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Schulich
MEDICINE & DENTISTRY

The History of Orthogonal Procrustes Analysis

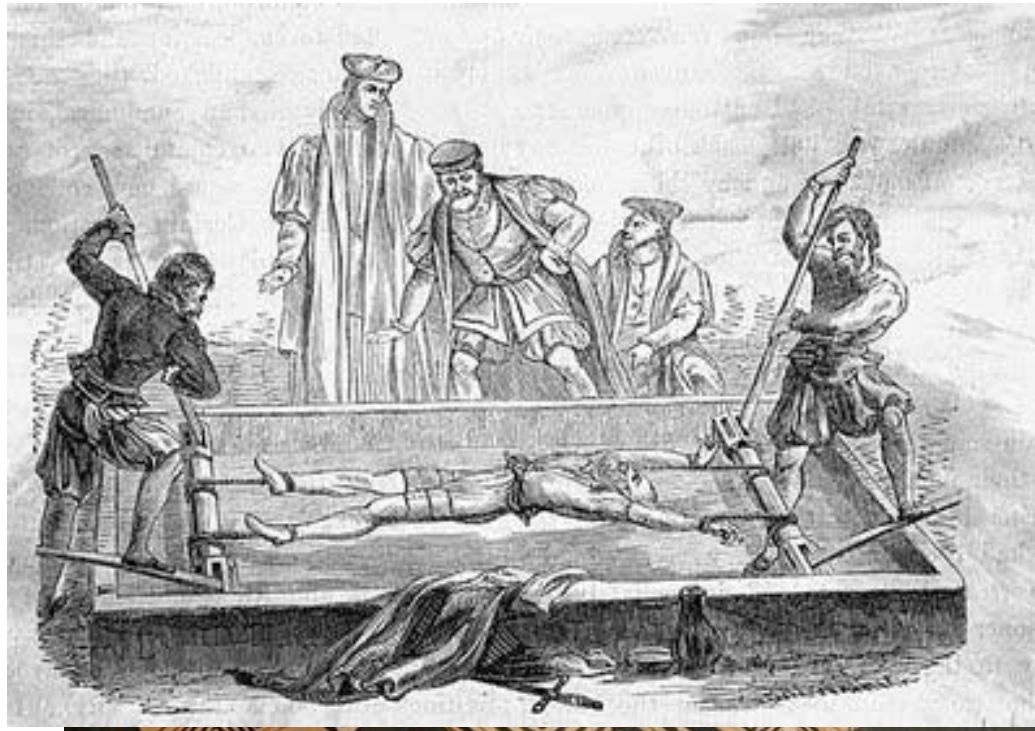
Elvis C.S. Chen

**Virtual Augmentation and Simulation for Surgery and Therapy (VASST) Lab,
Robarts Research Institute, London, Ontario**

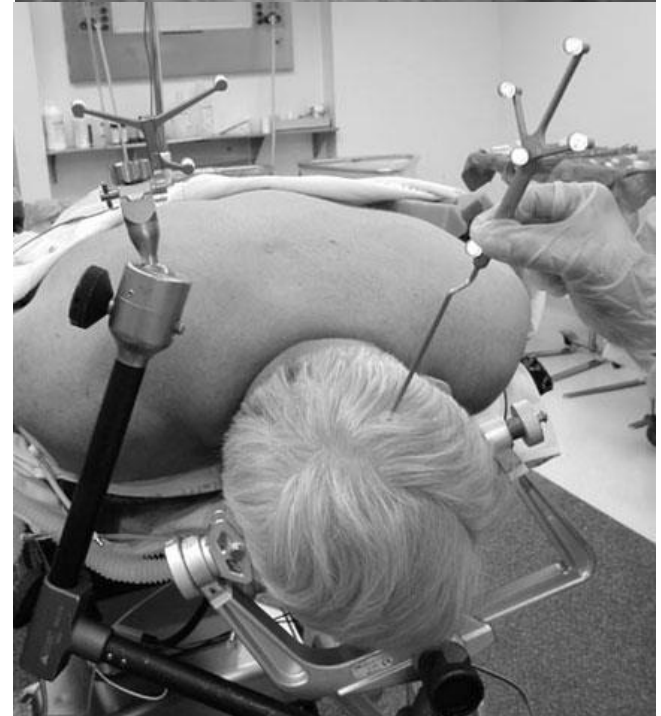
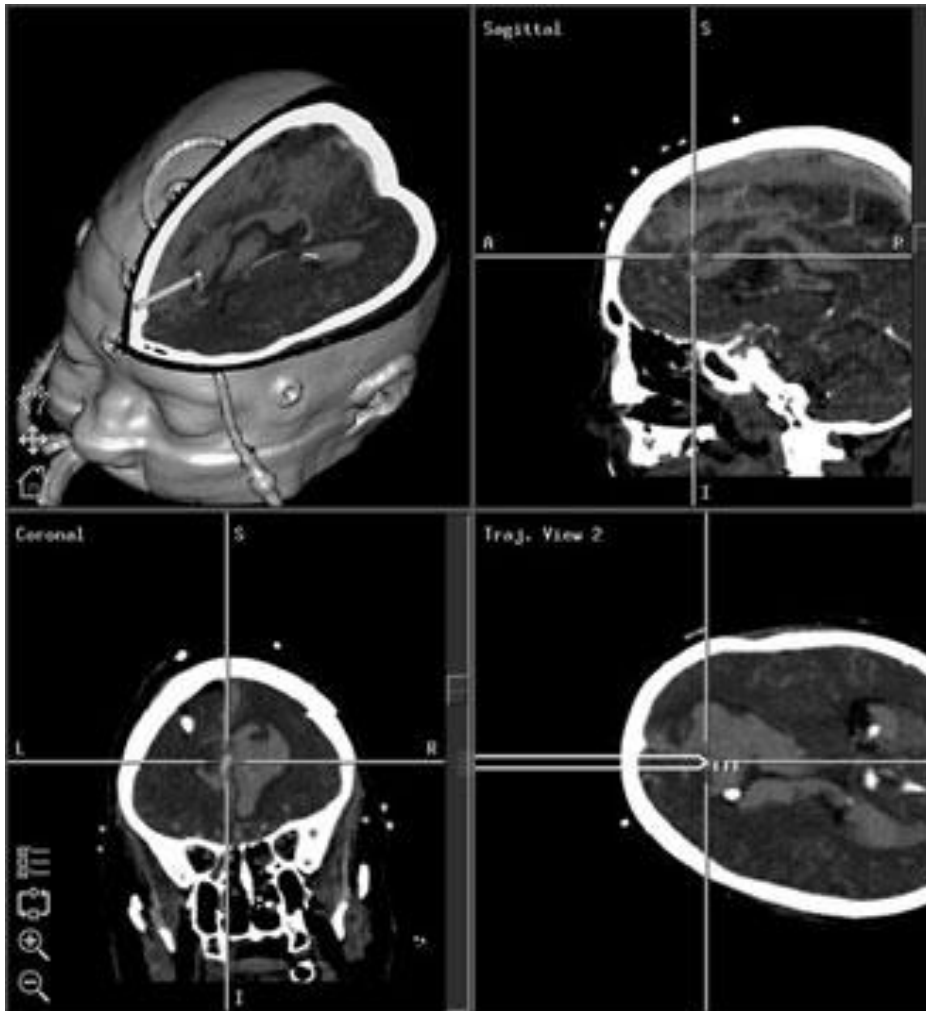


Who

- Son of Poseidon. He would invite traveler to his home, where he would “fit” the traveler to an iron bed: he’d stretch the travelers if they are too short, or amputate the excess length if they are too tall. Eventually he was fitted to his own bed by Theseus.



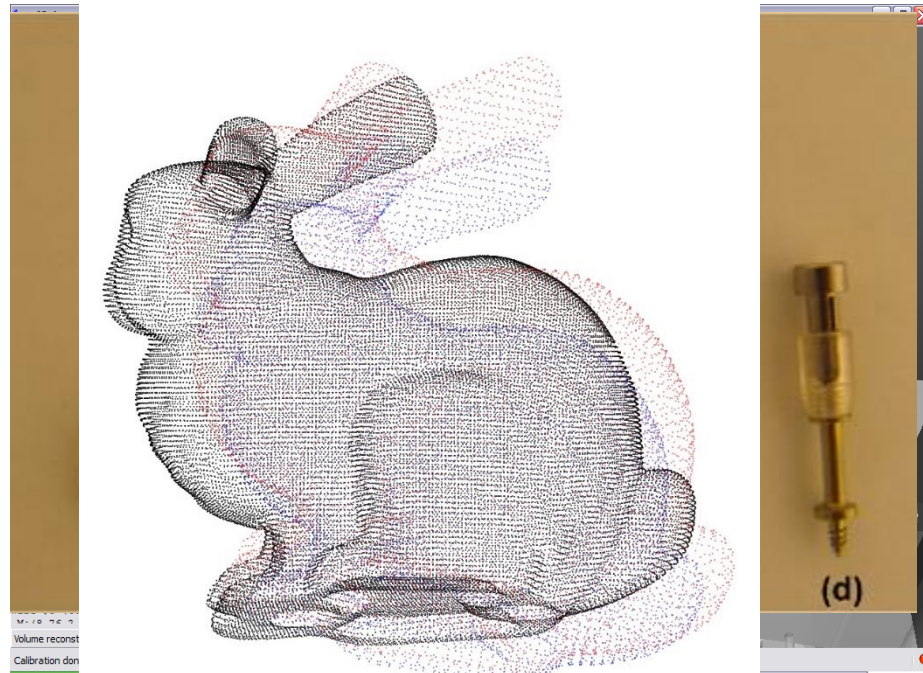
Where



Lemole et al, 2001

Where

- Point-to-point registration (n-to-n points)
 - Optical tracking
 - Ultrasound calibration
 - Image registration using anatomical landmarks
- Surface registration (n-to-m points)
 - Fundamental of the Iterative Closest Point algorithm



Where

The interpretation of generalized procrustes analysis and allied methods

GB Dijksterhuis, JC Gower - Food Quality and Preference, 1992 - Elsevier

Abstract We discuss various issues surrounding the use and interpretation of Generalized Procrustes Analysis and related methods. Included are considerations that have to be made before starting an analysis, how to handle different dimensionalities of data, when to ...

Cited by 123 Related articles All 4 versions Cite Save

Procrustes analysis in studying sensory-instrumental relations

G Dijksterhuis - Food quality and preference, 1994 - Elsevier

... Dijksterhuis and Gower, 1992; GB Dijksterhuis, JC Gower; The interpretation of Generalized Procrustes Analysis and allied methods. Food Quality and Preference, 3 (1992), pp. ... GB Dijksterhuis, PH Punter; Interpreting Generalised Procrustes Analysis 'Analysis of Variance' tables. ...

Cited by 26 Related articles All 3 versions Cite Save

[HTML] Assessing panel consonance

G Dijksterhuis - Food Quality and Preference, 1995 - Elsevier

... Volume I: Theory, Seminar Press, New York (1972), pp. 105-155. Dijksterhuis and Gower, 1991/2; GB Dijksterhuis, JC Gower; The interpretation of Generalized Procrustes Analysis and allied methods. J. Food Qual. Pref., 3 (1991/2), pp. 67-87. ...

Cited by 61 Related articles All 5 versions Web of Science: 41 Cite Save

A new significance test for consensus in generalized procrustes analysis

IANN WAKELING, MM RAATS... - Journal of sensory ..., 1992 - Wiley Online Library

... 92 IN WAKELING, MM RAATS and HJH MacFIE considerations when using GPA and a discussion on when and where to use scaling, refer to Dijksterhuis and Gower (1991). ... The Interpretation of Generalised Procrustes Analysis and Allied Methods. ... GOWER, JC 1975. ...

Cited by 59 Related articles All 2 versions Cite Save

[HTML] Sensory properties of hard cheese: identification of key attributes

DD Muir, EA Hunter, JM Banks, DS Horne - International Dairy Journal, 1995 - Elsevier

... 83-87. Dijksterhuis and Gower, 1991/1992; GB Dijksterhuis, JC Gower; The interpretation of Generalized Procrustes Analysis and allied methods. Food Quality & Preference, 3 (1991/1992), pp. 67-87. ... Gower; Generalized Procrustes Analysis. Psychometrika, 40 (1975), pp. 33-52 ...

Cited by 42 Related articles All 5 versions Web of Science: 34 Cite Save

[HTML] Generalized procrustes analysis of coffee brands tested by five European sensory panels

S de Jong, J Heidema, H van der Knaap - Food quality and preference, 1998 - Elsevier

... Dijksterhuis and Gower, 1992; GB Dijksterhuis, JC Gower; The interpretation of generalized Procrustes analysis and allied methods. Food Quality and Preference, 3 (1992), pp. 67-87. ...

Cited by 20 Related articles All 6 versions Web of Science: 17 Cite Save

[PDF] Procrustes analysis in sensory research

G Dijksterhuis - Data Handling in Science and Technology, 1996 - econ.upf.edu

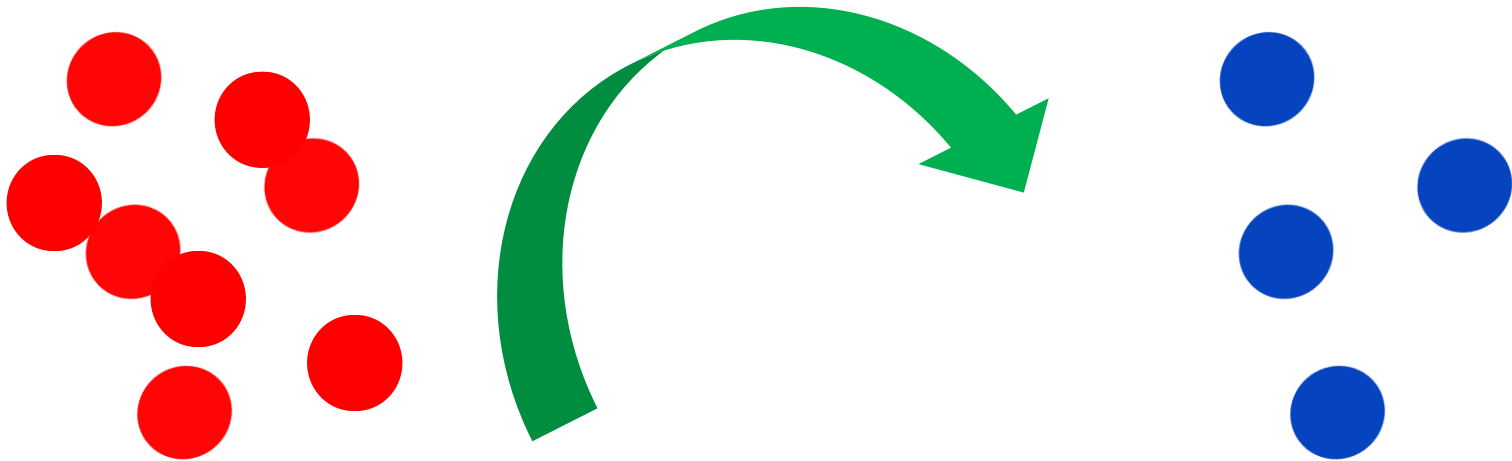
... A 3 — Total — i Assessor 1 — — — Residual — Assessor 2 A 'A — i Assessor 3 - Figure 9.

Why

- Name: given by Hurley and Cattell (1962, Behavioral Science) to a technique in which was originally developed for used in factor analysis (FA) and multidimensional scaling
 - Initially to “express disapproval of perceived tendency of some to distort one set of observations to support the claim that they fit another set” (Fitzpatrick et al. 2000)
- Other names:
 - landmark-based registration,
 - point registration with correspondence,
 - Absolute Orientation
 - Wahba’s problem (orientation only) and the associated Kabsch’s algorithm

What

- Three players:
 - Traveller (Measurement point-sets, X),
 - Procrustean bed (Model point-sets, Y), and
 - Procrustean solution (transformation, T)

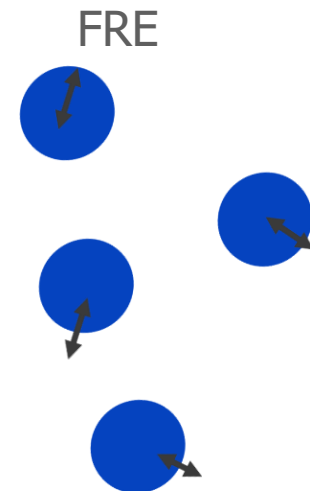
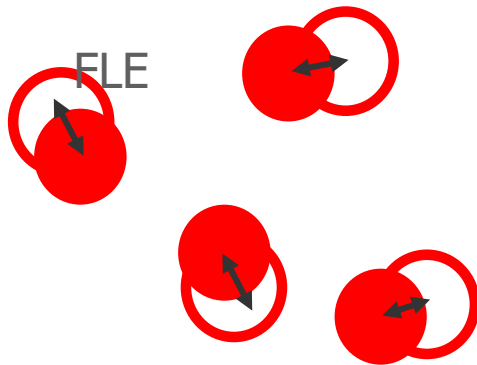


What

- $Y = R X + t$

- $$\begin{pmatrix} Y_{1x} & \dots & Y_{nx} \\ Y_{1y} & & Y_{ny} \\ Y_{1z} & \ddots & Y_{nz} \\ 1 & \dots & 1 \end{pmatrix} = \begin{pmatrix} R_{3 \times 3} & t_{3 \times 1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} X_{1x} & \dots & X_{nx} \\ X_{1y} & & X_{ny} \\ X_{1z} & \ddots & X_{nz} \\ 1 & \dots & 1 \end{pmatrix}$$

- $\text{FRE} = Y - (R X + t)$



What

- The objective is to find a transformation that satisfies some
 - optimality criterion: minimize FRE using a distance metric,
 - Proper rotation + translation (orthonormal),
 - Scaling + proper rotation + translation (orthogonal)
- More appropriately known as the Orthogonal Procrustes Problem (OPP)
 - Orthogonal == proper rotation although scaling is often involved

How, SVD

- a. Compute the weighted centroid of the fiducial configuration in each space:

$$\begin{aligned}\bar{\mathbf{x}} &= \sum_i^N w_i^2 \mathbf{x}_i / \sum_i^N w_i^2 \\ \bar{\mathbf{y}} &= \sum_i^N w_i^2 \mathbf{y}_i / \sum_i^N w_i^2 .\end{aligned}$$

- b. Compute the displacement from the centroid to each fiducial point in each space:

$$\begin{aligned}\tilde{\mathbf{x}}_i &= \mathbf{x}_i - \bar{\mathbf{x}} \\ \tilde{\mathbf{y}}_i &= \mathbf{y}_i - \bar{\mathbf{y}} .\end{aligned}$$

- c. Compute the weighted fiducial covariance matrix:

$$H = \sum_i^N w_i^2 \tilde{\mathbf{x}}_i \tilde{\mathbf{y}}_i^t ,$$

- d. Perform singular value decomposition of H :

$$H = U \Lambda V^t ,$$

where $U^t U = V^t V = I$, $\Lambda = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$, and $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq 0$.

- e. $R = V \text{diag}(1, 1, \det(VU)) U^t$.

- f. $\mathbf{t} = \bar{\mathbf{y}} - R \bar{\mathbf{x}}$.

How, Quaternion

- a. Compute the weighted centroid of the fiducial configuration in each space:

$$\bar{\mathbf{x}} = \sum_i^N w_i^2 \mathbf{x}_i / \sum_i^N w_i^2$$

$$\bar{\mathbf{y}} = \sum_i^N w_i^2 \mathbf{y}_i / \sum_i^N w_i^2 .$$

- b. Compute the displacement from the centroid to each fiducial point in each space:

$$\tilde{\mathbf{x}}_i = \mathbf{x}_i - \bar{\mathbf{x}}$$

$$\tilde{\mathbf{y}}_i = \mathbf{y}_i - \bar{\mathbf{y}} .$$

- c. Compute the weighted fiducial covariance matrix:

$$N = \begin{bmatrix} (S_{xx} + S_{yy} + S_{zz}) & S_{yz} - S_{zy} & S_{zx} - S_{xz} & S_{xy} - S_{yx} \\ S_{yz} - S_{zy} & (S_{xx} - S_{yy} - S_{zz}) & S_{xy} + S_{yx} & S_{zx} + S_{xz} \\ S_{zx} - S_{xz} & S_{xy} + S_{yx} & (-S_{xx} + S_{yy} - S_{zz}) & S_{yz} + S_{zy} \\ S_{xy} - S_{yx} & S_{zx} + S_{xz} & S_{yz} + S_{zy} & (-S_{xx} - S_{yy} + S_{zz}) \end{bmatrix} .$$

- e. $R = V \text{diag}(1, 1, \det(VU)) U^t$.

- f. $\mathbf{t} = \bar{\mathbf{y}} - R\bar{\mathbf{x}}$.

How, SVD vs. Quaternion

- Equivalent in terms of robustness, accuracy, and computational requirement
- Typically the SVD solution is preferred simply because the SVD itself is numerical robust,
 - SVD solution is generalizable to higher dimensions
- Quaternion solution works only with 3D dataset,
 - However, the solution always leads to proper solution

When (1952), matrix square root

- The first least-square solution was presented by Green (1952) using matrix square root, assuming full rank

**PSYCHOMETRIKA—VOL. 17, NO. 4
DECEMBER, 1952**

THE ORTHOGONAL APPROXIMATION OF AN OBLIQUE STRUCTURE IN FACTOR ANALYSIS

BERT F. GREEN

MASSACHUSETTS INSTITUTE OF TECHNOLOGY*



When (1966), SVD

- Schönemann presented the first generalized solution (1966) using Singular-Value Decomposition

TABLE 1

Flowchart for Orthogonal Procrustes
(General Solution)

(1) Read A

Read B

(2) Compute

$$S = A^T B$$

(3) Diagonalize

$$S^T S = V D_S V^T$$

$$S S^T = W D_S W^T$$

$$(4) T = W V^T$$

$$(5) B^* = A T$$

$$(6) E = B - B^*$$

$$(7) \text{Output } T, A T, E = B - A T$$

(8) End.

When (1966), SVD, proper rotation

- Farrell (1966) restricted the solution to proper rotation

Because $\det M$ is required to be $+1$, $\det X = \det (NM^TUN^T) = (\det N)^2 \cdot \det M \det U = \det U$. If $\det U = -1$, then it is required that $\det X = -1$, and it is not hard to see that

$$X = \begin{pmatrix} I_{k-1} & 0 \\ 0 & -1 \end{pmatrix}$$

second. That is, find M which minimizes

$$\sum_{j=1}^n \| \mathbf{v}_j^* - M\mathbf{v}_j \|^2.$$

When (1966), matrix square root

- Wessner presented a solution based on matrix square root

R. H. WESSNER (Hughes Aircraft Company) in his solution points out that if $\det A \neq 0$, then $V^*V^T = A = UP$,

$$U = (A^T)^{-1}(A^T A)^{1/2}, \quad P = (A^T A)^{1/2},$$

where $(A^T A)^{1/2}$ is the symmetric square root of $A^T A$ with positive eigenvalues, and, hence, for $\det A > 0$,

$$M_0 = (VV^{*T})^{-1}(VV^{*T}V^*V^T)^{1/2}.$$

When (1970),

- Schönemann and Carroll presented a solution with isotropic scaling (1970)

PSYCHOMETRIKA—VOL. 35, NO. 2
JUNE, 1970

$$(3.7) \quad u = \text{tr } B'QB / \text{tr } A'QA$$

PETER H. SCHÖNEMANN* AND ROBERT M. CARROLL†

THE OHIO STATE UNIVERSITY

A least squares method is presented for fitting a given matrix A to another given matrix B under choice of an unknown rotation, an unknown translation, and an unknown central dilation. The procedure may be useful to investigators who wish to compare results obtained with nonmetric scaling techniques across samples or who wish to compare such results with those obtained by conventional factor analytic techniques on the same sample.

When (1987), SVD

- Arun et al presented the SVD solution in PAMI (1987)

A. Algorithm

Step 1: From $\{p_i\}$, $\{p'_i\}$ calculate p , p' ; and then $\{q_i\}$, $\{q'_i\}$.

Step 2: Calculate the 3×3 matrix

$$H \triangleq \sum_{i=1}^N q_i q_i^t \quad (11)$$

where the superscript t denotes matrix transposition.

Step 3: Find the SVD of H ,

$$H = U \Lambda V^t. \quad (12)$$

Step 4: Calculate

$$X = V U^t. \quad (13)$$

Step 5: Calculate $\det(X)$, the determinant of X .

If $\det(X) = +1$, then $\hat{R} = X$.

If $\det(X) = -1$, the algorithm fails. (This case usually does not occur. See Sections IV and V.)

When (1991), SVD

- Umeyama presented the SVD solution in PAMI (1991)

Least-Squares Estimation of Transformation

$$\begin{aligned} R &= U Q V^T \\ &= U S V^T \end{aligned} \quad (30)$$

where

$$S = \begin{cases} I & \text{if } \det(U) \det(V) = 1 \\ \text{diag}(1, 1, \dots, 1, -1) & \text{if } \det(U) \det(V) = -1. \end{cases} \quad (31)$$

Q.E.D.

translation, and scaling) that give the least mean squared error between these point patterns. Recently Arun *et al.* and Horn *et al.* have presented a solution of this problem. Their solution, however, sometimes fails to give a correct rotation matrix and gives a reflection instead when the data is severely corrupted. The theorem given in this correspondence is a strict solution of the problem, and it always gives the correct transformation parameters even when the data is corrupted.

When (1986), quaternion

- Faugeras and Heberts presented a quaternion based solution (1986) in the context of fitting points to planes for range data

$$E = \text{Min} \sum_{i=1}^N (\mathbf{v} \cdot \mathbf{x}_i + d)^2 = \text{Min } F(\mathbf{v}, d). \quad (2)$$

O. D. Faugeras

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The Representation, Recognition, and Locating of 3-D Objects

Finally, the direction of the best-fitting plane is the vector \mathbf{v}_{\min} corresponding to the smallest eigenvalue λ_{\min} of the matrix

$$\mathbf{M} = \sum_{i=1}^N \mathbf{A}_i \mathbf{A}_i^T,$$

When (1986), quaternion

- Froimowitz and Matthysse presented a quaternion based solution (1986)

Appendix

Consider two rigid bodies K and K' , each composed of N points internally connected. Let \mathbf{X}_i ($i = 1, \dots, N$) and \mathbf{X}'_i ($i = 1, \dots, N$) be 3-vectors denoting the positions of the points of K and K' ; assume

$$\sum_{i=1}^N \mathbf{X}_i = \sum_{i=1}^N \mathbf{X}'_i = 0 \quad (1)$$

Let K' be subjected to a rotation \mathbf{R} followed by a translation \mathbf{T} ; the problem is to find \mathbf{R} and \mathbf{T} such that, after they are applied, K' is as closely as possible superimposed upon K . We use as a criterion of closeness the sum of the squares of the distances between corresponding pairs of points. Thus, the quantity

$$F = \sum_{i=1}^N \|\mathbf{X}_i - (\mathbf{T} + \mathbf{R}\mathbf{X}'_i)\|^2 \quad (2)$$

($\|\cdot\|$ denoting the Euclidean norm) is to be minimized. Because of (1), (2) reduces to $\sum_{i=1}^N \|\mathbf{X}_i - \mathbf{R}\mathbf{X}'_i\|^2 + N\|\mathbf{T}\|^2$; evidently $\mathbf{T} = 0$ is the optimal choice. $\sum_{i=1}^N \|\mathbf{X}_i - \mathbf{R}\mathbf{X}'_i\|^2$ can be expressed as

$$\sum_{i=1}^N \|\mathbf{X}_i\|^2 + \sum_{i=1}^N \|\mathbf{X}'_i\|^2 - 2 \sum_{i=1}^N \mathbf{X}_i \cdot \mathbf{R}\mathbf{X}'_i \quad (3)$$

(\cdot denoting the scalar product), so our task is to maximize

$$U = \sum_{i=1}^N \mathbf{X}_i \cdot \mathbf{R}\mathbf{X}'_i \quad (4)$$

According to a theorem of Cayley,⁶⁰ every rotation matrix can be expressed as eq 5 where $\sum_{i=1}^4 q_i^2 = 1$. Since \mathbf{R}

$$\mathbf{R} = \begin{bmatrix} q_4^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_1q_2 + q_3q_4) & 2(q_1q_3 - q_2q_4) \\ 2(q_1q_2 - q_3q_4) & q_4^2 + q_2^2 - q_1^2 - q_3^2 & 2(q_2q_3 + q_1q_4) \\ 2(q_1q_3 + q_2q_4) & 2(q_2q_3 - q_1q_4) & q_4^2 + q_3^2 - q_1^2 - q_2^2 \end{bmatrix} \quad (5)$$

is a quadratic form in q_1, \dots, q_4 , U is also, which we will denote by

$$U = \sum_{s,t=1}^4 H_{st} q_s q_t \quad H_{st} = H_{ts} \quad (6)$$

where the H_{st} depend on \mathbf{X}_i and \mathbf{X}'_i and can readily be calculated as functions of those variables. As q_1, \dots, q_4 are varied subject to the constraint $\sum_{i=1}^4 q_i^2 = 1$, the maximum value of U is achieved by setting the q 's equal to that eigenvector of \mathbf{H} which corresponds to the largest eigenvalue λ_m ; the constrained maximum of U is, indeed, λ_m .

When (1987), quaternion

- Horn presented a quaternion based solution (1987)

Reprinted from *Journal of the Optical Society of America A*, Vol. 4, page 629, April 1987

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Closed-form solution of absolute orientation using unit quaternions

Berthold K. P. Horn

Department of Electrical Engineering, University of Hawaii at Manoa, Honolulu, Hawaii 96720

$$N = \begin{bmatrix} (S_{xx} + S_{yy} + S_{zz}) & S_{yz} - S_{zy} & S_{zx} - S_{xz} & S_{xy} - S_{yx} \\ S_{yz} - S_{zy} & (S_{xx} - S_{yy} - S_{zz}) & S_{xy} + S_{yx} & S_{zx} + S_{xz} \\ S_{zx} - S_{xz} & S_{xy} + S_{yx} & (-S_{xx} + S_{yy} - S_{zz}) & S_{yz} + S_{zy} \\ S_{xy} - S_{yx} & S_{zx} + S_{xz} & S_{yz} + S_{zy} & (-S_{xx} - S_{yy} + S_{zz}) \end{bmatrix}.$$

When (1988), orthonormal matrices

- Horn presented a solution based on orthonormal matrices (1988)

Horn *et al.*

Vol. 5, No. 7/July 1988/J. Opt. Soc. Am. A 1127

Closed-form solution of absolute orientation using orthonormal matrices

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Received June 2, 1987; accepted March 25, 1988



When					
	Orthogonal Matrices	SVD	Quaternion	keyword	Note
Green (1952)	X				Factor Analysis
Schönemann (1966)		X		Procrustes	Psychometrika
Farrel (1966)		X		Proper rotation	aerospace
Wessner (1966)	X				aerospace
Schönemann (1970)					scaling
Kabsch (1976)		X			Crystallography
Faugeras (1986)			X		robotics
Froimowitz (1986)			X		chemistry
Arun (1987)		X			PAMI/EE
Horn (1987)			X	Absolute orientation	CV
Horn (1988)	X				CV
Umeyama (1991)		X			PAMI/EE

Does the history repeat?

- Let's consider the scenario of anisotropic noise

Iterative Solution for Rigid-Body Point-Based Registration with

APPENDIX

The following are Matlab functions that implement the algorithm presented in this paper:

```
function [R,t,FRE,n] = anisotropic_point_register(X,Y,W,threshold)
% X is the moving set, which is registered to the static set Y. Both are 3
% by N, where N is the number of fiducials. W is a 3-by-3-by-N array, with
% each page containing the weighting matrix for the Nth pair of points.
% THRESHOLD is the size of the change to the moving set above which the
% iteration continues.
```

- [6]^o N. Ohta and K. Kanatani, “Optimal estimation of three-dimensional rotation and reliability evaluation”, Computer Vision - ECCV 98', H. Burkhardt, B. Neumann Eds., Lecture Notes in Computer Science, Springer, pp. 175—187 (1998).

What: Anisotropic noise

Iterative Solution for Rigid-Body Point-Based Registration with Anisotropic Weighting

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IEEE TRANSACTIONS ON MEDICAL IMAGING, VOL. 30, NO. 3, MARCH 2011

General Approach to First-Order Error Prediction in Rigid Point Registration

Andrei Danilchenko* and J. Michael Fitzpatrick, *Fellow, IEEE*

1520

IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. 34, NO. 8, AUGUST 2012

679

Convergent Iterative Closest-Point Algorithm to Accomodate Anisotropic and Inhomogenous Localization Error

Lena Maier-Hein, Alfred M. Franz, Thiago R. dos Santos, Mirko Schmidt, Markus Fangerau, Hans-Peter Meinzer, and J. Michael Fitzpatrick, *Fellow, IEEE*

What: linearizing rotation

APPENDIX

The following are Matlab functions that implement the algorithm presented in this paper:

```
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% each page containing the weighting matrix for the Nth pair of points.
% THRESHOLD is the size of the change to the moving set above which the
% iteration continues.
o.
```

$$w = \begin{bmatrix} \sigma & 0 & 0 \\ 0 & \sigma & 0 \\ 0 & 0 & 5\sigma \end{bmatrix}$$

Optimal Rigid Motion Estimation and Performance Evaluation with Bootstrap

Bogdan Matei and Peter Meer*

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Nothing new under the sun?

- What has been will be again, what has been done will be done again; there is nothing new under the sun (quote from bible)
 - Your problem may have been solved by others
- “but there’s always a fresh way of looking at something”
 - Different solution to the same problem?
- Cite the “right” paper
- Google is your friend
 - Learn the correct keywords
 - Expand your search to other fields
- Don’t re-invent the wheel



Proof

- Let's derive the least-square solution for the Orthogonal Procrustes Analysis
 - "Closed-form solution of absolute orientation using unit quaternions" by B. K. P. Horn (1987)
 - "Least-Squares Fitting of Two 3-D Point Sets" by Arun et al. (1987)