Three dimensional least-squares fitting of ellipsoids and hyperboloids

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Abstract. Spatial continuity can be described as a variogram model that has an ellipsoid anisotropy. In previous research, two-dimensional least-square ellipse fitting method by Fitzgibbon, Pilu and Fisher has been applied to the analysis of spatial continuity for coal deposits. However, it is not easy to generalize their method to three-dimensional least-square ellipsoid fitting. In this research, we obtain a three-dimensional least-square fitting for ellipsoids and hyperboloids by generalizing two-dimensional least-square ellipse fitting method introduced by Gander, Golub and Strebel.

1. Introduction

Nowadays, it is undeniable that more and more researchers are applying the results of research in the field of mathematics to help facilitate their research. One of them is the application of fitting method with direct least-squares in the mining. The spatial continuity of a precipitate may be described as a variogram model having an elliptic anisotropy. This is demonstrated in a recent study by Fikri et al. [1]. They analyzed the continuity of spatial deposits of coal by applying the method introduced by Fitzgibbon et al. [2] (see also [3]).

Meanwhile, in 1994, Gander, Golub and Strebel in [4] introduced the method of elliptical fittings at measured data points by minimizing algebraic distance. The paper explained the fitting method in which the process utilized singular value decomposition in obtaining the shape of an ellipse or hyperbola from a distribution of data points.

The purpose of this research is to get the form of three dimensional least-squares fitting of ellipsoid and hyperboloid from a distribution of data points by generalizing the two dimensional least-squares fitting that were mentioned in previous researches. After getting the least-squares fitting as the result of the generalization, the obtained data [5] were fitted into a form of ellipsoid or hyperboloid by applying the obtained generalization method.

In section 2 we will present the underlying theories that were used to generalize the fitting method. In addition, an algorithm and a calculation sample will also be given at a data point deployment using the obtained method. In the end, the conclusion of the research will be presented at the end of the paper.
2. Basic theory

This research is based on two fitting methods on two dimensional with different constraints, which were introduced in [2] and [4]. However, this paper will discuss more on SVD method introduced by Golub, et al. Singular value decomposition, known as SVD technique, is a very useful technique to solve least-squares problems.

Initially given a form of presentation of the general equation three dimensional space as follows:

\[ x^T A x + b^T x + c = 0, \]  
with :

\[
\begin{aligned}
\begin{pmatrix} x_1 \\ x_2 \\ x_3 
\end{pmatrix} &= \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix},
\end{aligned}
\]

If equation (2.1) is described as follows:

\[
\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} a_{11} x_1^2 + 2a_{12} x_1 x_2 + 2a_{13} x_1 x_3 + 2a_{23} x_2 x_3 + a_{22} x_2^2 + a_{33} x_3^2 + b_1 x_1 + b_2 x_2 + b_3 x_3 + c = 0 \end{pmatrix}
\]
then we introduce new coordinates \( \vec{x} \) with \( x = Q \vec{x} + t \) so that the equation is rotated and shifted. Consequently, equation 2.1 changes to:

\[
\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_3^2 + c' = 0 \end{pmatrix}
\]

Further more defined \( \vec{A} = Q^T A \); \( \vec{b} = (2t^T A + b^T) \). So (2.3) may be written as \( \vec{x}^T \vec{A} \vec{x} + \vec{b}^T \vec{x} + c' = 0 \). We may choose \( \vec{Q} \) so that \( \vec{A} = diag (\lambda_1, \lambda_2, \lambda_3) = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \). As in [4], we can select \( \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \) so that \( \vec{b} = \vec{0} \). Hence, the equation may be written:

\[
\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_3^2 + c' = 0 \end{pmatrix}
\]

Similar to the two-dimensional method in paper [4], in generalizing the method to three-dimensional form, we need to find coefficient \( \vec{u} = (a_{11} \ 2a_{12} \ 2a_{13} \ 2a_{23} \ a_{22} \ a_{33} \ b_1 \ b_2 \ b_3 \ c)^T \) from the equation (2.2) with least-square method that minimize \( \|B \vec{u}\| \) subject to \( \|\vec{u}\| = 1 \) where

\[
B = \begin{pmatrix} x_{11} & x_{12} & x_{13} & x_{21} & x_{22} & x_{23} & x_{31} & x_{32} & x_{33} & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{1m} & x_{1m} & x_{1m} & x_{1m} & x_{1m} & x_{1m} & x_{1m} & x_{1m} & x_{1m} & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}
\]

The constraint \( \|\vec{u}\| = 1 \) was chosen to obtain a non-trivial solution [6].

But the constraint \( \|\vec{u}\| = 1 \) is not invariant for Euclidean coordinate transformation (rotating and shifting) \( x = Q \vec{x} + t \) where \( Q^T Q = I \). Therefore, in order to make the constraint invariant, a new constraint is defined as follow:

\[
\lambda_1^2 + \lambda_2^2 + \lambda_3^2 = a_{11}^2 + 2a_{12}^2 + 2a_{13}^2 + 2a_{23}^2 + a_{22}^2 + a_{33}^2 = 1
\]

Next to determine the vector \( \vec{u} \), we define the following two vectors:

\[
\vec{v} = (b_1 \ b_2 \ b_3 \ c)^T \quad \text{and} \quad \vec{w} = (a_{11} \ \sqrt{2}a_{12} \ \sqrt{2}a_{13} \ \sqrt{2}a_{23} \ a_{22} \ a_{33})^T
\]

As a result, the distribution of data owned is formed into a new coefficient matrix as follows:

\[
S = \begin{pmatrix} x_{11} & x_{21} & x_{31} & 1 & x_{11}^2 & \sqrt{2}x_{11}x_{21} & \sqrt{2}x_{11}x_{31} & \sqrt{2}x_{21}x_{31} & x_{21}^2 & x_{31}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{1m} & x_{2m} & x_{3m} & 1 & x_{1m}^2 & \sqrt{2}x_{1m}x_{2m} & \sqrt{2}x_{1m}x_{3m} & \sqrt{2}x_{2m}x_{3m} & x_{2m}^2 & x_{3m}^2 \end{pmatrix}
\]
So that the system of equation to be resolved can be rewritten to minimize \( \| S \left( \frac{v}{w} \right) \| \) with constraint \( \| w \| = 1 \).

To solve the problem, we use QR factorization for the matrix \( S \) to obtain a system involving \( w \) used as constraint in this equation. The result is obtained \( \| S \left( \frac{v}{w} \right) \| = \| QR \left( \frac{v}{w} \right) \| \). Because in the QR method of factorization, \( Q \) is an orthogonal matrix and \( R \) is the upper triangular matrix, consequently \( \| QR \left( \frac{v}{w} \right) \| = \| R \left( \frac{v}{w} \right) \| \) so the form can be written to be

\[
\begin{pmatrix}
R_{11} & R_{12} \\
0 & R_{22}
\end{pmatrix}
\begin{pmatrix}
\frac{v}{w}
\end{pmatrix}
\approx 0
\]

As a result, the problem has been simplified to minimize \( \| R_{22} w \| \) with constraint \( \| w \| = 1 \). If we do singular value decomposition to \( R_{22} \), say \( R_{22} = U \Sigma V^T \) then based on the singular value decomposition theorem \[7, Theorem 2.3\] we get \( w = v_n \), where \( v_n \) is the last column of the matrix \( V \) from the SVD of \( R_{22} \). Then we obtain \( v = -R_{11}^{-1} R_{12} w \) and thus the coefficient value of the equation is obtained (2.2).

### 3. Result

This section presents the result of generalizing the fitting method in three dimensional using the singular value decomposition approach. The data used in the calculation obtained from [5].

#### Table 1. Three dimensional data distribution.

| \( x_1 \) | 1 | -1 | 0 | -1 | 2 | 2 | 4 | 5 | 1 | -1 | 0 | -1 | 3 | 2 | 5 | 6 |
|----------|---|----|---|----|---|---|---|---|---|----|---|----|---|---|---|---|
| \( x_2 \) | 2 | 1 | 3 | 4 | 2 | 3 | 1 | 1 | 2 | 1 | 3 | 5 | 2 | 3 | 1 | 1 |
| \( x_3 \) | -1 | 0 | -1 | 6 | -1 | -1 | 6 | 4 | -2 | -1 | 2 | 7 | -2 | -2 | 6 | 5 |

The equation to be obtained is the equation

\[
a_{11} x_1^2 + 2a_{12} x_1 x_2 + 2a_{13} x_1 x_3 + 2a_{23} x_2 x_3 + a_{22} x_2^2 + a_{33} x_3^2 + b_1 x_1 + b_2 x_2 + b_3 x_3 + c = 0
\]

with \( u = (a_{11}, 2a_{12}, 2a_{13}, 2a_{23}, a_{22}, a_{33}, b_1, b_2, b_3, c)^T \).

The equation matrix is

\[
S = \begin{pmatrix}
1 & 2 & -1 & 1 & 1 & 2.83 & -1.41 & -2.83 & 4 & 1 \\
-1 & 1 & 0 & 1 & 1 & -1.41 & 0 & 0 & 1 & 0 \\
0 & 3 & -1 & 1 & 0 & 0 & 0 & -4.24 & 9 & 1 \\
-1 & 4 & 6 & 1 & 1 & -5.66 & -8.49 & 33.94 & 16 & 36 \\
2 & 2 & -1 & 1 & 4 & 5.66 & -2.83 & -2.83 & 4 & 1 \\
2 & 3 & -1 & 1 & 4 & 8.49 & -2.83 & -4.24 & 9 & 1 \\
4 & 1 & 6 & 1 & 16 & 5.66 & 33.94 & 8.49 & 1 & 36 \\
5 & 1 & 4 & 1 & 25 & 7.07 & 28.28 & 5.66 & 1 & 16 \\
1 & 2 & -2 & 1 & 1 & 2.83 & -2.83 & -5.66 & 4 & 4 \\
-1 & 1 & -1 & 1 & 1 & -1.41 & 1.41 & -1.41 & 1 & 1 \\
0 & 3 & -1 & 1 & 0 & 0 & 0 & -8.49 & 9 & 4 \\
-1 & 5 & 7 & 1 & 1 & -7.07 & -9.9 & 49.5 & 25 & 49 \\
3 & 2 & -2 & 1 & 9 & 8.49 & -8.49 & -5.66 & 4 & 4 \\
2 & 3 & -2 & 1 & 4 & 8.49 & -5.66 & -8.49 & 9 & 4 \\
5 & 1 & 6 & 1 & 25 & 7.07 & 42.43 & 8.49 & 1 & 36 \\
6 & 1 & 5 & 1 & 36 & 8.49 & 42.43 & 7.07 & 1 & 25
\end{pmatrix}
\]

After the decomposition of QR, then obtained matrix \( R \) as follows:
\[
R = \begin{pmatrix}
11.36 & 3.08 & 6.6 & 2.38 & 50.98 & 20.8 & 62.3 & 0.75 & 3.61 & 43.76 \\
0 & 9.46 & 3.03 & 2.92 & -0.27 & 12.5 & -9.84 & 27.49 & 52.86 & 6.63 & 55.86 \\
0 & 0 & 12.89 & -0.27 & 12.5 & -9.84 & 27.49 & 52.86 & 6.63 & 55.86 \\
0 & 0 & 0 & 1.31 & 6.26 & -0.58 & 16.66 & -7.8 & -6.03 & 0.83 \\
0 & 0 & 0 & 0 & 11.9 & -2.19 & 7.68 & 1.81 & 1 & -4.51 \\
0 & 0 & 0 & 0 & 0 & 4.38 & -4.67 & -0.82 & 0.24 & -2.97 \\
0 & 0 & 0 & 0 & 0 & 0 & 21.95 & -12.88 & -0.77 & 0.94 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 8.08 & 2.2 & 8.49 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.79 & 2.09 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 13.32
\end{pmatrix}
\]

where
\[
R_{22} = \begin{pmatrix}
11.9 & -2.19 & 7.68 & 1.81 & 1 & -4.51 \\
0 & 4.38 & -4.67 & -0.82 & 0.24 & -2.97 \\
0 & 0 & 21.95 & -12.88 & -0.77 & 0.94 \\
0 & 0 & 0 & 8.08 & 2.2 & 8.49 \\
0 & 0 & 0 & 0 & 1.79 & 2.09 \\
0 & 0 & 0 & 0 & 0 & 13.32
\end{pmatrix}
\]

Using the singular value decomposition, we get
\[
R_{22} = U \Sigma V^T
\]
for
\[
V = \begin{pmatrix}
-0.127 & -0.201 & -0.754 & 0.609 & 0.042 & -0.015 \\
0.045 & -0.013 & 0.196 & 0.302 & -0.889 & -0.276 \\
-0.866 & 0.152 & -0.203 & -0.37 & -0.179 & -0.122 \\
0.473 & 0.071 & -0.570 & -0.574 & -0.218 & -0.259 \\
0.031 & 0.046 & -0.142 & -0.107 & -0.352 & 0.917 \\
0.073 & 0.963 & -0.077 & 0.241 & 0.057 & -0.012
\end{pmatrix}
\]

By SVD theorem [7], \(w = v_6 = \begin{pmatrix}
-0.015 \\
-0.276 \\
-0.122 \\
-0.259 \\
0.917 \\
-0.012
\end{pmatrix}\) will minimize \(\|R_{22}w\|\). And we obtain \(v = \begin{pmatrix}
0.815 \\
-4.196 \\
0.796 \\
4.164
\end{pmatrix}\).

Hence the resulting quadratic equation is
\[-0.015x_1^2 - 0.39x_1x_2 - 0.17x_1x_3 - 0.37x_2x_3 + 0.917x_2^2 - 0.012x_3^2 + 0.815x_1 - 4.196x_2 + 0.796x_3 + 4.164 = 0\]
with the following picture

**Figure 1.** One sheet hyperboloid.

The following is also the result of three dimensional least-square fitting of some distribution of data points.
**Table 2.** The experimental result of some distributions of three dimensional data points.

| Number | Distribution of data points | Picture |
|--------|-----------------------------|---------|
| 1      | $x_1$ 0 0 -1 0 0 1 1 1 0  | ![Image](image1.png) |
|        | $x_2$ 0 1 0 -1 0 0 1 1 1  |         |
|        | $x_3$ 0 0 1 0 -1 -1 1 0 -1 |         |
|        | The equation: $0.34x_1^2 - 0.4x_1x_2 + 0.01x_1x_3 + 0.47x_2x_3 + 0.78x_2^2 + 0.28x_3^2 - 0.1x_1 - 0.22x_2 - 0.01x_3 - 0.41 = 0$ |         |
| 2      | $x_1$ -4 3 -1 -3 4 -2 -1 1 1 2 -2 | ![Image](image2.png) |
|        | $x_2$ -1 1 -3 -3 5 -1 1 -2 1 -2 1 1 |         |
|        | $x_3$ 5 -3 3 -3 1 -1 -5 4 1 3 3 2 |         |
|        | The equation: $0.43x_1^2 + x_1x_2 + 0.07x_1x_3 - 0.34x_2x_3 + 0.49x_2^2 + 0.03x_3^2 + 0.44x_1 + 0.43x_2 - 0.02x_3 - 3.56 = 0$ |         |
| 3      | $x_1$ 1 2 5 7 9 3 | ![Image](image3.png) |
|        | $x_2$ 1 2 3 4 5 6 |         |
|        | $x_3$ 7 6 8 7 5 7 |         |
|        | The equation: $-0.07x_1^2 + 0.64x_1x_2 + 0.49x_1x_3 + 0.25x_2x_3 + 0.02x_2^2 + 0.79x_3^2 - 5.01x_1 - 3.42x_2 - 13.24x_3 + 56.67 = 0$ |         |

4. Conclusion

We conclude that two dimensional least-square fitting method with Singular Value Decomposition method approach can be generalized to three dimensional form. For next research we will use this result to the analysis of spatial continuity for coal deposits in three dimensional.

Acknowledgments

This research is supported by Hibah P3MI Institut Teknologi Bandung

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