes, including Procrustes analysis, graphical displays, principal
components analysis, permutation and bootstrap tests, thin-plate
spline transformation grids and comparing covariance matrices.
See Dryden, I.L. and Mardia, K.V. (2016). Statistical shape analysis,
with Applications in R (2nd Edition), John Wiley and Sons.

Maintainer Ian Dryden <ian.dryden@nottingham.ac.uk>

Imports minpack.lm, scatterplot3d, rgl, MASS

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R topics documented:

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apes	*Great ape data*

Description

Great ape skull landmark data. 8 landmarks in 2 dimensions, 167 individuals

Usage

```
data(apes)
```

Format

apes$x : An array of dimension 8 x 2 x 167

apes$group : Species and sex of each specimen: "gorf" 30 female gorillas, "gorm" 29 male gorillas, "panf" 26 female chimpanzees, "pamm" 28 male chimpanzees, "pongof" 24 female orang utans, "pongom" 30 male orang utans.

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester.

O'Higgins, P. and Dryden, I. L. (1993). Sexual dimorphism in hominoids: further studies of craniofacial shape differences in Pan, Gorilla, Pongo, Journal of Human Evolution, 24, 183-205.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(apes)
par(mfrow=c(1,2))
plotshapes(apes$x[,,apes$group=="gorf"],symbol="f")
plotshapes(apes$x[,,apes$group=="gorm"],symbol="m")
```

---

backfit	*Backfit from scores to configuration*

Description

Backfit from PNSS or PCA scores to a representative configuration

Usage

```
backfit(scores, x, type="pnss", size=1)
```

Arguments

scores	n x p matrix of scores
x	An object that is the output of either pnss3d (if type="pnss") or procGPA (if type="pca")
type	Either "pnss" for PNSS or "pca" for PCA
size	The centroid size of the backfitted configuration. The default is 1 but one can rescale the backfitting if desired.

Value

A k x m matrix of co-ordinates of the backfitted configuration

Author(s)

Ian Dryden

References

Dryden, I.L., Kim, K., Laughton, C.A. and Le, H. (2019). Principal nested shape space analysis of molecular dynamics data. Annals of Applied Statistics, 13, 2213-2234.

Jung, S., Dryden, I.L. and Marron, J.S. (2012). Analysis of principal nested spheres. Biometrika, 99, 551-568.

See Also

pns, pns4pc, plot3darcs

Examples

```
ans <- pnss3d( macf.dat, sphere.type="BIC", n.pc=8)
y <- backfit( ans$PNS$scores[1,] , ans ,type="pnss")
riemdist( macf.dat[,,1] , y )  #should be close to zero

ans2 <- procGPA( macf.dat, tangentcoords="partial")
y <- backfit( ans2$scores[1,] , ans2 ,type="pca")
riemdist( macf.dat[,,1] , y )  #should be close to zero
```

---

bookstein2d	*Bookstein's baseline registration for 2D data*

Description

Carries out Bookstein's baseline registration and calculates a mean shape

Usage

```
bookstein2d(A,l1=1,l2=2)
```

Arguments

A	a k x 2 x n real array, or k x n complex matrix, where k is the number of land-marks, n is the number of observations
l1	l1: an integer : l1 is sent to (-1/2,0) in the registration
l2	l2: an integer : l2 is sent to (1/2,0) in the registration

Value

A list with components:

k	number of landmarks
n	sample size
mshape	Bookstein mean shape with baseline l1, l2
bshpv	the k x n x 2 array of Bookstein shape variables, including the baseline

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester. Chapter 2.

Bookstein, F. L. (1986) Size and shape spaces for landmark data in two dimensions (with discussion). Statistical Science, 1:181-242.

Examples

```
data(gorf.dat)
data(gorm.dat)

bookf<-bookstein2d(gorf.dat)
bookm<-bookstein2d(gorm.dat)

plotshapes(bookf$mshape,bookm$mshape,joinline=c(1,6,7,8,2,3,4,5,1))
```

---

brains	*Brain landmark data*

Description

24 landmarks located in 58 adult healthy brains

Usage

```
data(brains)
```

Format

A list with components:

brains$x : An array of dimension 24 x 3 x 58 containing the landmarks in 3D

brains$sex : Sex of each volunteer (m or f)

brains$age : Age of each volunteer

brains$handed : Handedness of each volunteer (r or l)

brains$grp : group label: 1= right-handed males, 2=left-handed males, 3=right-handed females, 4=left-handed females

References

Free, S.L., O'Higgins, P., Maudgil, D.D., Dryden, I.L., Lemieux, L., Fish, D.R. and Shorvon, S.D. (2001). Landmark-based morphometrics of the normal adult brain using MRI. Neuroimage , 13 , 801–813.

Examples

```
data(brains)
# plot first three brains
shapes3d(brains$x[,,1:3])
```

---

centroid.size   *Centroid size*

Description

Calculate cetroid size from a configuration or a sample of configurations.

Usage

```
centroid.size(x)
```

Arguments

x   For a single configuration k x m matrix or complex k-vector

                    For a sample of configurations k x m x n array or k x n complex matrix

Value

Centroid size(s)

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester.

Examples

```
data(mice)
centroid.size(mice$x[,,1])
```

---

cortical   *Cortical surface data*

Description

Cortical surface data, from MR scans. Axial slice outlines with 500 points on each outline. 68 individuals.

Usage

```
data(cortical)
```

Format

cortical$age (age) cortical$group (Control, Schizophrenia) cortical$sex (1 = male, 2 = female) cortical$symm (a symmetry measure from the original 3D cortical surface)

cortical$x (500 x , y coordinates of an axial slice through the cortical surface intersecting the anterior and posterior commissures)

cortical$r (500 radii from equal angular polar coordinates)

Source

Brignell, C.J., Dryden, I.L., Gattone, S.A., Park, B., Leask, S., Browne, W.J. and Flynn, S. (2010). Surface shape analysis, with an application to brain surface asymmetry in schizophrenia. Biostatistics, 11, 609-630.

Dryden, I.L. (2005). Statistical analysis on high-dimensional spheres and shape spaces. Annals of Statistics, 33, 1643-1665

References

Original MR data from Sean Flynn (UBC) in collaboration with Bert Park (Nottingham).

Examples

```
data(cortical)
plotshapes(cortical$x)
```

---

digit3.dat   *Digit 3 data*

Description

Handwritten digit '3' data. 13 landmarks in 2 dimensions, 30 individuals

Usage

```
data(digit3.dat)
```

Format

An array of dimension 13 x 2 x 30

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

http://www.maths.nott.ac.uk/personal/ild/bookdata/digit3.dat

Data from Cath Anderson

Examples

```
data(digit3.dat)
k<-dim(digit3.dat)[1]
n<-dim(digit3.dat)[3]
plotshapes(digit3.dat,joinline=c(1:13))
```

---

distcov   *Compute a distance between two covariance matrices*

Description

Compute a distance between two covariance matrices, with non-Euclidean options.

Usage

```
distcov(S1, S2, method="Riemannian",alpha=1/2)
```

Arguments

S1	Input a covariance matrix (square, symmetric, positive definite)
S2	Input another covariance matrix of the same size
method	The type of distance to be used: "Procrustes": Procrustes size-and-shape metric, "ProcrustesShape": Procrustes metric with scaling, "Riemannian": Riemannian metric, "Cholesky": Cholesky based distance, "Power: Power Euclidean, with power alpha, "Euclidean": Euclidean metric, "LogEuclidean": Log-Euclidean metric, "RiemannianLe": Another Riemannian metric.
alpha	The power to be used in the power Euclidean metric

Value

The distance

Author(s)

Ian Dryden

References

Dryden, I.L., Koloydenko, A. and Zhou, D. (2009). Non-Euclidean statistics for covariance matrices, with applications to diffusion tensor imaging. Annals of Applied Statistics, 3, 1102-1123.

See Also

estcov

Examples

```
A <- diag(5)
B <- A + .1*matrix(rnorm(25),5,5)
S1<-A
S2<- B

distcov( S1, S2, method="Procrustes")
```

---

dna.dat	*DNA data*

Description

Part of a 3D DNA molecule moving in time, k = 22 atoms, 30 time points

Usage

```
data(dna.dat)
```

Format

An array of dimension 22 x 3 x 30

Examples

```
data(dna.dat)
plotshapestime3d(dna.dat)
```

---

estcov   *Weighted Frechet mean of covariance matrices*

Description

Computes the weighted Frechet means of an array of covariance matrices, with different options for the covariance metric. Also carries out principal co-ordinate analysis of the covariance matrices

Usage

```
estcov(S , method="Riemannian",weights=1,alpha=1/2,MDSk=2)
```

Arguments

S	Input an array of covariance matrices of size k x k x n where each matrix is square, symmetric and positive definite
method	The type of distance to be used: "Procrustes": Procrustes size-and-shape metric, "ProcrustesShape": Procrustes metric with scaling, "Riemannian": Riemannian metric, "Cholesky": Cholesky based distance, "Power: Power Euclidean, with power alpha, "Euclidean": Euclidean metric, "LogEuclidean": Log-Euclidean metric, "RiemannianLe": Another Riemannian metric.
weights	The weights to be used for calculating the mean. If weights=1 then equal weights are used, otherwise the vector must be of length n.
alpha	The power to be used in the power Euclidean metric
MDSk	The number of MDS components in the principal co-ordinate analysis

Value

A list with values

mean	The weighted mean covariance matrix
sd	The weighted standard deviation
pco	Principal co-ordinates (from multidimensional scaling with the metric)
eig	The eigenvalues from the principal co-ordinate analysis

Author(s)

Ian Dryden

References

Dryden, I.L., Koloydenko, A. and Zhou, D. (2009). Non-Euclidean statistics for covariance matrices, with applications to diffusion tensor imaging. Annals of Applied Statistics, 3, 1102-1123.

See Also

distcov

Examples

```
S <- array(0,c(5,5,10) )
for (i in 1:10){
tem <- diag(5)+.1*matrix(rnorm(25),5,5)
S[,,i]<- tem
}

estcov( S , method="Procrustes")
```

---

frechet   *Mean shape estimators*

Description

Calculation of different types of Frechet mean shapes, or the isotropic offset Gaussian MLE mean shape

Usage

```
frechet(x, mean="intrinsic")
```

Arguments

x
: Input k x m x n real array, where k is the number of points, m is the number of dimensions, and n is the sample size.

mean
: Type of mean shape. The Frechet mean shape is obtained by minimizing sum $d(x_i,mu)^2$ with respect to mu. Different estimators are obtained with different choices of distance d. "intrinsic" intrinsic mean shape (d = rho = Riemannian distance); "partial.procrustes" partial Procrustes (d = 2*sin(rho/2)); "full.procrustes" full Procrustes (d = sin(rho)); h (positive real number) M-estimator ($d^2 = (1 - cos^{2h}(rho))/h$) Kent (1992); "mle" - isotropic offset Gaussian MLE of Mardia and Dryden (1989)

Value

A list with components

mshape	Mean shape estimate
var	Minimized Frechet variance (not available for MLE)
kappa	(if available) The estimated kappa for the MLE
code	Code from optimization, as given by function nlm - should be 1 or 2
gradient	Gradient from the optimization, as given by function nlm - should be close to zero

Author(s)

Ian Dryden

References

Dryden, I. L. (1991). Discussion to 'Procrustes methods in the statistical analysis of shape' by C.R. Goodall. Journal of the Royal Statistical Society, Series B, 53:327-328.

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester.

Kent, J. T. (1992). New directions in shape analysis. In Mardia, K. V., editor, The Art of Statistical Science, pages 115-127. Wiley, Chichester.

Mardia, K. V. and Dryden, I. L. (1989b). The statistical analysis of shape data. Biometrika, 76:271-282.

See Also

procGPA

Examples

```
#2D example : female and male Gorillas (cf. Dryden and Mardia, 2016)

data(gorf.dat)
frechet(gorf.dat[,,1:4],mean="intrinsic")
```

---

gels *Electrophoresis gel data*

Description

Electrophoresis gel data. 10 invariant spots have been picked out by an expert on two electrophoretic gels.

Usage

```
data(gels)
```

Format

An array of dimension 10 x 2 x 2

Source

Dryden, I. L. and Walker, G. (1999). Highly resistant regression and object matching. Biometrics, 55, 820-825.

References

Data from Chris Glasbey (BioSS)

Examples

```
data(gels)
plotshapes(gels)
```

---

gorf.dat *Female gorilla data*

Description

Female gorilla skull data. 8 landmarks in 2 dimensions, 30 individuals

Usage

```
data(gorf.dat)
```

Format

An array of dimension 8 x 2 x 30

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

O'Higgins, P. and Dryden, I. L. (1993). Sexual dimorphism in hominoids: further studies of craniofacial shape differences in Pan, Gorilla, Pongo, Journal of Human Evolution, 24, 183-205.

References

http://www.maths.nott.ac.uk/personal/ild/bookdata/gorf.dat

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(gorf.dat)
plotshapes(gorf.dat)
```

---

gorm.dat   *Male gorilla data*

Description

Male gorilla skull data. 8 landmarks in 2 dimensions, 29 individuals

Usage

```
data(gorm.dat)
```

Format

An array of dimension 8 x 2 x 29

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

O'Higgins, P. and Dryden, I. L. (1993). Sexual dimorphism in hominoids: further studies of craniofacial shape differences in Pan, Gorilla, Pongo, Journal of Human Evolution, 24, 183-205.

References

http://www.maths.nott.ac.uk/personal/ild/bookdata/gorm.dat

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(gorm.dat)
plotshapes(gorm.dat)
```

groupstack	*Combine two or more groups of configurations*

Description

Combine two or more groups of configurations and create a group label vector. (Maximum 8 groups).

Usage

```
groupstack(A1, A2, A3=0, A4=0, A5=0, A6=0, A7=0, A8=0)
```

Arguments

A1	Input k x m x n real array of the Procrustes transformed configurations, where k is the number of points, m is the number of dimensions, and n is the sample size.
A2	Input k x m x n real array of the Procrustes original configurations, where k is the number of points, m is the number of dimensions, and n is the sample size.
A3	Optional array
A4	Optional array
A5	Optional array
A6	Optional array
A7	Optional array
A8	Optional array

Value

A list with components

x	The combined array of all configurations
groups	The group labels (integers)

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester.

See Also

procGPA

Examples

```
#2D example : female and male Gorillas (cf. Dryden and Mardia, 2016)

data(gorf.dat)
data(gorm.dat)

groupstack(gorf.dat,gorm.dat)
```

---

humanmove   *Human movement data*

Description

Human movement data. 4 landmarks in 2 dimensions, 5 individuals observed at 10 times.

Usage

```
data(humanmove)
```

Format

humanmove: An array of landmark configurations 4 x 2 x 10 x 5

Source

Alshabani, A. K. S. and Dryden, I. L. and Litton, C. D. and Richardson, J. (2007). Bayesian analysis of human movement curves, J. Roy. Statist. Soc. Ser. C, 56, 415–428.

References

Data from James Richardson.

Examples

```
data(humanmove)
#plotshapes(humanmove[,,,1])
#for (i in 2:5){
#for (j in 1:4){
#for (k in 1:10){
#points(humanmove[j,,k,i],col=i)
#}
#}
#}
```

---

macaques   *Male and Female macaque data*

Description

Male and female macaque skull data. 7 landmarks in 3 dimensions, 18 individuals (9 males, 9 females)

Usage

```
data(macaques)
```

Format

macaques$x : An array of dimension 7 x 3 x 18

macaques$group : A factor indicating the sex ('m' for male and 'f' for female)

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

Dryden, I. L. and Mardia, K. V. (1993). Multivariate shape analysis. Sankhya Series A, 55, 460-480.

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(macaques)
shapes3d(macaques$x[,,1])
```

---

macf.dat   *Female macaque data*

Description

Female macaque skull data. 7 landmarks in 3 dimensions, 9 individuals

Usage

```
data(macf.dat)
```

Format

An array of dimension 7 x 3 x 9

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(macf.dat)
plotshapes(macf.dat)
```

---

macm.dat   *Male macaque data*

Description

Male macaque skull data. 7 landmarks in 3 dimensions, 9 individuals

Usage

```
data(macm.dat)
```

Format

An array of dimension 7 x 3 x 9

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(macm.dat)
plotshapes(macm.dat)
```

---

mice	*T2 mouse vertabrae data*

Description

T2 mouse vertebrae data - 6 landmarks in 2 dimensions, in 3 groups (30 Control, 23 Large, 23 Small mice). The 6 landmarks are obtained using a semi-automatic method at points of high curvature. This particular strain of mice is the 'QE' strain. In addition pseudo-landmarks are given around each outlines.

Usage

```
data(mice)
```

Format

mice$x : An array of dimension 6 x 2 x 76 of the two dimensional co-ordinates of 6 landmarks for each of the 76 mice.

mice$group : Group labels. "c" Control, "l" Large, "s" Small mice

mice$outlines : An array of dimension 60 x 2 x 76 containing the 6 landmarks and 54 pseudo-landmarks, with 9 pseudo-landmarks approximately equally spaced between each pair of landmarks.

Source

Dryden, I.L. and Mardia, K.V. (1998). Statistical Shape Analysis, Wiley, Chichester. p313

References

Mardia, K. V. and Dryden, I. L. (1989). The statistical analysis of shape data. Biometrika, 76, 271-281.

Data from Paul O'Higgins (Hull-York Medical School) and David Johnson (Leeds)

Examples

```
data(mice)
plotshapes(mice$x,symbol=as.character(mice$group),joinline=c(1,6,2:5,1))
```

---

panf.dat   *Female chimpanzee data*

Description

Female chimpanzee skull data. 8 landmarks in 2 dimensions, 26 individuals

Usage

```
data(panf.dat)
```

Format

An array of dimension 8 x 2 x 26

Source

O'Higgins, P. and Dryden, I. L. (1993). Sexual dimorphism in hominoids: further studies of craniofacial shape differences in Pan, Gorilla, Pongo, Journal of Human Evolution, 24, 183-205.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(panf.dat)
plotshapes(panf.dat)
```

---

panm.dat   *Male chimpanzee data*

Description

Male chimpanzee skull data. 8 landmarks in 2 dimensions, 28 individuals

Usage

```
data(panm.dat)
```

Format

An array of dimension 8 x 2 x 28

Source

O'Higgins, P. and Dryden, I. L. (1993). Sexual dimorphism in hominoids: further studies of cran-iofacial shape differences in Pan, Gorilla, Pongo, Journal of Human Evolution, 24, 183-205.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(panm.dat)
plotshapes(panm.dat)
```

---

plot3darcs   *Modes of variation plots for PCA and PNSS*

Description

Modes of variation plots for PCA and PNSS based on 3D views and arcs along a mode. c * sd : the extent along lower and upper principal arcs.

The lower principal arc -> 0 -> upper principal arc has a total of 2*nn+1 configurations with: nn configurations along the negative principal arc to 0; one configuration at the PNS mean; nn configurations along the positive principal arc.

Usage

```
plot3darcs(x,pcno=1,c=1,nn=100,boundary.data=TRUE,view.theta=0,view.phi=0,type="pnss")
```

Arguments

x	Output from pnss3d
pcno	The number of the PC/PNSS component. The default is 1, the first PC/PNSS
c	Number of standard deviations along each arc
nn	In total 2 * nn + 1 configurations: n configurations on arc from negative to 0; 1 configuration at 0; nn configurations from 0 to positive
boundary.data	Logical for whether to use boundary data or not.
view.theta	Viewing angle theta
view.phi	Viewing angle phi
type	"pnss" principal nested sphere mean and arc, or "pca" Procrustes mean and linear PC.

Value

A list with components

PNSmean	the PNSS mean
lu.arc	the configurations along the arc

Author(s)

Kwang-Rae Kim, Ian Dryden

References

Dryden, I.L., Kim, K., Laughton, C.A. and Le, H. (2019). Principal nested shape space analysis of molecular dynamics data. Annals of Applied Statistics, 13, 2213-2234.

Jung, S., Dryden, I.L. and Marron, J.S. (2012). Analysis of principal nested spheres. Biometrika, 99, 551-568.

See Also

pns, pns4pc, pnss3d

Examples

```
ans <- pnss3d(digit3.dat, sphere.type="BIC", n.pc=5)
#aa <- plot3darcs(ans,c=2,pcno=1)
#bb <- plot3darcs(ans,c=2,pcno=1,type="pca")
```

---

plotshapes   *Plot configurations*

Description

Plots configurations. Either one or two groups of observations can be plotted on the same scale.

Usage

```
plotshapes(A, B = 0, joinline = c(1, 1),orthproj=c(1,2),color=1,symbol=1)
```

Arguments

A	k x m x n array, or k x m matrix for first group
B	k x m x n array, or k x m matrix for 2nd group (can be missing)
joinline	A vector stating which landmarks are joined up by lines, e.g. joinline=c(1:n,1) will start at landmark 1, join to 2, ..., join to n, then re-join to landmark 1.
orthproj	A vector stating which two orthogonal projections will be used. For example, for m=3 dimensional data: X-Y projection given by c(1,2) (default), X-Z projection given by c(1,3), Y-Z projection given by c(2,3).
color	Colours for points. Can be a vector, e.g. 1:k gives each landmark a different colour for the specimens
symbol	Plotting symbols. Can be a vector, e.g. 1:k gives each landmark a different symbol for the specimens

Value

Just graphical output

Author(s)

Ian Dryden

See Also

shapepca,tpsgrid

Examples

```
data(gorf.dat)
data(gorm.dat)
plotshapes(gorf.dat,gorm.dat,joinline=c(1,6,7,8,2,3,4,5,1))

data(macm.dat)
data(macf.dat)
plotshapes(macm.dat,macf.dat)
```

---

pns   *Principal Nested Spheres*

Description

Calculation of Principal Nested Spheres

Usage

```
pns(x, sphere.type = "seq.test", alpha = 0.1, R = 100,
                        nlast.small.sphere = 1, output=TRUE)
```

Arguments

x	a (d + 1) x n data matrix where each column is a unit vector in S^d and n is the sample size.
sphere.type	a character string specifying the type of sphere fitting method. "seq.test" specifies sequential tests to decide either "small" or "great"; "small" specifies Principal Nested SMALL Sphere; "great" specifies Principal Nested GREAT Sphere (radius pi/2); "BIC" specifies BIC statistic to decide either "small" or "great"; and "bi.sphere" specifies Principal Nested GREAT Sphere for the first part and Principal Nested SMALL Sphere for last parts. The default is "seq.test".
alpha	significance level (0 < alpha < 1) used when sphere.type = "seq.test". The default is 0.1.
R	the number of bootstrap samples to be evaluated for the sequential test. The default is 100.

nlast.small.sphere

        the number of small spheres in the finishing part used when sphere.type = "bi.sphere".

output   Logical. If TRUE then plots and some brief printed summaries are given. If FALSE then no plots or output is given.

Value

A list with components

resmat	the residual matrix (X_PNS). Each entry in row k works like the kth principal component
$PNS	= the list with the following components.
radii	the size (radius) of PNS.
orthaxis	the orthogonal axis v_i of subspheres.
dist	the distance r_i of subspheres
pvalues	the p-values of LRT and parametric boostrap tests (if any).
ratio	the estimated ratios. Now unavailable.
mean	the location of the PNS mean.
sphere.type	the type of method for fitting subspheres.
percent	proportion of variances explained.
spherePNS	The co-ordinates of the data points projected to the sphere in 3D (also plotted)
circlePNS	The co-ordinates of the 2D circle projections on the sphere in 3D (also plotted)

Author(s)

Kwang-Rae Kim: R translation of Sungkyu Jung's matlab code

References

Dryden, I.L., Kim, K., Laughton, C.A. and Le, H. (2019). Principal nested shape space analysis of molecular dynamics data. Annals of Applied Statistics, 13, 2213-2234.

Jung, S., Dryden, I.L. and Marron, J.S. (2012). Analysis of principal nested spheres. Biometrika, 99, 551-568.

See Also

pns4pc, pnss3d

Examples

```
#  out <- pc2sphere(x = gorf.dat, n.pc = 2)
#  spheredata <- t(out$spheredata)
#  pns.out <- pns(x = spheredata)
```

---

pns4pc   *Principal Nested Shape Spaces from PCA*

Description

Approximation of Principal Nested Shapes Spaces using PCA

Usage

```
pns4pc(x, sphere.type = "seq.test", alpha = 0.1, R = 100, nlast.small.sphere = 1,n.pc=2)
```

Arguments

x	k x m x n array of landmark data.
sphere.type	a character string specifying the type of sphere fitting method. "seq.test" specifies sequential tests to decide either "small" or "great"; "small" specifies Principal Nested SMALL Sphere; "great" specifies Principal Nested GREAT Sphere (radius pi/2); "BIC" specifies BIC statistic to decide either "small" or "great"; and "bi.sphere" specifies Principal Nested GREAT Sphere for the first part and Principal Nested SMALL Sphere for The default is "seq.test".
alpha	significance level (0 < alpha < 1) used when sphere.type = "seq.test". The default is 0.1.
R	the number of bootstrap samples to be evaluated for the sequential test. The default is 100.
nlast.small.sphere	
	the number of small spheres in the finishing part used when sphere.type = "bi.sphere".
n.pc	the number of PC scores to be used (n.pc >= 2)

Value

A list with components

PNS	the output of the function pns
GPAout	the result of GPA
spheredata	transformed spherical data from the PC scores
percent	proportion of variances explained.

Author(s)

Kwang-Rae Kim

References

Dryden, I.L., Kim, K., Laughton, C.A. and Le, H. (2019). Principal nested shape space analysis of molecular dynamics data. Annals of Applied Statistics, 13, 2213-2234.

Jung, S., Dryden, I.L. and Marron, J.S. (2012). Analysis of principal nested spheres. Biometrika, 99, 551-568.

See Also

pns, pns4pc, pnss3d, plot3darcs

Examples

```
pns4pc(digit3.dat,n.pc=2)
```

---

pnss3d   *Principal Nested Shape Space Analysis*

Description

Approximation of Principal Nested Shapes Spaces using PCA: 2D or 3D data, small or large samples

Usage

```
pnss3d(x,sphere.type="seq.test",alpha = 0.1,R = 100,
                    nlast.small.sphere = 1,n.pc="Full",output=TRUE)
```

Arguments

x	k x m x n array of landmark data.
sphere.type	a character string specifying the type of sphere fitting method. "seq.test" specifies sequential tests to decide either "small" or "great"; "small" specifies Principal Nested SMALL Sphere; "great" specifies Principal Nested GREAT Sphere (radius pi/2); "BIC" specifies BIC statistic to decide either "small" or "great"; and "bi.sphere" specifies Principal Nested GREAT Sphere for the first part and Principal Nested SMALL Sphere for the last part. The default is "seq.test".
alpha	significance level ($0 <$ alpha < 1) used when sphere.type = "seq.test". The default is 0.1.
R	the number of bootstrap samples to be evaluated for the sequential test. The default is 100.
nlast.small.sphere	
	the number of small spheres in the finishing part used when sphere.type = "bi.sphere".
n.pc	the number of PC scores to be used (n.pc >= 2)
output	Logical. If TRUE then plots and some brief printed summaries are given. If FALSE then no plots or output is given.

Value

A list with components

PNS	the output of the function pns
GPAout	the result of GPA
spheredata	transformed spherical data from the PC scores
percent	proportion of variances explained.

Author(s)

Kwang-Rae Kim, Ian Dryden

References

Dryden, I.L., Kim, K., Laughton, C.A. and Le, H. (2019). Principal nested shape space analysis of molecular dynamics data. Annals of Applied Statistics, 13, 2213-2234.

Jung, S., Dryden, I.L. and Marron, J.S. (2012). Analysis of principal nested spheres. Biometrika, 99, 551-568.

See Also

pns, pns4pc, plot3darcs

Examples

```
ans <- pnss3d(digit3.dat, sphere.type="BIC", n.pc=5)
#aa <- plot3darcs(ans,c=2,pcno=1)
#bb <- plot3darcs(ans,c=2,pcno=1,type="pca")
```

---

pongof.dat   *Female orang utan data*

Description

Female orang utan skull data. 8 landmarks in 2 dimensions, 30 individuals

Usage

```
data(pongof.dat)
```

Format

An array of dimension 8 x 2 x 30

Source

O'Higgins, P. and Dryden, I. L. (1993). Sexual dimorphism in hominoids: further studies of craniofacial shape differences in Pan, Gorilla, Pongo, Journal of Human Evolution, 24, 183-205.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(pongof.dat)
plotshapes(pongof.dat)
```

---

pongom.dat   *Male orang utan data*

Description

Male orang utan skull data. 8 landmarks in 2 dimensions, 30 individuals

Usage

```
data(pongom.dat)
```

Format

An array of dimension 8 x 2 x 30

Source

O'Higgins, P. and Dryden, I. L. (1993). Sexual dimorphism in hominoids: further studies of craniofacial shape differences in Pan, Gorilla, Pongo, Journal of Human Evolution, 24, 183-205.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(pongom.dat)
plotshapes(pongom.dat)
```

---

procdist   *Procrustes distance*

Description

Calculates different types of Procrustes shape or size-and-shape distance between two configurations

Usage

```
procdist(x, y,type="full",reflect=FALSE)
```

Arguments

x	k x m matrix (or complex k-vector for 2D data) where k = number of landmarks and m = no of dimensions
y	k x m matrix (or complex k-vector for 2D data)
type	string indicating the type of distance; "full" full Procrustes distance, "partial" partial Procrustes distance, "Riemannian" Riemannian shape distance, "sizeand-shape" size-and-shape Riemannian/Procrustes distance
reflect	Logical. If reflect = TRUE then reflection invariance is included.

Value

The distance between the two configurations.

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester.

See Also

procOPA,procGPA

Examples

```
data(gorf.dat)
data(gorm.dat)
gorf<-procGPA(gorf.dat)
gorm<-procGPA(gorm.dat)
distfull<-procdist(gorf$mshape,gorm$mshape)
cat("Full Procustes distance between mean shapes is ",distfull," \n")
```

procGPA   *Generalised Procrustes analysis*

Description

Generalised Procrustes analysis to register landmark configurations into optimal registration using translation, rotation and scaling. Reflection invariance can also be chosen, and registration without scaling is also an option. Also, obtains principal components, and some summary statistics.

Usage

```
procGPA(x, scale = TRUE, reflect = FALSE, eigen2d = FALSE,
tol1 = 1e-05, tol2 = tol1, tangentcoords = "residual", proc.output=FALSE,
distances=TRUE, pcaoutput=TRUE, alpha=0, affine=FALSE)
```

Arguments

x	Input k x m x n real array, (or k x n complex matrix for m=2 is OK), where k is the number of points, m is the number of dimensions, and n is the sample size.
scale	Logical quantity indicating if scaling is required
reflect	Logical quantity indicating if reflection is required
eigen2d	Logical quantity indicating if complex eigenanalysis should be used to calculate Procrustes mean for the particular 2D case when scale=TRUE, reflect=FALSE
tol1	Tolerance for optimal rotation for the iterative algorithm: tolerance on the mean sum of squares (divided by size of mean squared) between successive iterations
tol2	tolerance for rescale/rotation step for the iterative algorithm: tolerance on the mean sum of squares (divided by size of mean squared) between successive iterations
tangentcoords	Type of tangent coordinates. If (SCALE=TRUE) the options are "residual" (Procrustes residuals, which are approximate tangent coordinates to shape space), "partial" (Kent's partial tangent co-ordinates), "expomap" (tangent coordinates from the inverse of the exponential map, which are the similar to "partial" but scaled by (rho/sin(rho)) where rho is the Riemannian distance to the pole of the projection. If (SCALE=FALSE) then all three options give the same tangent co-ordinates to size-and-shape space, which is simply the Procrustes residual X^P - mu.
proc.output	Logical quantity indicating if printed output during the iterations of the Procrustes GPA algorithm should be given
distances	Logical quantity indicating if shape distances and sizes should be calculated
pcaoutput	Logical quantity indicating if PCA should be carried out
alpha	The parameter alpha used for relative warps analysis, where alpha is the power of the bending energy matrix. If alpha = 0 then standard Procrustes PCA is carried out. If alpha = 1 then large scale variations are emphasized, if alpha = -1 then small scale variations are emphasised. Requires m=2 and m=3 dimensional data if alpha $!=$ 0.

affine   Logical. If TRUE then only the affine subspace of shape variability is considered.

Value

A list with components

k	no of landmarks
m	no of dimensions (m-D dimension configurations)
n	sample size
mshape	Procrustes mean shape. Note this is unit size if complex eigenanalysis used, but on the scale of the data if iterative GPA is used.
tan	The tangent shape (or size-and-shape) coordinates
rotated	the k x m x n array of full Procrustes rotated data
pcar	the columns are eigenvectors (PCs) of the sample covariance Sv of tan
pcasd	the square roots of eigenvalues of Sv using tan (s.d.'s of PCs)
percent	the percentage of variability explained by the PCs using tan. If alpha $!=0$ then it is the percent of non-affine variation of the relative warp scores. If affine is TRUE it is the percentage of total shape variability of each affine component.
size	the centroid sizes of the configurations
stdscores	standardised PC scores (each with unit variance) using tan
rawscores	raw PC scores using tan
rho	Kendall's Riemannian shape distance rho to the mean shape
rmsrho	root mean square (r.m.s.) of rho
rmsd1	r.m.s. of full Procrustes distances to the mean shape d_F
GSS	Minimized Procrustes sum of squares

Author(s)

Ian Dryden, with input from Mohammad Faghihi and Alfred Kume

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester. Chapter 7.

Goodall, C.R. (1991). Procrustes methods in the statistical analysis of shape (with discussion). Journal of the Royal Statistical Society, Series B, 53: 285-339.

Gower, J.C. (1975). Generalized Procrustes analysis, Psychometrika, 40, 33–50.

Kent, J.T. (1994). The complex Bingham distribution and shape analysis, Journal of the Royal Statistical Society, Series B, 56, 285-299.

Ten Berge, J.M.F. (1977). Orthogonal Procrustes rotation for two or more matrices. Psychometrika, 42, 267-276.

See Also

procOPA,riemdist,shapepca,testmeanshapes

Examples

```
#2D example : female and male Gorillas (cf. Dryden and Mardia, 2016)

data(gorf.dat)
data(gorm.dat)

plotshapes(gorf.dat,gorm.dat)
n1<-dim(gorf.dat)[3]
n2<-dim(gorm.dat)[3]
k<-dim(gorf.dat)[1]
m<-dim(gorf.dat)[2]
gor.dat<-array(0,c(k,2,n1+n2))
gor.dat[,,1:n1]<-gorf.dat
gor.dat[,,(n1+1):(n1+n2)]<-gorm.dat

gor<-procGPA(gor.dat)
shapepca(gor,type="r",mag=3)
shapepca(gor,type="v",mag=3)

gor.gp<-c(rep("f",times=30),rep("m",times=29))
x<-cbind(gor$size,gor$rho,gor$scores[,1:3])
pairs(x,panel=function(x,y) text(x,y,gor.gp),
    label=c("s","rho","score 1","score 2","score 3"))


###########################################################
#3D example

data(macm.dat)
out<-procGPA(macm.dat,scale=FALSE)

par(mfrow=c(2,2))
plot(out$rawscores[,1],out$rawscores[,2],xlab="PC1",ylab="PC2")
title("PC scores")
plot(out$rawscores[,2],out$rawscores[,3],xlab="PC2",ylab="PC3")
plot(out$rawscores[,1],out$rawscores[,3],xlab="PC1",ylab="PC3")
plot(out$size,out$rho,xlab="size",ylab="rho")
title("Size versus shape distance")
```

---

procOPA   *Ordinary Procrustes analysis*

Description

Ordinary Procrustes analysis : the matching of one configuration to another using translation, rotation and (possibly) scale. Reflections can also be included if desired. The function matches configuration B onto A by least squares.

Usage

```
procOPA(A, B, scale = TRUE, reflect = FALSE)
```

Arguments

A   k x m matrix (or complex k-vector for 2D data), of k landmarks in m dimensions. This is the reference figure.

B   k x m matrix (or complex k-vector for 2D data). This is the figure which is to be transformed.

scale   logical indicating if scaling is required

reflect   logical indicating if reflection is allowed

Value

A list with components:

R   The estimated rotation matrix (may be an orthogonal matrix if reflection is allowed)

s   The estimated scale matrix

Ahat   The centred configuration A

Bhat   The Procrustes registered configuration B

OSS   The ordinary Procrustes sum of squares, which is $\|Ahat-Bhat\|^2$

rmsd   rmsd = sqrt(OSS/(km))

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester. Chapter 7.

See Also

procGPA,riemdist,tpsgrid

Examples

```
data(digit3.dat)

A<-digit3.dat[,,1]
B<-digit3.dat[,,2]
ans<-procOPA(A,B)
plotshapes(A,B,joinline=1:13)
plotshapes(ans$Ahat,ans$Bhat,joinline=1:13)

#Sooty Mangabey data
data(sooty.dat)
A<-sooty.dat[,,1]    #juvenile
B<-sooty.dat[,,2]    #adult
par(mfrow=c(1,3))
par(pty="s")
plot(A,xlim=c(-2000,3000),ylim=c(-2000,3000),xlab=" ",ylab=" ")
lines(A[c(1:12,1),])
points(B)
lines(B[c(1:12,1),],lty=2)
title("Juvenile (-------) Adult (- - - -)")
#match B onto A
out<-procOPA(A,B)
#rotation angle
print(atan2(out$R[1,2],out$R[1,1])*180/pi)
#scale
print(out$s)
plot(A,xlim=c(-2000,3000),ylim=c(-2000,3000),xlab=" ",ylab=" ")
lines(A[c(1:12,1),])
points(out$Bhat)
lines(out$Bhat[c(1:12,1),],lty=2)
title("Match adult onto juvenile")
#match A onto B
out<-procOPA(B,A)
#rotation angle
print(atan2(out$R[1,2],out$R[1,1])*180/pi)
#scale
print(out$s)
plot(B,xlim=c(-2000,3000),ylim=c(-2000,3000),xlab=" ",ylab=" ")
lines(B[c(1:12,1),],lty=2)
points(out$Bhat)
lines(out$Bhat[c(1:12,1),])
title("Match juvenile onto adult")
```

---

procWGPA   *Weighted Procrustes analysis*

Description

Weighted Procrustes analysis to register landmark configurations into optimal registration using translation, rotation and scaling. Registration without scaling is also an option. Also, obtains principal components, and some summary statistics.

Usage

```
procWGPA(x, fixcovmatrix=FALSE, initial="Identity", maxiterations=10, scale=TRUE,
 reflect=FALSE, prior="Exponential",diagonal=TRUE,sampleweights="Equal")
```

Arguments

x	Input k x m x n real array, where k is the number of points, m is the number of dimensions, and n is the sample size.
fixcovmatrix	If FALSE then the landmark covariance matrix is estimated. If a fixed covariance matrix is desired then the value should be given here, e.g. fixcovmatrix=diag(8) for the identity matrix with 8 landmarks.
initial	The initial value of the estimated covariance matrix. "Identity" - identity matrix, "Rawdata" - based on sample variance of the raw landmarks. Also, could be a k x k symmetric positive definite matrix.
maxiterations	The maximum number of iterations for estimating the covariance matrix,
scale	Logical quantity indicating if scaling is required,
reflect	Logical quantity indicating if reflection invariance is required,
prior	Indicates the type of prior. "Exponential" is exponential for the inverse eigenvalues. "Identity" is an inverse Wishart with the identity matrix as parameters.
diagonal	Logical. Indicates if the diagonal of the landmark covariance matrix (only) should be used. Diagonal matrices can lead to some landmarks having very small variability, which may or may not be desirable.
sampleweights	Gives the weights of the observations in the sample, rather than the landmarks. This is a fixed quatity. "Equal" indicates that all observations in the sample have equal weight. The weights do not need to sum to 1.

Details

The factored covariance model is assumed: $Sigma\_k \ x \ I\_m$ with $Sigma\_k$ being the covariance matrix of the landmarks, and the cov matrix at each landmark is the identity matrix.

Value

A list with components

k	no of landmarks
m	no of dimensions (m-D dimension configurations)
n	sample size
mshape	Weighted Procrustes mean shape.
tan	This is the mk x n matrix of Procrustes residuals X_i^P - Xbar.
rotated	the k x m x n array of weighted Procrustes rotated data
pcar	the columns are eigenvectors (PCs) of the sample covariance Sv of tan
pcasd	the square roots of eigenvalues of Sv using tan (s.d.'s of PCs)
percent	the percentage of variability explained by the PCs using tan.

size	the centroid sizes of the configurations
scores	standardised PC scores (each with unit variance) using tan
rawscores	raw PC scores using tan
rho	Kendall's Riemannian distance rho to the mean shape
rmsrho	r.m.s. of rho
rmsd1	r.m.s. of full Procrustes distances to the mean shape d_F
Sigmak	Estimate of the sample covariance matrix of the landmarks

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester.

Goodall, C.R. (1991). Procrustes methods in the statistical analysis of shape (with discussion). Journal of the Royal Statistical Society, Series B, 53: 285-339.

See Also

procGPA

Examples

```
#2D example : female Gorillas (cf. Dryden and Mardia, 2016)

data(gorf.dat)

gor<-procWGPA(gorf.dat,maxiterations=3)
```

---

qcet2.dat	*Control T2 mouse vertabrae data*

Description

T2 mouse vertebrae data - control group. 6 landmarks in 2 dimensions, 30 individuals

Usage

```
data(qcet2.dat)
```

Format

An array of dimension 6 x 2 x 30

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

http://www.maths.nott.ac.uk/personal/ild/bookdata/qcet2.dat

Data from Paul O'Higgins (Hull-York Medical School) and David Johnson (Leeds)

Examples

```
data(qcet2.dat)
plotshapes(qcet2.dat)
```

---

qlet2.dat   *Large T2 mouse vertabrae data*

Description

T2 mouse vertebrae data - large group. 6 landmarks in 2 dimensions, 23 individuals

Usage

```
data(qlet2.dat)
```

Format

An array of dimension 6 x 2 x 23

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

http://www.maths.nott.ac.uk/personal/ild/bookdata/qlet2.dat

Data from Paul O'Higgins (Hull-York Medical School) and David Johnson (Leeds)

Examples

```
data(qlet2.dat)
plotshapes(qlet2.dat)
```

---

qset2.dat   *Small T2 mouse vertabrae data*

Description

T2 mouse vertebrae data - small group. 6 landmarks in 2 dimensions, 23 individuals

Usage

```
data(qset2.dat)
```

Format

An array of dimension 6 x 2 x 23

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

http://www.maths.nott.ac.uk/personal/ild/bookdata/qset2.dat

Data from Paul O'Higgins (Hull-York Medical School) and David Johnson (Leeds)

Examples

```
data(qset2.dat)
plotshapes(qset2.dat)
```

---

rats   *Rat skulls data*

Description

Rat skulls data, from X rays. 8 landmarks in 2 dimensions, 18 individuals observed at 7, 14, 21, 30, 40, 60, 90, 150 days.

Usage

```
data(rats)
```

Format

rats$x: An array of landmark configurations 144 x 2 x 2

rats$no: Individual rat number (note rats 3, 13, 20 missing due to incomplete data)

rats$time observed time in days

Source

Vilmann's rat data set (Bookstein, 1991, Morphometric Tools for Landmark Data: Geometry and Biology, pp. 408-414)

References

Bookstein, F.L. (1991). Morphometric tools for landmark data: geometry and biology, Cambridge University Press.

Examples

```
data(rats)
plotshapes(rats$x,col=1:8)
```

---

resampletest	*Tests for mean shape difference using complex arithmetic, including bootstrap and permutation tests.*

Description

Carries out tests to examine differences in mean shape between two independent populations. For 2D data the methods use complex arithmetic and exploit the geometry of the shape space (which is the main use of this function). An alternative faster, approximate procedure using Procrustes residuals is given by the function 'testmeanshapes'. For 3D data tests are carried out on the Procrustes residuals, which is an approximation suitable for small variations in shape.

Up to four test statistics are calculated:

lambda : the asymptotically pivotal statistic $lambda\_min$ from Amaral et al. (2007), equ.(14),(16) (m=2 only)

H : Hotelling T^2 statistic (see Amaral et al., 2007, equ.(23), Dryden and Mardia, 2016, equ.(9.4))

J : James' statistic (see Amaral et al., 2007, equ.(24)) (m=2 only)

G : Goodall's F statistic (see Amaral et al., 2007, equ.(25), Dryden and Mardia, 2016, equ.(9.9))

p-values are given based on resampling as well as the usual table based p-values.

Note when the sample sizes are low (compared to the number of landmarks) some regularization is carried out. In particular if Sw is a singular within group covariance matrix, it is replaced by Sw + 0.000001 (Identity matrix) and a '*' is printed in the output.

Usage

```
resampletest(A, B, resamples = 200, replace = TRUE)
```

Arguments

`A`	The random sample for group 1: k x m x n1 array of data, where k is the number of landmarks and n1 is the sample size. (Alternatively a k x n1 complex matrix for 2D)
`B`	The random sample for group 3: k x m x n2 array of data, where k is the number of landmarks and n2 is the sample size. (Alternatively a k x n2 complex matrix for 2D)
`resamples`	Integer. The number of resampling iterations. If resamples = 0 then no resampling procedures are carried out, and the tabular p-values are given only.
`replace`	Logical. If replace = TRUE then for 2D data bootstrap resampling is carried out with replacement *within* each group. If replace = FALSE then permutation resampling is carried out (sampling without replacement in *pooled* samples).

Value

A list with components (or a subset of these)

`lambda`	λ_{min} statistic
`lambda.pvalue`	p-value for λ_{min} test based on resampling
`lambda.table.pvalue`	
	p-value for λ_{min} test based on the asymptotic chi-squared distribution (large n1,n2)
`H`	The Hotelling T^2 statistic
`H.pvalue`	p-value for the Hotelling T^2 test based on resampling
`H.table.pvalue`	p-value for the Hotelling T^2 test based on the null F distribution, assuming normality and equal covariance matrices
`J`	The Hotelling T^2 statistic
`J.pvalue`	p-value for the Hotelling T^2 test based on resampling
`J.table.pvalue`	p-value for the Hotelling T^2 test based on the null F distribution, assuming normality and unequal covariance matrices
`G`	The Goodall F statistic
`G.pvalue`	p-value for the Goodall test based on resampling
`G.table.pvalue`	p-value for the Goodall test based on the null F distribution, assuming normality and equal isotropic covariance matrices)

Author(s)

Ian Dryden

References

Amaral, G.J.A., Dryden, I.L. and Wood, A.T.A. (2007) Pivotal bootstrap methods for k-sample problems in directional statistics and shape analysis. Journal of the American Statistical Association. 102, 695-707.

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 9.

Goodall, C. R. (1991). Procrustes methods in the statistical analysis of shape (with discussion). Journal of the Royal Statistical Society, Series B, 53: 285-339.

See Also

testmeanshapes

Examples

```
#2D example : female and male Gorillas

data(gorf.dat)
data(gorm.dat)

#just select 3 landmarks and the first 10 observations in each group
select<-c(1,2,3)
A<-gorf.dat[select,,1:10]
B<-gorm.dat[select,,1:10]
resampletest(A,B,resamples=100)
```

---

riemdist	*Riemannian shape distance*

Description

Calculates the Riemannian shape distance rho between two configurations

Usage

```
riemdist(x, y, reflect=FALSE)
```

Arguments

x	k x m matrix (or complex k-vector for 2D data) where k = number of landmarks and m = no of dimensions
y	k x m matrix (or complex k-vector for 2D data)
reflect	Logical. If reflect = TRUE then reflection invariance is included.

Value

The Riemannian shape distance rho between the two configurations. Note $0 \le rho \le pi/2$ if no reflection invariance. (for the Riemannian size-and-shape distance use ssriemdist)

Author(s)

Ian Dryden

References

Kendall, D. G. (1984). Shape manifolds, Procrustean metrics and complex projective spaces, Bulletin of the London Mathematical Society, 16, 81-121.

See Also

procOPA,procGPA

Examples

```
data(gorf.dat)
data(gorm.dat)
gorf<-procGPA(gorf.dat)
gorm<-procGPA(gorm.dat)
rho<-riemdist(gorf$mshape,gorm$mshape)
cat("Riemannian distance between mean shapes is ",rho," \n")
```

---

rigidbody	*Rigid body transformations*

Description

Applies a rigid body transformations to a landmark configuration or array

Usage

```
rigidbody(X,transx=0,transy=0,transz=0,thetax=0,thetay=0,thetaz=0)
```

Arguments

X	k x m matrix, or k x m x n array where k = number of landmarks and m = no of dimensions and n is no of specimens
transx	negative shift in x-coordinates
transy	negative shift in y-coordinates
transz	negative shift in z-coordinates
thetax	Rotation about x-axis in degrees
thetay	Rotation about y-axis in degrees
thetaz	Rotation about z-axis in degrees

Value

The transformed coordinates (X - trans) Rx Ry Rz

Author(s)

Ian Dryden

Examples

```
data(gorf.dat)
plotshapes ( rigidbody(gorf.dat , 0, 0, 0, 0, 0, -90 ) )
```

---

sand   *Sand particle outline data*

Description

50 points on 24 sea sand and 25 river sand grain profiles in 2D. The original data were kindly provided by Professor Dietrich Stoyan (Stoyan and Stoyan, 1994; Stoyan, 1997). The 50 points on each outline were extracted at approximately equal arc-lengths by the method described in Kent et al. (2000, section 8.1)

Usage

```
data(sand)
```

Format

A list with components:

sea$x : An array of dimension 50 x 2 x 49 containing the 50 point co-ordinates in 2D for each grain

sea$group : The types of the sand grains: "sea", 24 particles from the Baltic Sea

"river", 25 particles from the Caucasian River Selenchuk

References

Kent, J. T., Dryden, I. L. and Anderson, C. R. (2000). Using circulant symmetry to model featureless objects. Biometrika, 87, 527–544.

Stoyan, D. (1997). Geometrical means, medians and variances for samples of particles. Particle Particle Syst. Charact. 14, 30–34.

Stoyan, D. and Stoyan, H. (1994). Fractals, Random Shapes and Point Fields: Methods of Geometric Statistics, John Wiley, Chichester.

Examples

```
data(sand)
plotshapes(sand$x[,,sand$group=="sea"],sand$x[,,sand$group=="river"],joinline=c(1:50))
```

---

schizophrenia   *Bookstein's schizophrenia data*

Description

Bookstein's schizophrenia data. 13 landmarks in 2 dimensions, 28 individuals. The first 14 individuals are controls. The last fourteen cases were diagnosed with schizophrenia. The landmarks were taken in the near midline from MR images of the brain: (1) splenium, posteriormost point on corpus callosum; (2) genu, anteriormost point on corpus callosum; (3) top of corpus callosum, uppermost point on arch of callosum (all three to an approximate registration on the diameter of the callosum); (4) top of head, a point relaxed from a standard landmark along the apparent margin of the dura; (5) tentorium of cerebellum at dura; (6) top of cerebellum; (7) tip of fourth ventricle; (8) bottom of cerebellum; (9) top of pons, anterior margin; (10) bottom of pons, anterior margin; (11) optic chiasm; (12) frontal pole, extension of a line from landmark 1 through landmark 2 until it intersects the dura; (13) superior colliculus.

Usage

```
data(schizophrenia.dat)
```

Format

schizophrenia$x : An array of dimension 13 x 2 x 28

schizophrenia$group : A factor of group labels 'con' for Controls and 'scz' for the schizophrenia patients.

Source

Bookstein, F. L. (1996). Biometrics, biomathematics and the morphometric synthesis, Bulletin of Mathematical Biology, 58, 313–365.

References

Data kindly provided by Fred Bookstein (University of Washington and University of Vienna)

Examples

```
data(schizophrenia)
plotshapes(schizophrenia$x,symbol=as.integer(schizophrenia$group))
```

`schizophrenia.dat`   *Bookstein's schizophrenia data*

Description

Bookstein's schizophrenia data. 13 landmarks in 2 dimensions, 28 individuals. The first 14 individuals are controls. The last fourteen cases were diagnosed with schizophrenia. The landmarks were taken in the near midline from MR images of the brain: (1) splenium, posteriormost point on corpus callosum; (2) genu, anteriormost point on corpus callosum; (3) top of corpus callosum, uppermost point on arch of callosum (all three to an approximate registration on the diameter of the callosum); (4) top of head, a point relaxed from a standard landmark along the apparent margin of the dura; (5) tentorium of cerebellum at dura; (6) top of cerebellum; (7) tip of fourth ventricle; (8) bottom of cerebellum; (9) top of pons, anterior margin; (10) bottom of pons, anterior margin; (11) optic chiasm; (12) frontal pole, extension of a line from landmark 1 through landmark 2 until it intersects the dura; (13) superior colliculus.

Usage

```
data(schizophrenia.dat)
```

Format

An array of dimension 13 x 2 x 28

Source

Bookstein, F. L. (1996). Biometrics, biomathematics and the morphometric synthesis, Bulletin of Mathematical Biology, 58, 313–365.

References

Data kindly provided by Fred Bookstein (University of Washington and University of Vienna)

Examples

```
data(schizophrenia.dat)
k<-dim(schizophrenia.dat)[1]
n<-dim(schizophrenia.dat)[3]
plotshapes(schizophrenia.dat)
```

---

shapepca   *Principal components analysis for shape*

Description

Provides graphical summaries of principal components for shape.

Usage

```
shapepca(proc, pcno = c(1, 2, 3), type = "r", mag = 1, joinline = c(1, 1),
        project=c(1,2),scores3d=FALSE,color=2,axes3=FALSE,rglopen=TRUE,zslice=0)
```

Arguments

proc	List given by the output from `procGPA()`
pcno	A vector of the PCs to be plotted
type	Options for the types of plot for the $m=2$ planar case: "r" : rows along PCs evaluated at c = -3,0,3 sd's along PC, "v" : vectors drawn from mean to +3 sd's along PC, "s" : plots along c= -3, -2, -1, 0, 1, 2, 3 superimposed, "m" : movie backward and forwards from -3 to +3 sd's along PC, "g" : TPS grid from mean to +3 sd's along PC.
mag	Magnification of the effect of the PC (scalar multiple of sd's)
joinline	A vector stating which landmarks are joined up by lines, e.g. joinline=c(1:n,1) will start at landmark 1, join to 2, ..., join to n, then re-join to landmark 1.
project	The default orthogonal projections if in higher than 2 dimensions
scores3d	Logical. If TRUE then a 3D scatterplot of the first 3 raw PC scores with labels in 'pcno' is given, instead of the default plot of the mean and PC vectors.
color	Color of the spheres used in plotting. Default color = 2 (red). If a vector is given then the points are colored in that order.
axes3	Logical. If TRUE then the axes are plotted in a 3D plot.
rglopen	Logical. If TRUE open a new RGL window, otherwise plot in current window.
zslice	For 3D case, type = "g": the z co-ordinate(s) for the grid slice(s)

Details

The mean and PCs are plotted.

Value

No value is returned

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 7.

See Also

procGPA

Examples

```
#2d example
data(gorf.dat)
data(gorm.dat)

gorf<-procGPA(gorf.dat)
gorm<-procGPA(gorm.dat)
shapepca(gorf,type="r",mag=3)
shapepca(gorf,type="v",mag=3)
shapepca(gorm,type="r",mag=3)
shapepca(gorm,type="v",mag=3)

#3D example
#data(macm.dat)
#out<-procGPA(macm.dat)
#movie
#shapepca(out,pcno=1)
```

---

shapes.cva   *Canonical variate analysis for shapes*

Description

Carry out canonical variate analysis for shapes (in two or more groups)

Usage

```
shapes.cva(X,groups,scale=TRUE,tangentcoords = "residual",ncv=2)
```

Arguments

X	Input k x m x n real array of the configurations, where k is the number of points, m is the number of dimensions, and n is the sample size.
groups	The group labels
scale	Logical, indicating if Procrustes scaling should be carried out
tangentcoords	The type of Procrustes tangent coordinates to use (as for procGPA)
ncv	Number of canonical variates to display

Value

A plot if ncv=2 or 3 and the Canonical Variate Scores

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester.

See Also

procGPA

Examples

```
#2D example : female and male apes   (cf. Dryden and Mardia, 2016)

data(pongof.dat)
data(pongom.dat)
data(panm.dat)
data(panf.dat)

apes   <- groupstack( pongof.dat , pongom.dat , panm.dat, panf.dat )

shapes.cva( apes$x, apes$groups)
```

---

shapes3d   *Plot 3D data*

Description

Plot the landmark configurations from a 3D dataset

Usage

```
shapes3d(x,loop=0,type="p", color = 2, joinline=c(1:1), axes3=FALSE, rglopen=TRUE)
```

Arguments

x   An array of size k x 3 x n, where k is the number of landmarks and n is the
            number of observations

loop   gives the number of times an animated loop through the observations is dis-
            played (in order 1 to n). loop > 0 is suitable when a time-series of shapes is
            available. loop = 0 gives a plot of all the observations on the same figure.

type	Type of plot: "p" points, "dots" dots (quicker for large plots), "l" dots and lines though landmarks 1:k if 'joinline' not stated
color	Colour of points (default color = 2 (red)). If a vector is given then the points are coloured in that order.
joinline	Join the numbered landmarks by lines
axes3	Logical. If TRUE then plot the axes.
rglopen	Logical. If TRUE then open a new RGL window, if FALSE then plot in current window.

Value

None

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester.

Examples

```
data(dna.dat)
shapes3d(dna.dat)
```

---

shells   *Microfossil shell data*

Description

Microfossil shell data. Triangles from 21 individuals. Lohmann (1983) published 21 mean outlines of the microfossil which were based on random samples of organisms taken at different latitudes in the South Indian Ocean.

Usage

```
data(shells)
```

Format

shells$uv Scaled shape coordinates (Bookstein shape co-ordinates with base (0,0) and (1,0). shells$size Centroid size

Source

Bookstein, F. L. (1986). Size and shape spaces for landmark data in two dimensions (with discussion). Statistical Science, 1:181-242.

Lohmann, G. P. (1983). Eigenshape analysis of microfossils: a general morphometric procedure for describing changes in shape. Mathematical Geology, 15:659-672.

References

The data have been extracted from Fig. 7 of Bookstein (1986).

Examples

```
data(shells)
plotshapes(shells$uv)
```

---

sooty   *Sooty mangabey data*

Description

Sooty mangabey data skull data. 12 landmarks in 2 dimensions, 2 individuals (juvenile and male adult) followed by three individuals, female adult, male adult. The first entries are rotated, translated versions of the 3rd and 7th figure.

Usage

```
data(sooty)
```

Format

An array of dimension 12 x 2 x 7

Source

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 1.

References

Data from Paul O'Higgins (Hull-York Medical School)

Examples

```
data(sooty)
plotshapes(sooty,joinline=c(1:12,1))
```

---

ssriemdist   *Riemannian size-and-shape distance*

Description

Calculates the Riemannian size-and-shape distance d_S between two configurations

Usage

```
ssriemdist(x, y, reflect=FALSE)
```

Arguments

x	k x m matrix (or complex k-vector for 2D data) where k = number of landmarks and m = no of dimensions
y	k x m matrix (or complex k-vector for 2D data)
reflect	Logical. If reflect = TRUE then reflection invariance is included.

Value

The Riemannian size-and-shape distance d_S between the two configurations. (for the Riemannian shape distance use riemdist)

Author(s)

Ian Dryden

References

Le, H.-L. (1995). Mean size-and-shapes and mean shapes: a geometric point of view. Advances in Applied Probability, 27:44-55.

See Also

procOPA,procGPA,riemdist

Examples

```
data(gorf.dat)
data(gorm.dat)
gorf<-procGPA(gorf.dat,scale=FALSE)
gorm<-procGPA(gorm.dat,scale=FALSE)
ds<-ssriemdist(gorf$mshape,gorm$mshape)
cat("Riemannian size-and-shape distance between mean size-and-shapes is ",ds," \n")
```

---

steroids	*Steroid data*

Description

Steroid data. Between 42 and 61 atoms for each of 31 steroid molecules.

Usage

```
data(steroids)
```

Format

steroids$x : An array of dimension 61 x 3 x 31 of 3D co-ordinates of the 31 steroids. If a molecules has less than 61 atoms then the remaining co-ordinates are all zero.

steroids$activity : Activity class ('1' = high, '2' = intermediate, and '3' = low binding affinities to the corticosteroid binding globulin (CBG) receptor)

steroids$radius : van der Waals radius (0 = missing value)

steoirds$atom : atom type (0 = missing value)

steroids$charge : partial charge (0 = missing value)

steroids$names : steroid names

Source

This particular version of the steroids data set of (x, y, z) atom co-ordinates and partial charges was constructed by Jonathan Hirst and James Melville (School of Chemistry, University of Nottingham).

Also see Wagener, M., Sadowski, J., Gasteiger, J. (1995). J. Am. Chem. Soc., 117, 7769-7775.

http://www2.ccc.uni-erlangen.de/services/steroids/

References

Dryden, I.L., Hirst, J.D. and Melville, J.L. (2007). Statistical analysis of unlabelled point sets: comparing molecules in chemoinformatics. Biometrics, 63, 237-251.

Czogiel I., Dryden, I.L. and Brignell, C.J. (2011). Bayesian matching of unlabeled point sets using random fields, with an application to molecular alignment. Annals of Applied Statistics, 5, 2603-2629.

Examples

```
data(steroids)
shapes3d(steroids$x[,,1])
```

testmeanshapes	*Tests for mean shape difference, including permutation and bootstrap tests*

Description

Carries out tests to examine differences in mean shape between two independent populations, for $m=2$ or $m=3$ dimensional data. Tests are carried out using tangent co-ordinates.

H : Hotelling T^2 statistic (see Dryden and Mardia, 2016, equ.(9.4))

G : Goodall's F statistic (see Dryden and Mardia, 2016, equ.(9.9))

J : James T^2 statistic (see Amaral et al., 2007)

p-values are given based on resampling (either a bootstrap test or a permutation test) as well as the usual table based p-values. Bootstrap tests involve sampling with replacement under H0 (as in Amaral et al., 2007).

Note when the sample sizes are low (compared to the number of landmarks) some minor regularization is carried out. In particular if Sw is a singular within group covariance matrix, it is replaced by Sw + 0.000001 (Identity matrix) and a '*' is printed in the output.

Usage

```
testmeanshapes(A, B, resamples = 1000, replace = FALSE, scale= TRUE)
```

Arguments

A	The random sample for group 1: k x m x n1 array of data, where k is the number of landmarks and n1 is the sample size. (Alternatively a k x n1 complex matrix for 2D)
B	The random sample for group 2: k x m x n2 array of data, where k is the number of landmarks and n2 is the sample size. (Alternatively a k x n2 complex matrix for 2D)
resamples	Integer. The number of resampling iterations. If resamples = 0 then no resampling procedures are carried out, and the tabular p-values are given only.
replace	Logical. If replace = TRUE then bootstrap resampling is carried out with replacement *within* each group. If replace = FALSE then permutation resampling is carried out (sampling without replacement in *pooled* samples).
scale	Logical. Whether or not to carry out Procrustes with scaling in the procedure.

Value

A list with components

H	The Hotelling statistic (F statistic)
H.pvalue	p-value for the Hotelling test based on resampling
H.table.pvalue	p-value for the Hotelling test based on the null F distribution, assuming normality and equal covariance matrices

J	The James T^2 statistic
J.pvalue	p-value for the James T^2 test based on resampling
J.table.pvalue	p-value for the James T^2 test based on the null F distribution, assuming normality but unequal covariance matrices
G	The Goodall F statistic
G.pvalue	p-value for the Goodall test based on resampling
G.table.pvalue	p-value for the Goodall test based on the null F distribution, assuming normality and equal isotropic covariance matrices)

Author(s)

Ian Dryden

References

Amaral, G.J.A., Dryden, I.L. and Wood, A.T.A. (2007) Pivotal bootstrap methods for k-sample problems in directional statistics and shape analysis. Journal of the American Statistical Association. 102, 695-707.

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with applications in R (Second Edition). Wiley, Chichester. Chapter 9.

Goodall, C. R. (1991). Procrustes methods in the statistical analysis of shape (with discussion). Journal of the Royal Statistical Society, Series B, 53: 285-339.

See Also

resampletest

Examples

```
#2D example : female and male Gorillas

data(gorf.dat)
data(gorm.dat)

A<-gorf.dat
B<-gorm.dat
testmeanshapes(A,B,resamples=100)
```

---

tpsgrid   *Thin-plate spline transformation grids*

Description

Thin-plate spline transformation grids from one set of landmarks to another.

Usage

```
tpsgrid(TT, YY, xbegin=-999, ybegin=-999, xwidth=-999, opt=1, ext=0.1, ngrid=22,
             cex=1, pch=20, col=2,zslice=0, mag=1, axes3=FALSE)
```

Arguments

TT	First object (source): (k x m matrix)
YY	Second object (target): (k x m matrix)
xbegin	lowest x value for plot: if -999 then a value is determined
ybegin	lowest y value for plot: if -999 then a value is determined
xwidth	width of plot: if -999 then a value is determined
opt	Option 1: (just deformed grid on YY is displayed), option 2: both grids are displayed
ext	Amount of border on plot in 2D case.
ngrid	Number of grid points: size is ngrid * (ngrid -1)
cex	Point size
pch	Point symbol
col	Point colour
zslice	For 3D case the scaled z co-ordinate(s) for the grid slice(s). The values are on a standardized scale as a proportion of height from the middle of the z-axis to the top and bottom. Values in the range -1 to 1 would be sensible.
mag	Exaggerate effect (mag > 1). Standard effect has mag=1.
axes3	Logical. If TRUE then the axes are plotted in a 3D plot.

Details

A square grid on the first configuration is deformed smoothly using a pair of thin-plate splines in 2D, or a triple of splines in 3D, to a curved grid on the second object. For 3D data the grid is placed at a constant z-value on the first figuure, indicated by the value of zslice.

For 2D data the covariance function in the thin-plate spline is $sigma(h) = |h|^2 \log |h|^2$ and in 3D it is given by $sigma(h) = -| h |$.

Value

No returned value

Author(s)

Ian Dryden

References

Bookstein, F.L. (1989). Principal warps: thin-plate splines and the decomposition of deformations, IEEE Transactions on Pattern Analysis and Machine Intelligence, 11, 567–585.

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester. Chapter 12.

See Also

procGPA

Examples

```
data(gorf.dat)
data(gorm.dat)

#TPS grid with shape change exaggerated (2x)
gorf<-procGPA(gorf.dat)
gorm<-procGPA(gorm.dat)
TT<-gorf$mshape
YY<-gorm$mshape
tpsgrid(TT,YY,mag=2)
title("TPS grid: Female mean (left) to Male mean (right)")
```

---

transformations	*Calculate similarity transformations*

Description

Calculate similarity transformations between configurations in two arrays.

Usage

```
transformations(Xrotated,Xoriginal)
```

Arguments

Xrotated	Input k x m x n real array of the Procrustes transformed configurations, where k is the number of points, m is the number of dimensions, and n is the sample size.
Xoriginal	Input k x m x n real array of the Procrustes original configurations, where k is the number of points, m is the number of dimensions, and n is the sample size.

Value

A list with components

translation	The translation parameters. These are the relative translations of the centroids of the individuals.
scale	The scale parameters
rotation	The rotation parameters. These are the rotations between the individuals after they have both been centred.

Author(s)

Ian Dryden

References

Dryden, I.L. and Mardia, K.V. (2016). Statistical Shape Analysis, with Applications in R (Second Edition). Wiley, Chichester.

See Also

procGPA

Examples

```
#2D example : female and male Gorillas (cf. Dryden and Mardia, 2016)

data(gorf.dat)

Xorig <- gorf.dat
Xrotated <- procGPA(gorf.dat)$rotated

transformations(Xrotated,Xorig)
```

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