STA 5707

Spring 2007

Procrustes Analysis

$\mathcal{NB}$

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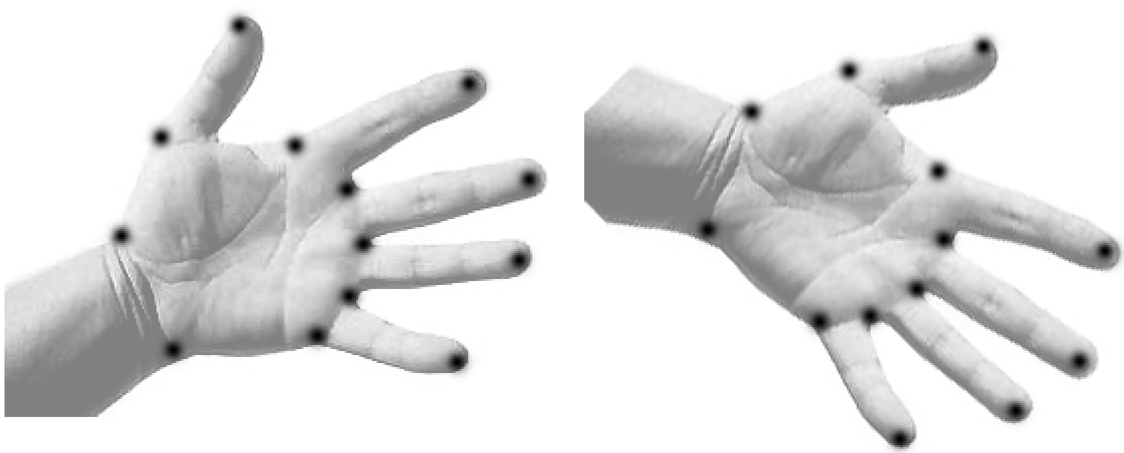
A Method for Statistical Shape Analysis

In statistics, Procrustes analysis is a form of *shape analysis* used for studying distributions of geometric configurations or shapes.

Consider sets of n points in $\mathbb{R}^p$, also called *landmark points*. We think of each set as a representation of a configuration (shape).



A Method for Statistical Shape Analysis

Two configurations are considered equivalent if one of them can be obtain from the other by rotation and translation *(Orthogonal Procrustes)*. By defining a suitable distance between two configurations one can find the distance between corresponding equivalent classes and solve the problem for optimal matching between them.

A more general approach includes scaling invariance in addition to rotation and translation invariance of shapes *(Extended Orthogonal Procrustes)*.

There is also the so called *Generalized Procrustes Analysis* that considers more than two shapes and tries to align them optimaly.

Procrustes Analysis is sometimes called *least-squares orthogonal* mapping, when the distance is the usual euclidean distance.

Comparing Configurations

Suppose we are given two configurations in $\mathbb{R}^p$, $\{x_j\}$ and $\{y_j\}$, j=1,...,n, represented by their data $n \times p$ matrices
$X = \{x_j^i\}_{i=1,j=1}^{p,n}$ and $Y = \{y_j^i\}_{i=1,j=1}^{p,n}$.

The goal is to find linear transformation of y-configuration in the form

$$y_j \mapsto Qy_j + b,$$

where Q is an orthogonal $p \times p$ matrix and $b \in \mathbb{R}^p$, so it matches x-configuration as close as possible. We will measure the proximity by Euclidean distance in $\mathbb{R}^p$.

This problem has an exact solution, which we present below.

Orthogonal Procrustes

Consider following objective function for assessing the matching

$$PR^2 \doteq \sum_{j=1}^{n} (x_j - Qy_j - b)'(x_j - Qy_j - b) =$$

$$tr\{(X - YQ' - b)'(X - YQ' - b)\}.$$

We call PR^2 *Procrustes measure*. The, optimality problem is

$$(\hat{b}, \hat{Q}) = \min_{Q \in O(p), b \in \mathbb{R}^p} PR^2.$$

In other words, we want to find a rotation matrix Q and translation vector b that minimize PR^2.

Orthogonal Procrustes

Without loss of generality we assume samples are centered, $\sum_j x_j = 0$ and $\sum_j y_j = 0$. Then we calculate the Procrustes measure

$$PR^2 = \sum_{j=1}^{n} (x_j - Qy_j)'(x_j - Qy_j) + nb'b =$$

$$\sum_j x_j' x_j + \sum_j y_j' y_j - \sum_j y_j' Q' x_j - \sum_j x_j' Q y_j + nb'b.$$

First two terms are constants and $b'b \geq 0$. So we conclude that $\hat{b} = 0$ and therefore

$$\min\{PR^2\} = const + 2 \min_Q \{-\sum_j tr\{x_j' Q y_j\}\} =$$

$$const - 2 \max_Q \{\sum_j tr\{Q y_j x_j'\}\}.$$

Next, observe that $\sum_j y_j x_j' = Y'X$. Then our problem can be formulated as

$$\hat{Q} = argmin\ _Q\ PR^2 = argmax\ _Q\ tr\{QY^t X\}.$$

Orthogonal Procrustes

SVD (Singular Value Decomposition) of $p \times p$ matrix $Y^t X$ is $Y^t X = U \Lambda V'$, for orthogonal matrices U and V and the diagonal matrix of singular values $\Lambda = diag\{\lambda_i\}_{i=1}^p$.

We have

$$\sum_{j=1}^n y_j x_j' = Y^t X = U \Lambda V' = \sum_{i=1}^p \lambda_i u_i v_i'.$$

Therefore

$$\sum_{j=1}^n tr\{Q y_j x_j'\} = \sum_{i=1}^p \lambda_i tr\{Q u_i v_i'\} = \sum_{i=1}^p \lambda_i v_i' Q u_i.$$

By Cauchy-Schwartz inequality,

$$v_i' Q u_i \leq \sqrt{v_i' Q Q' v_i} \sqrt{u_i' u_i} \leq 1,$$

with equality if and only if $u_i = Q^t v_i$. The last condition is nothing but $U = Q^t V$, or equivalently $Q = (V')^{-1} U' = V U'$. Thus

$$\hat{Q} = argmin_{Q,b} PR^2 = V U',$$

is the exact solution of our optimality problem.

Extended Orthogonal Procrustes

Extended Procrustes Analysis, in addition to translation and rotation, tries to adjust for scaling also.

Consider following objective function

$$PR^2 = \sum_{j=1}^{n} (x_j - cQy_j - b)'(x_j - cQy_j - b),$$

where c is a scale factor. Our problem now formulates as

$$(\hat{b}, \hat{Q}, \hat{c}) = argmin\ _{b,Q,c}\ PR^2.$$

We have

$$PR^2 = \sum_j x_j' x_j + c^2 \sum_j y_j' y_j - 2c \sum_j x_j' Q y_j + n b' b.$$

Again, by assuming x and y samples are centered, we need $\hat{b} = 0$.

As before, rotation matrix Q should satisfy

$\hat{Q} = argmax\ _Q\ tr\{QY^t X\}$, and hence $\hat{Q} = VU'$, where $Y^t X = U \Lambda V'$.

Extended Orthogonal Procrustes

In order to minimize PR^2 we set the derivative in respect to c to 0

$$\frac{\partial PR^2}{\partial c} = c\sum_j |y_j|^2 - tr(Q\sum_j y_j x_j') = 0.$$

Since $\sum_j y_j' y_j = tr(Y'Y)$ and $\sum_j y_j x_j' = Y^t X$, we finaly have

$$\hat{c} = \frac{tr(\hat{Q}Y^t X)}{tr(YY')} = \frac{tr(V\Lambda V')}{tr(YY')},$$

which is the desired optimal scale factor.

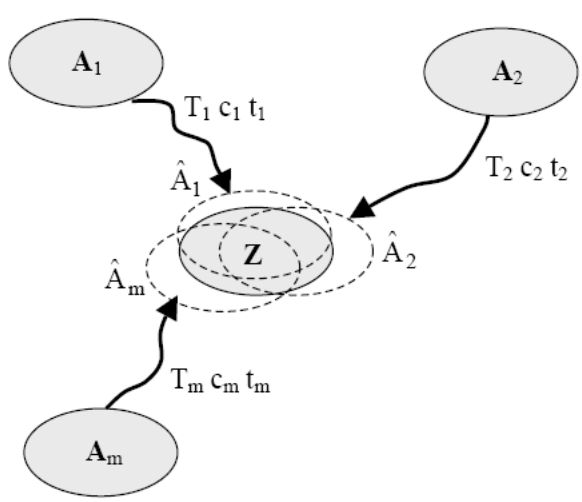
Generalized Orthogonal Procrustes

In this setup we are given m sets of samples in $\mathbb{R}^p$, Y_1, Y_2, ..., Y_m, each containing same number of points, n. The problem is to minimize

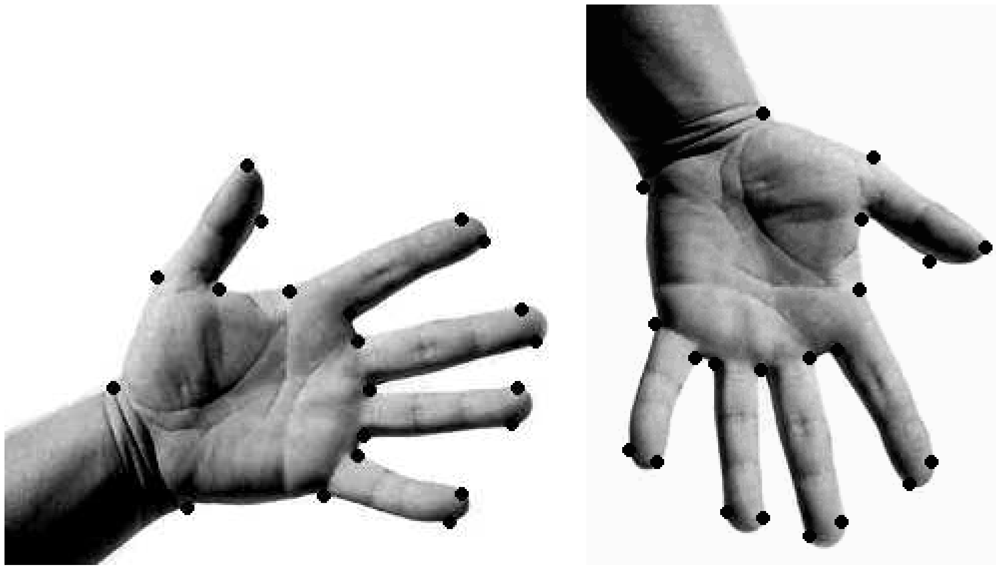
$$PR^2 = \sum_{i=1}^{m} \sum_{k=i+1}^{m}$$

$$(c_iY_iQ_i+b_i-c_kY_kQ_k-b_k)'(c_iY_iQ_i+b_i-c_kY_kQ_k-b_k).$$

If $\hat{A}_i = c_iY_iQ_i + b_i$, one of the problem formulation (Goodall, 1991) is to find a matrix Z, called *consensus matrix*, such that $\hat{A}_i = Z + E_i$ and E_i are iid $N_p(0, \Sigma)$.



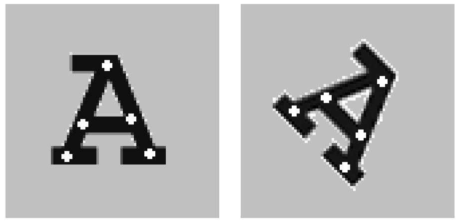
Hands Example - SAS Code.



```
/* Procrustes Analysis of Hand Rotation */
proc iml;
X = { /* p=2, n=21 */
54 126, 77 69, 122 8, 130 38, 110 75,
144 76, 233 36, 246 48, 175 88, 180 103, 264 84,
271 103, 188 128, 262 129, 260 146, 185 154,
180 164, 237 186, 228 201, 163 185, 93 193 };
Y = {
97 56, 156 80, 217 125, 185 132, 148 112,
148 148, 186 236, 176 246, 137 177, 122 181,
138 266, 122 272, 93 187, 96 264, 76 262,
69 184, 59 180, 37 235, 22 229,36 164,30 96 };
```

```
/* center X-sample */
colsum = X[+,]; nrows = nrow(X);
colsum = colsum / nrows;
XX = colsum @  j(nrows,1,1); X = X - XX;

/* center Y-sample */
colsum = Y[+,]; nrows = nrow(Y);
colsum = colsum / nrows;
YY = colsum @  j(nrows,1,1); Y = Y - YY;

YY = t(Y);
S = YY*X;

call svd(u, L, v, S);

Q = v*t(u); QQ = round(Q, 0.1);
print Q, QQ;

/* Q =
-0.006432 0.9999793
-0.999979 -0.006432 */

/* Rotation: arcsin (alpha) = 1,
and alpha = 90 */
```

Letter A Example - SAS Code.



```
proc iml;
X = { /* p=2, n=5 */
23 68, 27 53, 37 24, 48 53, 53 67
};
Y = {
23 47, 38 43, 64 33, 52 61, 48 73
};

/* Q =
 0.6634123  0.748254
-0.748254 0.6634123
*/

/* Rotation: arcsin (alpha) = 0.748,
   and alpha = 41.58 (degrees) */
```

Etymology

In Greek Mythology, Procrustes(the stretcher) was a bandit from Atica, who lured travelers passing by his stronghold by offering them a bed for the night. Then he forced the victims to fit the exact length of his iron bed either by stretched them or cut down to size. Nobody would ever fit the bed since Procrustes secretly adjusted it upon victims arival. Procrustes was killed by Theseus.

(Wikipedia)