

# Package ‘shapes’

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**Title** Statistical Shape Analysis

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**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.

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**Imports** scatterplot3d, rgl, MASS

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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. (1998). Statistical Shape Analysis, 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")
```

---

 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 $k \times 2 \times n$ real array, or $k \times n$ complex matrix, where $k$ is the number of landmarks, $n$ 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. (1998) *Statistical Shape Analysis*. 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	<i>Centroid size</i>
---------------	----------------------

---

**Description**

Calculate centroid 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. (1998). *Statistical Shape Analysis*, Wiley, Chichester.

**Examples**

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

---

cortical	<i>Cortical surface data</i>
----------	------------------------------

---

**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. (1998). Statistical Shape Analysis, Wiley, Chichester. p318

**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)
plotshape3d(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 $k \times k \times n$ 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 $k \times m \times n$ 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 ( $d = 2 \cdot \sin(\rho/2)$ ); "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. (1998). *Statistical Shape Analysis*. 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, 1998)

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. (1998). *Statistical Shape Analysis*, Wiley, Chichester. p317

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	<i>Male gorilla data</i>
----------	--------------------------

---

**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. (1998). Statistical Shape Analysis, Wiley, Chichester. p317

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 $k \times m \times n$ 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 $k \times m \times n$ 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. (1998). Statistical Shape Analysis, Wiley, Chichester.

### See Also

procGPA

**Examples**

```
#2D example : female and male Gorillas (cf. Dryden and Mardia, 1998)

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

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

---

humanmove	<i>Human movement data</i>
-----------	----------------------------

---

**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. (1998). Statistical Shape Analysis, Wiley, Chichester.

**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. (1998). Statistical Shape Analysis, Wiley, Chichester. p16

**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. (1998). Statistical Shape Analysis, Wiley, Chichester. p16

**References**

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

**Examples**

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

---

mice

*T2 mouse vertebrae 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	<i>Female chimpanzee data</i>
----------	-------------------------------

---

**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	<i>Male chimpanzee data</i>
----------	-----------------------------

---

**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 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(panm.dat)
plotshapes(panm.dat)
```

---

plotshapes	<i>Plot configurations</i>
------------	----------------------------

---

**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)
```

---

pongof.dat	<i>Female orang utan data</i>
------------	-------------------------------

---

**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. (1998). Statistical shape analysis. 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 Procrustes 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 coordinates 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 $\neq$ 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 $S_v$ of $\tan$
pcasd	the square roots of eigenvalues of $S_v$ using $\tan$ (s.d.'s of PCs)
percent	the percentage of variability explained by the PCs using $\tan$ . If $\alpha \neq 0$ 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 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 $S_{d\_F}$
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. (1998). Statistical Shape Analysis, 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.
- 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, 1998)

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. (1998). Statistical shape analysis. Wiley, Chichester.

**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 quantity. "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:  $\Sigma_k \times I_m$  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 $m_k \times n$ matrix of Procrustes residuals $X_i^P - \bar{X}$ .
rotated	the $k \times m \times n$ array of weighted Procrustes rotated data
pcar	the columns are eigenvectors (PCs) of the sample covariance $S_v$ of tan
pcasd	the square roots of eigenvalues of $S_v$ 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. (1998). Statistical Shape Analysis, 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, 1998)

data(gorf.dat)

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

---

qcet2.dat

*Control T2 mouse vertebrae 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. (1998). Statistical Shape Analysis, Wiley, Chichester. p313

**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	<i>Large T2 mouse vertebrae data</i>
-----------	--------------------------------------

---

**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. (1998). Statistical Shape Analysis, Wiley, Chichester. p313

**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	<i>Small T2 mouse vertebrae data</i>
-----------	--------------------------------------

---

**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. (1998). Statistical Shape Analysis, Wiley, Chichester. p313

**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	<i>Tests for mean shape difference using complex arithmetic, including bootstrap and permutation tests.</i>
--------------	-------------------------------------------------------------------------------------------------------------

---

## 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, 1998, equ.(7.4))

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, 1998, equ.(7.9))

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 <i>*within*</i> each group. If replace = FALSE then permutation resampling is carried out (sampling without replacement in <i>*pooled*</i> samples).

**Value**

A list with components (or a subset of these)

lambda	\$lambda_min\$ statistic
lambda.pvalue	p-value for \$lambda_min\$ test based on resampling
lambda.table.pvalue	p-value for \$lambda_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. (1998) *Statistical Shape Analysis*, 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.

**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	<i>Riemannian shape distance</i>
----------	----------------------------------

---

### 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  $0 \leq \rho \leq \pi/2$  if no reflection invariance

### 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. (1998) *Statistical Shape Analysis*. Wiley, Chichester.

**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,ncv=2)
```

**Arguments**

X	Input $k \times m \times n$ 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
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. (1998). Statistical Shape Analysis, Wiley, Chichester.

**See Also**

procGPA

**Examples**

```
#2D example : female and male apes (cf. Dryden and Mardia, 1998)

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 $k \times 3 \times n$ , 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 displayed (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. (1998) *Statistical Shape Analysis*. 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. (1998). Statistical Shape Analysis, Wiley, Chichester. p17, 42

**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**

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

**Value**

The Riemannian size-and-shape distance  $\rho$  between the two configurations.

**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`

**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 molecule 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)

steroids\$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	<i>Tests for mean shape difference, including permutation and bootstrap tests</i>
----------------	-----------------------------------------------------------------------------------

---

### 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, 1998, equ.(7.4))

G : Goodall's F statistic (see Dryden and Mardia, 1998, equ.(7.9))

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  $H_0$  (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  $S_w$  is a singular within group covariance matrix, it is replaced by  $S_w + 0.000001$  (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: $k \times m \times n_1$ array of data, where $k$ is the number of landmarks and $n_1$ is the sample size. (Alternatively a $k \times n_1$ complex matrix for 2D)
B	The random sample for group 2: $k \times m \times n_2$ array of data, where $k$ is the number of landmarks and $n_2$ is the sample size. (Alternatively a $k \times n_2$ complex matrix for 2D)
resamples	Integer. The number of resampling iterations. If <code>resamples = 0</code> then no resampling procedures are carried out, and the tabular p-values are given only.
replace	Logical. If <code>replace = TRUE</code> then bootstrap resampling is carried out with replacement *within* each group. If <code>replace = FALSE</code> 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. (1998) *Statistical Shape Analysis*, 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.

**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 figure, 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. (1998) Statistical Shape Analysis. Wiley, Chichester. Chapter 10.

**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  $k \times m \times n$  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  $k \times m \times n$  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. (1998). *Statistical Shape Analysis*, Wiley, Chichester.

**See Also**

procGPA

**Examples**

```
#2D example : female and male Gorillas (cf. Dryden and Mardia, 1998)

data(gorf.dat)

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

transformations(Xrotated,Xorig)
```

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