Using SVD for some fitting problems

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This is some notes on how to use the singular value decomposition (SVD) for solving some fitting problems. The problems are considered in the PhD-course in data analysis at Luleå University of Technology.

1 The Singular Value Decomposition

The singular value decomposition of a matrix $A \in \mathbb{R}^{m\times n}$ is

$$A = USV^T,$$

where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal matrices, and $S \in \mathbb{R}^{m\times n}$ is a diagonal matrix containing the singular values $\sigma_1 \geq \sigma_2 \geq \cdots, \geq \sigma_r \geq 0,\ r = \min(m, n)$.

2 The Rigid Body Movement Problem

Assume that we have n landmarks in a rigid body and let $\{x_1, \ldots, x_n\}$ be the 3-D positions of these landmarks before the movement and $\{y_1, \ldots, y_n\}$ be the positions after the movement. We want to determine a rotation matrix R and a translation vector d that map the points x_i to the points $y_i, i = 1, \ldots, n$. Because of measurement errors the mapping is not exact and we use the following least-squares problem

$$\min_{R\in\Omega,d} \sum_{i=1}^{n} \| Rx_i + d - y_i \|^2, \tag{1}$$

where

$$\Omega = \{R \,|\, R^T R = RR^T = I_3; det(R) = 1\},$$

is the set of orthogonal rotation matrices. Problem (1) is linear with respect to the vector d but it is nonlinear with respect to the rotation matrix R (that is because of the orthogonality condition of R). Introducing $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i,\ \ \overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$, and the matrices

$$A = [x_1 - \overline{x}, \ldots, x_n - \overline{x}]\,,\ \ B = [y_1 - \overline{y}, \ldots, y_n - \overline{y}]\,,$$

the problem of determining the rotation matrix becomes

$$\min_{R\in\Omega} \|RA - B\|_F, \tag{2}$$

where the Frobenius norm of a matrix Z is defined as $\|Z\|_F^2 = \sum_{i,j} z_{i,j}^2$. In e.g. [1, 3] it is shown that this *Orthogonal Procrustes problem* can be solved using the singular value decomposition of the matrix $C = BA^T$. An algorithm is presented below.

Algorithm 2.1 *Algorithm for solving problem (1) by using the SVD-method.*

1. $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \;\; \overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$
2. $A = [x_1 - \overline{x}, \ldots, x_n - \overline{x}]\,, \;\; B = [y_1 - \overline{y}, \ldots, y_n - \overline{y}]$
3. $C = BA^T$
4. $U\,S\,V^T = C$ *(Computation of the singular decomposition of C)*
5. $R = U\,diag(1, 1, det(UV^T))\,V^T$
6. $d = \overline{y} - R\overline{x}$

The solution to problem (2) is unique if $\sigma_2(C)$ is nonzero. (More strictly, the solution is not unique if $\sigma_2(C)$ equals zero or if $\sigma_2(C) = \sigma_3(C)$ and $det(UV^T) = -1$. But the latter situation implies that a reflection is the best orthogonal matrix describing the movement. This situation will seldom occur when studying rigid bodies and indicates that something is wrong.)

Algorithm 2.1 can be used also in 2-D settings when a movement in the plane is to be determined.

More about the rigid body movement problem and its sensitivity with respect to perturbations in the positions of the landmarks can be found in [4, 5, 6].

3 Fitting Planes and Lines by Orthogonal Distance Regression

Assume that we want to find the plane that are as close as possible to a set of n 3-D points $(p_1, \ldots, p_n)$ and that the closeness is measured by the square sum of the orthogonal distances between the plane and the points.

Let the position of the plane be repreented by a point c belonging to the plane and let the unit vector n be the normal to the plane determining its direction. The orthogonal distance between a point p_i and the plane is then $(p_i - c))^T n$. Thus the plane can be found by solving

$$\min_{c, \|n\|=1} \sum_{i=1}^{n} ((p_i - c)^T n)^2. \tag{3}$$

Solving this for c gives $c = 1/n \sum_{i=1}^{n} p_i$, see e.g [2]. Introducing the $3 \times n$ matrix

$$A = [p_1 - c, p_2 - c, \ldots, p_n - c]$$

problem (3) can be formulated as

$$\min_{\|n\|=1} \|A^T n\|_2^2. \tag{4}$$

Using the singular decomposition $A = USV^T$, of A, we have

$$\|A^T n\|_2^2 = \|VS^T U^T n\|_2^2 = \|S^T U^T n\|_2^2 = (\sigma_1 y_1)^2 + \sigma_2 y_2)^2 + (\sigma_3 y_3)^2,$$

where y is the unit vector $y = U^T n$. Thus, $\|A^T n\|_2^2$ is minimised for $y = (0,0,1)^T$ or equivalently, for $n = U(:,3)$. The minimal value of $\sum_{i=1}^n ((p_i - c)^T n)^2$ is σ_3^2. To summerize we present the following algorithm for fitting the plane.

Algorithm 3.1 *Algorithm for fitting a plane using orthogonal distance regression and singular value decomposition.*

1. $c = \frac{1}{n}\sum_{i=1}^n p_i$
2. $A = [p_1 - c, \ldots, p_n - c]$
3. $U\,S\,V^T = A$ *(Computation of the singular decomposition of A)*
4. $n = U(:,3)$, *i.e., the normal is given as the third column of* U.

Since the normal is given by $U(:,3)$ it follows from the orthogonality of U that the plane is spanned by the two first columns of U.

Similarly, we can obtain the best fitted line as the first column of U. The square sum of distances between the "best "plane and the points are given by σ_3^3 and the square sum of distances between the "best" line and the points is given by $\sigma_2^2 + \sigma_3^2$.

A similar technique can be used also for fitting a line in 2-D.

References

[1] K.S. Arun, T.S. Huang, and S.D. Blostein. Least-Squares Fitting of Two 3-D Point Sets. *IEEE Trans. Patt. Anal. Machine Intell.*, Pami-9:698–700, 1987.

[2] W. Gander and J. Hrebicek. *Solving Problems in Scientific Computing using Matlab and Maple.* Springer Verlag, 1993.

[3] R.J. Hanson and M.J. Norris. Analysis of Measurements Based on the Singular Value Decomposition. *SIAM J. Sci. Stat. Comput.*, 2:363–373, 1981.

[4] I. Söderkvist. Perturbation Analysis of the Orthogonal Procrustes Problem. *BIT*, 33:687–694, 1993.

[5] I. Söderkvist and P.-Å. Wedin. Determining the Movements of the Skeleton Using Well-Configured Markers. *Journal of Biomechanics*, 26(12):1473–1477, 1993.

[6] I. Söderkvist and P.-Å. Wedin. On Condition Numbers and Algorithms for Determining a Rigid Body Movement. *BIT*, 34:424–436, 1994.