R package procrustes: Several algorithms from the procrustes family of transformations

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https://github.com/markheckmann/procrustes

Abstract

This document describes several features of the **procrustes** package. The procrustes package was written to facilitate my PhD work which includes several types of procrustes transformations. The available package lacked some features I needed, so I implemented them myself.

Keywords: procrustes, configurations, fitting, R.

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1. Quick start

To use the `procrustes` package, install

```
library(devtools)
install_github("procrustes", "markheckmann")
```

and load it.

```
library(procrustes)
```

2. Orthogonal procrustes analysis

Mathematically a configuration is represented by a $m \times n$ matrix, where each row represents a point and each column a dimension. Let the matrix $\mathbf{A}$ represent a small configuration with three points in $\mathbf{R}^2$.

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ -1 & -1 \\ 1 & -0 \end{pmatrix}$$

The standard orthogonal procrustes analysis (OPA) has the goal to fit a configuration $\mathbf{A}$ to a another configuration $\mathbf{B}$ as closely as possible by scaling, rotating and reflecting, and

translating configuration $\mathbf{A}$.

$$\mathbf{B} = \underset{\text{scaling}}{c}\ \mathbf{A}\ \underset{\substack{\text{rotation}+\\ \text{reflection}}}{\mathbf{Q}} + \underset{\text{translation}}{J\gamma^T} + \underset{\text{error}}{\mathbf{Q}} \tag{1}$$

Closeness is measured as the sum of squared distances between the row vectors (homologous points) of the two configurations. So the goal is to minimize the function

$$f(c, \mathbf{Q}, \gamma) = tr\ \mathbf{E^T E} \tag{2}$$

with respect to the transformations that are allowed. The function `opa` performs this type of analysis. `opa` also allows to one apply a subset of the possible transformations.[1] The following subsets are allowed:

1. Scaling only $f(c)$
2. Rotation only $f(\mathbf{Q})$
3. Rotation and scaling $f(c, \mathbf{Q})$
4. Rotation, scaling and translation $f(c, \mathbf{Q}, \gamma)$

The solution to these problems are special cases of the generalized solution to the orthogonal procrustes problem as outlined by SchÃűnemann and Carroll (1970).

3. Scaling only

This is a very unsual case, as it only makes sense if the configureations already have a natural center. The formulation is.

$$\mathbf{B} = \underset{\text{scaling}}{c}\ \mathbf{A} + \mathbf{E} \tag{3}$$

The solution to this problem is. All the three seperate transformations given (3) can be switched on or off. This was

4. Basic transformations

4.1. Translation

References

[1] One of the main reasons to write this package was that I needed a function where I can do this.

SchÃűnemann PH, Carroll RM (1970). "Fitting one matrix to another under choice of a central dilation and a rigid motion." *Psychometrika*, **35**(2), 245–255. ISSN 0033-3123, 1860-0980. doi:10.1007/BF02291266. URL http://www.springerlink.com/content/gq1933g700170w46/.

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