

An algorithm for fitting an ellipsoid to data

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Abstract

The ability to approximate a set of data by an ellipsoid is required in a diverse range of fields including robotics, astronomy and metrology. In this paper, we present techniques for ellipsoid fitting which are based on minimizing the sum of the squares of the geometric distances between the data and the ellipsoid. Although methods for solving this non-linear problem already exist, they are susceptible to numerical difficulties if the data approximate a “near-spherical” surface.

Initially, we consider an algebraic representation of an ellipsoid and develop a linear least squares approach to the fitting problem (this does not, in general, yield the best geometric fit). This representation is then used as the basis for a parametric form for expressing ellipsoids, and we are able to derive an iterative algorithm for obtaining the best geometric fit, using the algebraic fit as a first estimate. By means of numerical examples, this new method is shown to be particularly suited to fitting near-spherical data with an ellipsoid, as well as being effective for data sets representing more eccentric ellipsoids.

1 Introduction

In this paper, we describe techniques for fitting an ellipsoid to a prescribed set of data points $\{\mathbf{x}_i\}_{i=1}^m$. Ellipsoid fitting now has a large number of applications and is found, for example, in robotics [17], [18], astronomy [21] and metrology [19], [20]. Methods which fit ellipsoids to data are currently in existence, and we describe one such approach below.

Conventionally, an ellipsoid is defined in terms of centre co-ordinates (a, b, c) , semi-axes (r_x, r_y, r_z) and angles θ_1, θ_2 and θ_3 which represent rotations around the z -, y - and x -axes respectively. These angles control the orientation of the ellipsoid. The above ellipsoid can be defined parametrically by

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = R_1 R_2 R_3 \begin{bmatrix} r_x \cos u \cos v \\ r_y \sin u \cos v \\ r_z \sin v \end{bmatrix} + \begin{bmatrix} a \\ b \\ c \end{bmatrix}, \quad (1)$$

where $-\pi \leq u < \pi$ and $-\pi/2 \leq v < \pi/2$ are scalar auxiliary parameters. Here,

$$R_1 = \begin{bmatrix} c_1 & s_1 & 0 \\ -s_1 & c_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R_2 = \begin{bmatrix} c_2 & 0 & s_2 \\ 0 & 1 & 0 \\ -s_2 & 0 & c_2 \end{bmatrix} \quad \text{and} \quad R_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & c_3 & s_3 \\ 0 & -s_3 & c_3 \end{bmatrix}$$

are plane rotation matrices with $c_k = \cos \theta_k$ and $s_k = \sin \theta_k, k = 1, 2, 3$. Then, an ellipsoid E^* of best fit in the least squares sense to the given data points can be found by minimizing the sum of the squares of the geometric distances from the data to the ellipsoid. The geometric distance is defined to be the distance between a data point and its closest point on the ellipsoid [14]. Algorithms for finding the geometric distances from a set of points to a general surface are given in [1], [3].

Determining E^* is a non-linear problem which in principle can be solved by using the Gauss-Newton algorithm or one of its variants [15]. To illustrate the application of this algorithm, suppose that we have a parameter set $\mathbf{s} = [\hat{a}, \hat{b}, \hat{c}, \hat{r}_x, \hat{r}_y, \hat{r}_z, \hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3]^T$ that defines an estimate \hat{E} of E^* . For each data point, we find its geometric distance to \hat{E} and hence determine the vector \mathbf{d} whose i th component is the geometric distance to data point \mathbf{x}_i . If J is the associated Jacobian matrix defined at \mathbf{s} by

$$J_{ij} = \frac{\partial d_i}{\partial s_j},$$

then an updated estimate of the solution is given by $\mathbf{s} + \mathbf{p}$, where \mathbf{p} is the least squares solution of the (generally over-determined) linear system

$$J\mathbf{p} = -\mathbf{d}.$$

The ellipsoid fitting approach we have described suffers from two difficulties. Firstly, the provision of accurate estimates of the parameters \mathbf{s} is a complicated problem, and there appears to be no simple, generally effective manner of generating initial estimates of these parameters. Secondly, the fitting technique can suffer from numerical difficulties if we have data whose best fitting ellipsoid is near-spherical. For instance, we may wish to model a planetary body, such as the Earth. It is well known that a sphere provides a reasonable approximation to this, but that an ellipsoid gives a better model. In such a case, small changes to the data may result in large changes to the estimates of the rotation parameters, and hence the Jacobian matrix has a high condition number. Indeed, when an ellipsoid becomes a sphere, the rank of the Jacobian changes from nine to six.

In this paper, we present a technique for finding the best geometric fitting ellipsoid to data by deriving an alternative parametrization for an ellipsoid. The fitting problem is again non-linear and solved using the Gauss-Newton algorithm, but the numerical difficulties that occur if the data are near-spherical are avoided. A key consideration of our method is the determination of good starting values for the Gauss-Newton algorithm. Hence, we describe an approach for obtaining an accurate initial estimate of the solution parameters, which not only ensures that the Gauss-Newton algorithm converges to the correct solution, but also that it does so rapidly for representative data, thus reducing the computational cost. Necessary conditions for this minimization problem to have a unique solution are that $m \geq 9$ and the \mathbf{x}_i lie in general position (e.g., do not all lie in an elliptic plane). Throughout this paper, we assume that these conditions are satisfied.

2 An algorithm for a linear least squares estimated ellipsoid

We adopt a linear least squares approach to determine an estimated ellipsoid \hat{E} , which provides the initial estimate for the best fitting ellipsoid E^* . An ellipsoid with general orientation can be expressed as [9]

$$\mathbf{x}^T \bar{A} \mathbf{x} + \bar{\mathbf{b}}^T \mathbf{x} + \bar{c} = 0,$$

with the matrix \bar{A} symmetric and positive definite, $\bar{\mathbf{b}}$ a vector and \bar{c} a scalar. Setting

$$\bar{A} = \begin{bmatrix} A & D/2 & E/2 \\ D/2 & B & F/2 \\ E/2 & F/2 & C \end{bmatrix}, \quad \bar{\mathbf{b}} = \begin{bmatrix} G \\ H \\ K \end{bmatrix}, \quad \bar{c} = L, \quad \mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix},$$

we obtain the quadric equation

$$Ax^2 + By^2 + Cz^2 + Dxy + Exz + Fyz + Gx + Hy + Kz + L = 0, \quad (2)$$

subject to the constraints that $D^2 < 4AB$, $E^2 < 4AC$ and $F^2 < 4BC$ (these constraints ensure that \bar{A} is positive definite). Equation (2) contains ten parameters, one too many for a general ellipsoid. Therefore, we must either impose some suitable constraint upon equation (2), or eliminate a parameter. In order to maintain a linear problem, such a constraint must be linear. The simplest method is to fix one of the parameters in equation (2) equal to a prescribed constant. However, if that parameter is close to zero in the best fitting ellipsoid when it is unconstrained, numerical difficulties may arise if it is fixed to be a non-zero constant when it is constrained. Instead, we derive an approach based upon examining how the parameters A, B, C , etc relate to the ellipsoid's centre, semi-axes and orientation. From equation (1) we deduce that a point (x, y, z) on an ellipsoid satisfies

$$\begin{aligned} & \frac{1}{r_x^2} [(x-a)c_1c_2 + (y-b)(s_1c_3 - c_1s_2s_3) + (z-c)(c_1s_2c_3 + s_1s_3)]^2 \\ & + \frac{1}{r_y^2} [-(x-a)s_1c_2 + (y-b)(s_1s_2s_3 + c_1c_3) + (z-c)(c_1s_3 - s_1s_2c_3)]^2 \\ & + \frac{1}{r_z^2} [-(x-a)s_2 - (y-b)c_2s_3 + (z-c)c_2c_3]^2 = 1. \end{aligned} \quad (3)$$

Comparing coefficients of x^2, y^2 and z^2 in equations (2) and (3),

$$\begin{aligned} A &= \frac{c_1^2c_2^2}{r_x^2} + \frac{s_1^2c_2^2}{r_y^2} + \frac{s_2^2}{r_z^2}, \\ B &= \frac{(s_1c_3 - c_1s_2s_3)^2}{r_x^2} + \frac{(s_1s_2s_3 + c_1c_3)^2}{r_y^2} + \frac{c_2^2s_3^2}{r_z^2}, \\ C &= \frac{(c_1s_2c_3 + s_1s_3)^2}{r_x^2} + \frac{(c_1s_3 - s_1s_2c_3)^2}{r_y^2} + \frac{c_2^2c_3^2}{r_z^2}. \end{aligned}$$

By inspection, A, B and C are all strictly positive. We can similarly derive expressions in terms of a, b, c , etc for the other coefficients. The mathematics is cumbersome and we do not describe it in detail here. Instead, we note that D, E and F are near zero if θ_1, θ_2 and θ_3 are near zero. Further, G, H and K are near zero for ellipsoids centred near the origin (G, H and K are near zero in certain other cases also). Likewise, L can be shown to be near zero in a number of instances. Hence, only A, B and C

can be guaranteed to be non-zero, and so our constraint should be based upon these parameters.

We could constrain equation (2) by setting the largest in magnitude of A, B or C equal to a constant. However, given an arbitrary data set we have no *a priori* knowledge of which is largest and so instead set $A + B + C$ equal to a constant (which is larger than any of the individual parameters A, B or C), after rearranging the equation appropriately. Now, equation (2) can be rewritten as

$$\frac{1}{3}[(A + B + C)(x^2 + y^2 + z^2) + (A - C)(x^2 + y^2 - 2z^2) + (A - B)(x^2 - 2y^2 + z^2)] + Dxy + Exz + Fyz + Gx + Hy + Kz + L = 0. \quad (4)$$

Hence, upon multiplying the equation (4) by $3/(A + B + C)$ we have

$$x^2 + y^2 + z^2 - U(x^2 + y^2 - 2z^2) - V(x^2 - 2y^2 + z^2) - 4Mxy - 2Nxz - 2Pyz - Qx - Ry - Sz - T = 0, \quad (5)$$

where the coefficients in equation (5) are simple linear combinations of those in equation (4). To give some idea of the geometrical significance of these coefficients, we note that M, N and P are zero for the degenerate case of a sphere. Given the data set $\{\mathbf{x}_i = (x_i, y_i, z_i)\}_{i=1}^m$, the estimated ellipsoid \hat{E} is found by obtaining the solution in the least squares sense of the linear algebraic equations

$$\Lambda \mathbf{s}_{LS} = \mathbf{e},$$

where $\mathbf{s}_{LS} = (U, V, M, N, P, Q, R, S, T)^T$, the i th element of \mathbf{e} is $x_i^2 + y_i^2 + z_i^2$ and the i th row of the $m \times 9$ matrix Λ is

$$\left[x_i^2 + y_i^2 - 2z_i^2, \quad x_i^2 - 2y_i^2 + z_i^2, \quad 4x_i y_i, \quad 2x_i z_i, \quad 2y_i z_i, \quad x_i, \quad y_i, \quad z_i, \quad 1 \right].$$

Unfortunately, the elements of the vector \mathbf{e} are not, in general, measures of the geometric distances so this method does not normally provide the best geometric fitting ellipsoid. In fact, a major drawback of this algorithm is that it is difficult to interpret the residuals minimized in this method in a geometric sense. However, practical experiments have indicated that the estimation of E^* improves as the data become more spherical.

3 An algorithm for computing the ellipsoid of best geometric fit

In this section, we find the best fitting ellipsoid E^* by minimizing the sum of the squares of the geometric distances from the data $\{\mathbf{x}_i\}_{i=1}^m$ to the ellipsoid, whilst avoid-

ing the numerical difficulties described in Section 1. This non-linear problem is solved using an iterative technique, and we show how the linear least squares ellipsoid algorithm described in Section 2 can be used to provide initial estimates of the solution parameters.

One possible approach is to apply implicit orthogonal distance regression [6] to equation (5). However, we prefer to seek an alternative parametrization of an ellipsoid, since the parametric form more readily lends itself to distance regression. From equation (5), an ellipsoid centred at the origin with general orientation can be written as

$$x^2 + y^2 + z^2 = U(x^2 + y^2 - 2z^2) + V(x^2 - 2y^2 + z^2) + 4Mxy + 2Nxz + 2Pyz + T.$$

Introducing spherical polar co-ordinates $x = r \cos u \cos v$, $y = r \sin u \cos v$ and $z = r \sin v$ we obtain

$$r^2 = T + r^2[M(1 + \cos 2v) \sin 2u + N \cos u \sin 2v + P \sin u \sin 2v + U(3 \cos 2v - 1)/2 + 3V(\cos 2u \cos 2v + \cos 2u - \cos 2v + 1/3)/4].$$

Hence,

$$r^2 = T/[1 - M(1 + \cos 2v) \sin 2u - N \cos u \sin 2v - P \sin u \sin 2v - U(3 \cos 2v - 1)/2 - 3V(\cos 2u \cos 2v + \cos 2u - \cos 2v + 1/3)/4]. \quad (6)$$

Therefore, an ellipsoid centred at (a, b, c) can be specified as

$$\begin{aligned} x^* &= a + r(u, v) \cos u \cos v, \\ y^* &= b + r(u, v) \sin u \cos v, \\ z^* &= c + r(u, v) \sin v, \end{aligned} \quad (7)$$

with $r(u, v)$ given by equation (6) and $x^* = x + a$, etc. The best fitting ellipsoid can now be found by using the Gauss-Newton algorithm in a manner similar to that described in Section 1, except that the ellipsoid is defined by equation (7) and the minimization parameters are $\mathbf{s}^* = [a, b, c, M, N, P, T, U, V]^T$. The parametrization results in a well-conditioned problem for near-spherical data, as is demonstrated in Section 4. It is also effective for data sets approximating more eccentric ellipsoids. The provision of accurate starting values for the Gauss-Newton algorithm is discussed below.

It is important to note that, given identical values of M, N, P, T, U, V , equations (5) and (7) are only equivalent for ellipsoids centred at the origin, since T is dependent upon (a, b, c) in equation (5) but not in equation (7). However, we can exploit this

fact in order to obtain initial estimates for the Gauss-Newton algorithm, as we now describe. We find the linear least squares ellipsoid to the data set $\{\mathbf{x}_i\}_{i=1}^m$ and retrieve its centre, and then translate the data so that the linear least squares ellipsoid of the translated data is centred at the origin. Since we would expect the centre of the best fitting ellipsoid to the translated data to be close to the origin, we solve the linear least squares ellipsoid problem for the translated data and this provides initial estimates of M, N, P, T, U, V , with the centre initially estimated at $(0, 0, 0)$.

4 Numerical examples

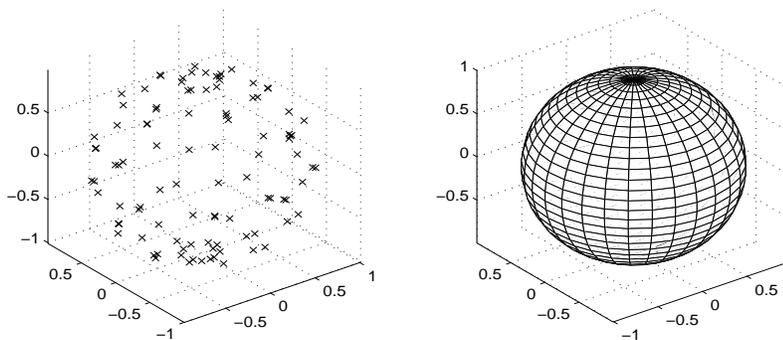


Figure 1: Synthesised near-spherical data set and best fit ellipsoid.

We have tested extensively the ellipsoid fitting technique described in Section 3, and Figures 1 and 2 show two synthesised data sets and their best fitting ellipsoids. The parameters $\mathbf{s}^* = [a, b, c, M, N, P, T, U, V]^T$ corresponding to the best fitting ellipsoids are given in Tables 1 and 3, along with the initial estimates $\hat{\mathbf{s}}$ which were provided by the linear least squares ellipsoid of Section 2. In both cases, the data set was translated so that the linear least squares ellipsoid was centred at the origin.

Table 2 shows the progress of the Gauss-Newton algorithm in fitting the near-spherical data shown in Figure 1. Successive columns represent (i) the condition number of the Jacobian matrix at each iteration and the 2-norms of (ii) the update step, (iii) the gradient vector and (iv) the vector of geometric distances (residuals). Table 4

	$\hat{\mathbf{s}}$	\mathbf{s}^*
a	0.000e+00	-9.191e-03
b	0.000e+00	-1.440e-03
c	0.000e+00	1.149e-03
M	-4.497e-03	-4.396e-03
N	-3.776e-04	-3.656e-04
P	-8.691e-03	-8.323e-03
T	9.986e-01	9.986e-01
U	-1.005e-03	-1.084e-03
V	-3.051e-04	-7.381e-04

Table 1: Details of the initial estimates and solution to the ellipsoid fitting problem for the data of Figure 1.

cond(Jacobian)	norm(step)	norm(gradient)	norm(residual)
3.124e+00	9.391e-03	2.884e-01	1.358e-01
3.123e+00	9.601e-05	2.322e-03	1.255e-01
3.123e+00	7.390e-07	9.037e-06	1.255e-01
3.123e+00	6.275e-09	9.917e-08	1.255e-01

Table 2: Progress of the Gauss-Newton algorithm when fitting an ellipsoid to the data of Figure 1.

shows corresponding results for the data set approximating a more eccentric ellipsoid shown in Figure 2. The convergence criterion was that both the 2-norm of the update step and the 2-norm of the gradient should be less than 10^{-8} .

Despite the residuals of the fit rendering quadratic convergence impossible, the Gauss-Newton algorithm converges at a reasonable rate. Further, we observe from the tables that the linear least squares ellipsoid provides excellent initial estimates $\hat{\mathbf{s}}$ to \mathbf{s}^* in both cases. From this estimate the Gauss-Newton algorithm provides a solution having sufficient accuracy for most practical purposes after two or three iterations. Indeed, if computational time is more important to the user than accuracy, the user may wish to implement only the linear least squares method. A study of Table 2 also shows that our parametrization leads to a well-conditioned problem for near-spherical data. In fact, comparison with Table 4 suggests rather that it is for ellipsoids with high eccentricity that ill-conditioning is now more likely to be a problem. This contrasts sharply with

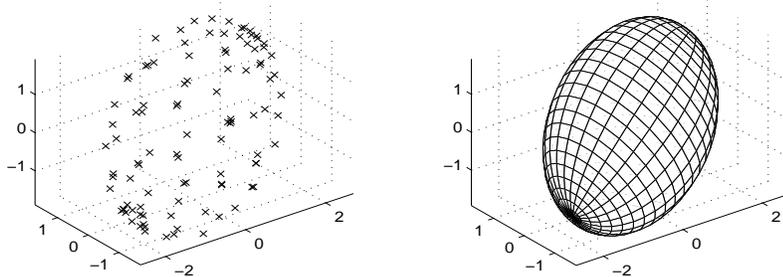


Figure 2: Synthesised data set and best fit ellipsoid.

the parametrization of Section 1, for which we found that the Gauss-Newton algorithm failed to converge for the data set of Figure 1.

5 Conclusions and further remarks

This paper has presented a method for fitting an ellipsoid to data, describing a technique for finding the best geometric fitting ellipsoid. In particular, if the data is near-spherical, we have demonstrated that our method can avoid the numerical difficulties suffered by existing approaches and provide a well-conditioned non-linear problem. Further, we have discussed how to achieve accurate initial estimates of the solution parameters. An additional feature of our method is that the ideas expressed in this paper can be generalised to certain other curves and surfaces.

Although not considered in this paper, we can extend the algorithm to take account of measurement error in the data. Further complications would appear to arise if the x, y and z co-ordinates were in some way correlated. However, in practice the theory of this paper remains valid, and compensation for the bias in the solution that would otherwise be obtained is made by introducing diagonal weighting matrices, or covariance matrices if the data co-ordinates are known to be correlated. In fact, surprisingly little additional effort is required. The mathematical details of how this can be done, in the context of fitting general surfaces to data, are given in [13].

	$\hat{\mathbf{s}}$	\mathbf{s}^*
a	0.000e+00	-2.498e-03
b	0.000e+00	9.520e-03
c	0.000e+00	-1.563e-03
M	2.635e-01	2.638e-01
N	-1.477e-01	-1.492e-01
P	6.765e-01	6.769e-01
T	2.197e+00	2.203e+00
U	1.343e-01	1.329e-01
V	3.868e-01	3.845e-01

Table 3: Details of the initial estimates and solution to the ellipsoid fitting problem for the data of Figure 2.

cond(Jacobian)	norm(step)	norm(gradient)	norm(residual)
3.604e+01	1.225e-02	2.111e+00	2.858e-01
3.589e+01	2.480e-04	1.648e-02	2.739e-01
3.589e+01	1.399e-06	8.981e-05	2.739e-01
3.589e+01	2.734e-10	1.049e-06	2.739e-01
3.589e+01	3.755e-10	9.464e-09	2.739e-01

Table 4: Progress of the Gauss-Newton algorithm when fitting an ellipsoid to the data of Figure 2.

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