A mechanical interpretation of least squares fitting in 3D

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Abstract

We address the computation of the line that minimizes the sum of the least squared distances with respect to a given set of n points in 3-space. This problem has a well known satisfying solution by means of PCA. We offer an alternative interpretation for this optimal line as the center of the screw motion that minimizes the sum of squared velocities in the given points. The numerical translation of this viewpoint is a generalized eigenproblem, where the total residue of the optimal line appears as the smallest generalized eigenvalue.

1 Introduction

In many practical problems, as the result of measurements or computations, we obtain a set of n collinear points in 3-space. However, due to (random) noise or round off errors the points do not lie on one line anymore. Although the exact position of the line is lost forever, one can still try to find the "most likely" line, according to some model assumption (e.g. gaussian noise). To "recover" the original line by means of the disturbed point set, one usually performs a two step procedure:

1. Elimination of outliers by means of some robust method (e.g. RANSAC, [1]).
2. Compute the line in euclidean 3-space that minimizes the sum of squared distances to the given points (the *least squared distances line*).

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The second step is the subject of this paper. As a matter of fact, the problem of finding the lsd-line has an elegant solution that is known for several decennia, namely by means of *principal component analysis*. We will refer to it as the PCA-method, and it is built on two observations. First, there is the property that a lsd-line always contains the mean of the data. It is convenient to translate the origin to this mean. Secondly, the direction of the lsd-line is given by the principal direction of the *scatter matrix* S, that is, the eigenvector belonging to the largest eigenvalue of S. This matrix S is a 3 by 3 matrix that is obtained as $A^T A$, with A the n by 3 matrix where each row contains the coordinates of a data point. Or equivalently , S is $(n-1)$ times the covariance matrix of the n 3D points.

A numerical improvement of the previous algorithm is given in [2]. In this article the author avoids to form the scatter matrix $A^T A$, directly operating on A, which is numerically more stable. See also [3] for a discussion of this method.

The purpose of this article is to present a mechanical interpretation of this lsd-line, providing a description in terms of Plücker coordinates. Although our description leads to an alternative algorithm for computing the lsd-line, we strongly suggest to keep on using the algorithm of [2], which is numerically superior.

Our starting point will be *screw centers*, real 6-vectors that represent infinitesimal rigid motions in 3-space. We recall the necessary fundamentals of kinematics in Section 2. It is well known that lines in (projective) 3-space can be represented by a 6-tuple of *Plücker coordinates*. However, not every 6-vector can be regarded as a line; it has to satisfy a quadratic equation (*GP-relation*). But it can always be regarded as a screw center, only corresponding to a line in the case of a special screw motion, namely a rotation (pitch 0) or a translation (pitch ∞, but that will be not the issue here as this case corresponds to a line at infinity).

In Section 3 we solve the problem of finding the optimal (normalized) screw center for the given set of n points, in the sense that it minimizes the sum of the squared velocities in each point. We can show almost immediately that this problem can be transformed to the minimization of a *generalized Raleigh quotient*, and hence to a *generalized eigenproblem*. Section 3 exhibits this known theory in a self-contained style for our special case. The conclusion of Section 3 is that the optimal screw center will correspond to the "smallest" generalized eigenvalue of a pair of symmetric 6 by 6 matrices. Our procedure is very similar to the solution by Pottmann and Wallner (see [4]) to reconstruct rotational or helical surfaces from measurement points.

The key observation is made in Section 4. It tells that the optimal screw center for a set of points has always pitch 0, and so it represents the Plücker coordinates of a line. Furthermore, after normalizing the screw center, the implied velocities are just the euclidean distances between the given points and this line. So, it appears that we have computed the lsd-line by this method. The generalized eigenvalue associated with our solution exactly equals the residue of the lsd-line with respect to the given set of points.

2 Screw centers

If we consider the first order approximation of a continuous, smooth motion in 3-space ($\mathbb{R}^3$) then we obtain a so-called *infinitesimal* or *instantaneous* motion that assigns a velocity vector V_p to each point p. A *rigid motion* is characterized by the property that the distance between each pair of points p and q is preserved:

$$||p(t) - q(t)||^2 = \text{constant}$$

or infinitesimally (taking the derivative in $t = 0$ and putting $p = p(0)$ and $q = q(0)$):

$$(p - q) \cdot (V_p - V_q) = 0$$

called the *preserved distance property (PDP)* for rigid infinitesimal motions.

From the PDP it can be deduced that infinitesimally every rigid motion can be represented by a 6-vector $C \in \mathbb{R}^6$, the *center* of the motion. More precisely, if $C = (c, \overline{c})$ with $c, \overline{c} \in \mathbb{R}^3$ then the velocity V_p in a point p is given by

$$V_p = V_p(C) = -\overline{c} + p \times c$$

It is easy to verify the PDP for these velocities, but conversely one can prove that every rigid infinitesimal motion has this form. We refer to [5]. Sometimes, by abuse of language, we will identify C with the motion it represents.

Example 1. If $\overline{c} = c = 0$ then $C = 0$ represents the zero motion (nothing moves).

Example 2. If $c = 0$ then each point p is subject to the same velocity vector: $V_p = -\overline{c}$. So, C is the center of an infinitesimal translation.

Example 3. If $c \neq 0$ but $c \cdot \overline{c} = 0$ then there exists a fixed point $z \in \mathbb{R}^3$ such that $\overline{c} = z \times c$. Consequently, for each point p, $V_p = (p - z) \times c$, and hence C represents an infinitesimal rotation about the line that goes through z and is directed by c.

Definition 1. *Let $C = (c, \overline{c})$ be a given center of motion such that $c \neq 0$ (no translation). The* pitch *of C is defined as*

$$\rho = \rho_C = \frac{c \cdot \overline{c}}{c^2}$$

Usually, the pitch of a translation is defined as ∞. Notice that the centers of a rotation are characterized as those with pitch zero.

Because $c \cdot (\overline{c} - \rho_C c) = 0$, the center $A = (c, \overline{c} - \rho c)$ represents a rotation.

Definition 2. *If C is a center with finite pitch ρ then the corresponding rotation $A = (c, \overline{c} - \rho c)$ is called the* axis *of C. To avoid confusion we will use the term* euclidean axis *if we mean the geometric line about which is rotated.*

If C is the center of a translation ($c = 0$) then the line at infinity of the planes perpendicular to $\overline{c}$ is often called the axis of C. If C represents a rotation then it equals its own axis. In general, $C = (c, \overline{c}) = A + (0, \rho c)$. This proves that (infinitesimally) a rigid motion is a translation, a rotation or a composition of both. Furthermore, we see that in this last composition the translation is directed along the axis of the rotation A. This is called an (infinitesimal) *screw motion*. If we are willing to regard rotations and translations as special cases of screw motions (with pitch 0 and ∞ respectively) then we can always refer to C as a *screw center*. In the literature this claim is known as the **Central Axis Theorem of Poinsot** ([5]).

Remark. The *Plücker coordinates* L of a line in $\mathbb{RP}^3$ through points with homogeneous coordinates $(x_0 : x_1 : x_2 : x_3)$ and $(y_0 : y_1 : y_2 : y_3)$ are defined by

$$L = (L_{01} : L_{02} : L_{03} : L_{23} : L_{31} : L_{12})$$

where L_{ij} is defined as the following 2 by 2 determinant:

$$L_{ij} = \begin{vmatrix} x_i & x_j \\ y_i & y_j \end{vmatrix}$$

It can be verified that L is determined as a point in $\mathbb{RP}^5$ by the given line in 3-space, rather than by the choice of the two projective points. If we choose $x_0 = 0$ as the plane at infinity of $\mathbb{RP}^3$ then we obtain a canonical embedding of affine 3-space $\mathbb{R}^3$ (equipped with the standard euclidean norm).

One can check that each 6-vector of Plücker coordinates for a line in $\mathbb{R}^3$ yields the center of a rotation with the given line as euclidean axis. Conversely, each center C of a rotation can be considered as the Plücker coordinates for the euclidean axis of this rotation. The different choices of scalar multiples correspond to different angular velocities. If the given line lies at infinity then each 6-vector of Plücker coordinates represents a translation in a direction orthogonal to the affine planes that contain the given line in the projective completion.
The points in $\mathbb{RP}^5$ that are the Plücker coordinates of some line in 3-space are characterized by the famous *Grassmann-Plücker relation*:

$$L_{01}L_{23} + L_{02}L_{31} + L_{03}L_{12} = 0$$

defining the *Klein quadric* in $\mathbb{RP}^5$ ([6, 7, 4]). Translated to screw centers $C = (c, \overline{c})$, the GP-relation comes down to $c \cdot \overline{c} = 0$, yielding pitch ∞ (translation) or pitch 0 (rotation).

If $C = (c, \overline{c})$ represents a rotation (or equivalently, the Plücker coordinates of a finite line), then both c and $\overline{c}$ have geometric interpretations in terms of the euclidean axis L_C:

1. c directs L_C (a vector parallel to L_C)
2. $\overline{c} = q \times c$ for a point q on L_C; so, it can be considered as the moment of L_C. We can always choose $q \cdot c = 0$.

From this it is immediate to deduce a euclidean representation for L_C from C. We refer to [4] for a splendid treatment on line geometry.

3 Optimal screw center

Let $\mathcal{P} = \{p_1, \ldots, p_n\}$ be a finite point set in the euclidean space $\mathbb{R}^3$. If $C = (c, \overline{c})$ is a given screw center then we can record the *global motion* of $\mathcal{P}$ in one $3n$-vector:

$$V_{\mathcal{P}}(C) = (V_1, \ldots, V_n)$$

with $V_i = V_{p_i}(C) = -\overline{c} + p_i \times c$.

In this section we look for the "optimal screw center" C for a given cloud of points $\mathcal{P}$ in 3-space, in the sense that $||V_{\mathcal{P}}(C)||^2 = \sum_{i=1}^{n} ||V_i||^2$ is minimized. As usual, we have to constraint C by some normalization in order to exclude the trivial solution $C = 0$ and to guarantee in the same time that the minimum still exists. Furthermore, we choose to exclude translations, that is, we avoid $c = 0$. Indeed, we may look for a screw C now, but in our hidden agenda we are aiming for the best fitting line; because the axis of a translation lies at infinity, it does not suit our purposes. This brings us to the following constrained minimization problem:

$$\min ||V_{\mathcal{P}}(C)||^2 \quad \text{subject to } ||c|| = 1$$

where $C = (c, \overline{c})$.

For each point $p_i = (x_i, y_i, z_i)$ of $\mathcal{P}$ we consider the following 3 by 6 *motion matrix*:

$$M(p_i) = \begin{pmatrix} 0 & -z_i & y_i & -1 & 0 & 0 \\ z_i & 0 & -x_i & 0 & -1 & 0 \\ -y_i & x_i & 0 & 0 & 0 & -1 \end{pmatrix}$$

This enables us to write

$$V_{p_i}(C) = M(p_i) \cdot C^T$$

where the screw center C now appears as a column vector C^T. Next, we concatenate the matrices $M(p_1), \ldots, M(p_n)$ and obtain one $3n$ by 6 *global motion matrix* $M = M(\mathcal{P})$ such that

$$V_{\mathcal{P}}(C) = M \cdot C^T.$$

Notice that a solution of the system $MC^T = 0$ corresponds to a center C of a screw that does not move the points of $\mathcal{P}$. The only centers $C \neq 0$ that keep points in $\mathbb{R}^3$ fixed correspond to rotations, fixing the points of the euclidean rotation axis. This leads us to the following description for the degenerate case for M:

Lemma 1. *If M is the global motion matrix of a point set $\mathcal{P}$ in $\mathbb{R}^3$ then the rank of M is 6 (maximal) if and only if $\mathcal{P}$ is not collinear.*

Next, we introduce the matrix

$$D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

With the previous notations our minimization problem can be reformulated with the objective function CM^TMC^T under the constraint $CD^TDC^T = CDC^T = 1$. This is equivalent to minimizing the *Raleigh quotient*

$$\frac{CM^TMC^T}{CDC^T},$$

a well-known problem that is solved by the "generalized eigenvector" corresponding to the smallest "generalized eigenvalue" of the pair of symmetric matrices (M^TM, D) ([8]). Due to the symmetry of the involved matrices, the (finite) generalized eigenvalues $\lambda_1, \lambda_2, \lambda_3$ are known to be real numbers, that can be easily seen to be positive in this case.

Finally, if $M^TMC^T = \lambda DC^T$ then

$$||V_{\mathcal{P}}(C)||^2 = \lambda CDC^T = \lambda||c||^2$$

yielding the following solution of our constrained minimization problem:

Theorem 1. *Let M be the $3n$ by 6 global motion matrix corresponding to a non-collinear set $\mathcal{P}$ of n points in $\mathbb{R}^3$ and let $N = M^TM$. Then the pair (N, D) has 3 finite generalized eigenvalues all positive and real: $\lambda_1 \leq \lambda_2 \leq \lambda_3$. Furthermore, if $C = (c, \overline{c})$ is a generalized eigenvector corresponding to λ_1, rescaled such that $||c|| = 1$ then it minimizes $||V_{\mathcal{P}}(C)||^2$ subject to $||c|| = 1$. The residue for this optimal solution exactly equals λ_1.*

Numerical remark. A convenient way to solve a generalized eigenvalue problem goes by way of the *Cholesky decomposition*. Since D is singular we must rewrite our matrix equation as

$$DC^T = \mu NC^T$$

where $N = M^TM$ is assumed to be regular (Lemma 1). Since N is positive definite, it can be decomposed as a product of a triangular matrix and its transpose, $N = LL^T$ or U^TU (with L lower and U upper triangular). The problem can now be transformed to the common eigenvalue problem for $L^{-1}DU^{-1}$. Because the smallest value for λ corresponds to the largest value for μ, the wanted eigenvector Z can be found by the *power method*. Finally, our solution equals $C = U^{-1}Z$.
However, in our case this procedure is not expected to be more accurate, because the computational bottleneck of the direct method is solving a cubic equation, which can be done exactly!

4 From optimal screws to optimal lines

We start this section with the observation that the optimal screw in the sense of Section 3 is of a special type:

Theorem 2. *If $\mathcal{P}$ is a set of n points in $\mathbb{R}^3$ then the screw $C = (c, \overline{c})$ with $||c|| = 1$ that minimizes $||V_{\mathcal{P}}(C)||^2$ is a rotation.*

Proof. The condition $||c|| = 1$ prevents C from being a translation, so it has a finite pitch ρ. Consider the rotation A that is the axis of C, $A = (a, \overline{a})$ with $a = c$ and $\overline{a} = \overline{c} - \rho c$ (see Section 2). For any point p in $\mathcal{P}$ we observe

$$a \cdot V_p(A) = a \cdot (-\overline{a} + p \times a) = 0$$

as $a \cdot \overline{a} = 0$ for a rotation. Applying Pythagoras' formula on $V_p(C) = V_p(A) + (-\rho a)$ we obtain

$$||V_p(C)||^2 = ||V_p(A)||^2 + \rho^2||a||^2$$

and hence, $||V_p(A)||^2 \leq ||V_p(C)||^2$. This yields that $\rho = 0$ or that $C = A$ or that C is a rotation. ■

Remark. In computational issues concerning lines in 3-space it has become common use to work with Plücker coordinates (screw centers). In doing so one has to cope with two technical problems:

- Plücker coordinates are determined up to a scalar multiple. This inconvenience is often overcome by normalization: $||c|| = 1$, as we did in Section 3. By this normalization we lose lines at infinity, but this might be an advantage in many applications (as in ours).
- Not every 6-vector represents the Plücker coordinates of a line (not every screw is a rotation). This problem often forces us to add the (nonlinear!) GP-relation to the algorithm. In our situation we appear to get this quadratic equation for free.

So far it may be not clear why we chose the velocities $V_p(C)$ as the residues to be minimized. The reason is that $V_p(C)$ is related to the euclidean distance between the point p and the line that is associated with the axis of C. This relation is most transparent when C is a rotation, the case that is relevant for our purposes. Indeed, if $A = (a, \overline{a})$ represents a rotation with L_A the associated euclidean axis, and if p is a point in $\mathbb{R}^3$ then it is well-known that

$$||V_p(A)|| = |pL_A| \cdot ||a||$$

with $|pL_A|$ the euclidean distance between the point and the line.

Using this last remark, combined with Theorem 2 and Theorem 1, we arrive at the main result of this article.

Theorem 3. *If $\mathcal{P}$ is a set of n points in $\mathbb{R}^3$ then the screw $C = (c, \overline{c})$ with $||c|| = 1$ that minimizes $||V_{\mathcal{P}}(C)||^2$ yields the Plücker coordinates of the line that minimizes the sum of the squared distances to the given points. This minimal residue is equal to the smallest generalized eigenvalue of the pair $(M^T M, D)$, and the optimal screw (line) is the corresponding generalized eigenvector.*

Remark. This algorithm has been checked in several simulations, in each case yielding the same line as compared to PCA.

5 Conclusion

We presented an alternative approach for computing the line that optimally fits a given 3D data set in the least squared distances sense. Likewise the classical solution (by PCA) a closed form is obtained by solving a cubic equation. Our new approach provides a new interpretation for this optimal line: the axis of the screw motion that minimizes the global velocity magnitude. A crucial step in our arguments is the observation that this screw motion always represents a rotation, and so it equals

the Plücker coordinates of a line (Theorem 2). After normalization, the velocities of the individual points get the meaning of euclidean distances to this line.
We translated the problem of the optimal screw motion to the minimization of a generalized Raleigh quotient, and hence to a generalized eigenproblem. The "smallest" generalized eigenvalue can be interpreted as the global residue of the optimal line.

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