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Type-Constrained Total Least Squares Fitting of Curved Surfaces to 3D Point Clouds

Lehmann R*

University of Applied Sciences Dresden, Faculty of Spatial Information, Germany

***Corresponding author:** Lehmann R, University of Applied Sciences Dresden, Faculty of Spatial Information, Friedrich-List-Platz 1, D-01069 Dresden, Germany, Fax: +49 351 462 2191, Tel: +49 351 462 3146,
E-mail: r.lehmann@htw-dresden.de

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Abstract

We present a unified approach to curved surface fitting in the framework of total least squares. Compared to algebraic and geometric fitting of surface models to 3D point cloud, this approach is relatively new. It has the largest degree of generality, such that any conceivable surface fitting problem can be formulated within this framework. In our contribution we consider quadric surfaces, which represent a very large and most popular class of curved surfaces. We discuss aspects of parametrizations and the use of constraints to restrict the set of solutions to special types of quadrics, like planes, spheres, ellipsoids, hyperboloids, cubes, cuboids, toroids, cylinders, cones, pyramids etc. Then we propose an iterative solution using Lagrange multipliers and the Newton method. The choice of an initial guess is discussed. Finally, we present a numerical example: fitting an elliptic cylinder with oblique axis to 20 data points. The results show that the total least squares fitting using type-constraints can be generally recommended to fit curved surfaces to point clouds.

Keywords: Quadric Surfaces; Point Cloud Fitting; Newton Method; Total Least Squares; Lagrange Multipliers

Introduction

Many measuring technologies only yield point observations, but actually a surface model is desired. Examples are the terrestrial and the airborne laser scanner technology, which are more and more applied in many branches, most of all in geodesy and photogrammetry. Today, a large number of such points is measurable in almost no time, forming huge point clouds in 3D space. See Yang *et al.* (2017) for the general relevance of point clouds in laser scanning technology [1].

This requires fitting surface models to such clouds. In computer graphics and CAD simple surface models are also known as geometric primitives: planes, spheres, ellipsoids, hyperboloids, cubes, cuboids, toroids, cylinders, cones, pyramids etc. Numerically, this fitting is an optimization: The optimally fitting surface is desired. This task is challenging for three reasons: The optimization problem

1. is usually nonlinear, requiring good initial guesses for the parameters to be optimized and a fastly converging iterative procedure,
2. often involves a large number of data points, possibly affected by outliers, and
3. is sometimes unstable or ill-posed because only small parts of the surface are covered by point observations.

In this contribution we deal with quite a general class of surfaces, known as quadric surfaces. Planes, spheres, spheroids, ellipsoids, hyperboloids, paraboloids, cylinders and cones belong to this class. They can be used as a model surface for fitting planar as well as most curved surfaces [2,3].

Optimal fitting requires a definition of optimality. This definition essentially determines the mathematical tools to be used as well as the computational costs. Two different definitions are customary: algebraic and geometric. The algebraic fitting is the most common technique applied in CAD, reverse engineering and computer vision technology [4]. It extends the equation of the quadric by a residual term. Optimality is now defined as the sum of squared residuals at the data points being a minimum.

Geometric fitting uses the spatial geometric distances of the data points from the quadric surface as a criterion of optimality [5-7]. It is more intuitive, but often computational much more costly than algebraic fitting. The author believes that when fitting surface models, computational costs should not be a criterion for exclusion of a method today.

Golub and Van Loan (1980) introduced total least squares (TLS) estimation. For the relationship of TLS to the errors-in-variables (EIV) model and the Gauss-Helmert model used in geodesy see (Neitzel 2010) Recently, Malissiovas *et al.* (2016) investigate 3D plane fitting by TLS [8-10].

When fitting surfaces to data points, the TLS approach is very much related to geometric fitting, but seen from a viewpoint, which is statistical rather than geometrical. The residual vector is orthogonal to the surfaces, which motivates using the term "orthogonal regression". The TLS approach to quadric surface fitting goes back to Späth (2004), but in principle the author also uses the geometric viewpoint. Up to now, the statistical viewpoint has not yet been consistently presented and fully exploited. Moreover, the idea of using type-constraints has not yet been consistently implemented into TLS. These are the mainstays of our contribution [4].

The outline of the paper is as follows: After deriving the geometry and parametrizations of a general quadric surface and all common special cases of it, we review the algebraic, geometric and TLS approaches found in the literature. The latter is then elaborated towards a unified approach applicable to all quadric surfaces by using type-constraints. These constraints restrict the set of admissible surfaces and are implemented in the framework of Lagrange multipliers. Finally, we apply this unified approach to the problem of fitting an elliptical cylinder with oblique axis to a number of 3D data points. The performance of TLS fitting is compared to the classical algebraic fitting.

General Quadrics as models of a curved surface

We start with a parametric model of a curved surface in three-dimensional space. For this purpose, the model of a quadric surface is well suited for most practical purposes. A quadric exists also in other dimensions (quadric curve, quadric hyper surface etc.). But since we deal here only with quadric surfaces, we call them 'quadrics' for short.

Let x,y,z be Cartesian coordinates of the 3D space. A point with coordinate vector $q=(x,y,z)^T$ is situated on a quadric, if and only if it satisfies the equation

$$q^T U q + v^T q = w \tag{1}$$

The elements of the 3x3-matrix U, the 3-vector and the scalar w are the parameters of the quadric. It would not be useful to consider nonsymmetric matrices U, because

$$\frac{1}{2} q^T \left(U + U^T\right) q + v^T q = w \tag{2}$$

would describe the same quadric as (1), with the now symmetric matrix $\left(U+U^T\right)/2$ in place of U. Let us therefore restrict to the case that U is symmetric:

$$U = \begin{pmatrix} u_{xx} & u_{xy} & u_{xz} \\ u_{xy} & u_{yy} & u_{yz} \\ u_{xz} & u_{yz} & u_{zz} \end{pmatrix}, v = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} \tag{3}$$

However, the remaining 10 parameters, collected in a vector

$$\beta = \left(u_{xx}, u_{xy}, u_{xz}, u_{yy}, u_{yz}, u_{zz}, v_x, v_y, v_z\right) \tag{4}$$

still exhibit a nonuniqueness, which causes trouble, when trying to fit a quadric to data points: All parameters multiplied by an arbitrary nonzero scalar describe the same quadric. At first dash it seems possible to solve this problem by introducing an arbitrary linear constraint

$$c^T \beta = 1 \tag{5a}$$

With some arbitrarily chosen vector c. But this solution fails if the vector space of equivalent parameters β happens to be perpenticular to c.

A simple constraint would be , i.e. in (5a) we get $c=(0,\dots.0,1)$. But this would be bad because a quadric passing through $q=0$ can no longer be represented. Moreover, moving the quadric by a small amount can cause jumps in some of the remaining 9 parameters. This also would cause numerical trouble, when trying to fit a quadric to data points.

Therefore, we propose a different approach to the parametrization of a quadric: We introduce a nonlinear constraint on the parameters in (4). The simplest one is

$$u_{xx}^2 + u_{xy}^2 + u_{xz}^2 + u_{yy}^2 + u_{yz}^2 + u_{zz}^2 + v_x^2 + v_y^2 + v_z^2 = 1 \tag{5b}$$

A constraint of type (5a) or (5b) will be called "uniqueness constraint" in the following. (5b) almost completely fixes the nonuniqueness described above, but leaves three minor problems unsolved:

1. The degenerate quadric β=0 , i.e. , $U = 0,$ $V = 0,$ w = 0, must be excluded from consideration.
2. If β satisfies (1) and (5b), so does -β. But as long as we keep away from the degenerate case β=0, we do not expect numerical problems.
3. (5b) is not invariant under translation and rotation of the coordinate system.

Let U be an invertible matrix. In this case, by a transformation

$$\tilde{q} = -\frac{1}{2}U^{-1}v,\ \tilde{w} = w + \frac{1}{4}v^T U^{-1} v \tag{6}$$

we can rewrite (1) in the equivalent form

$$(q-\tilde{q})^T U (q-\tilde{q}) = \tilde{w} \tag{7}$$

A reverse transformation from (7) to (1) is

$$v = -2U\tilde{q},\ w = \tilde{w} - \tilde{q}^T U \tilde{q} \tag{8}$$

Closely examined, for the existance of an expression (8) it is not necessary that U is regular. It is sufficient that v is in the range space of U, such that (8) has a solution $\tilde{q}, \tilde{w}$. Nonetheless, there are quadrics, which can be expressed in the form (1), but not in the form (7). Conversely, a quadric of the form (7) can always be expressed in the form (1). Thus, (1) is the more general form.

If we want to define parameters based on the form (7) we can replace v_x, v_y, v_z, w in (4) by $\tilde{q}_x, \tilde{q}_y, \tilde{q}_z, \tilde{w}$:

$$\tilde{\beta} = \left(u_{xx}, u_{xy}, u_{xz}, u_{yy}, u_{yz}, u_{zz}, \tilde{q}_x, \tilde{q}_y, \tilde{q}_z, \tilde{w}\right)^T \tag{9}$$

However, we also face an equivalent problem regarding uniqueness of the parametrization as in the form (1): All parameters $u_{xx}, \ldots, u_{zz}, \tilde{w}$ multiplied by an arbitrary nonzero scalar would describe the same quadric.

Again, a uniqueness constraint must be added to (7). The simplest one is here

$$u_{xx}^2 + u_{xy}^2 + u_{xz}^2 + u_{yy}^2 + u_{yz}^2 + u_{zz}^2 = 1 \tag{10}$$

But again leaves three minor problems unsolved:

1. The degenerate quadric $U = 0, \tilde{w} = 0$, must be excluded from consideration.
2. If $U, \tilde{q}, \tilde{w}$ satisfies (7) and (10), so does $-U, \tilde{q}, -\tilde{w}$. But as long as we keep away from the degenerate case $U = 0, \tilde{w} = 0$, we do not expect numerical problems.
3. (10) is invariant under translation, but not under rotation of the coordinate system.

Summarizing, (1) together with (5a) or (5b) is the optimal parametrization. While (1),(5a) is a linear system of equations for the parameters β, (7) is always nonlinear for the parameters $\tilde{\beta}$. However, the expression (7) is often useful for studying the geometric shape of a quadric, which will be done in the next section.

Special quadrics and principal axes transformation

A number of important special cases are included in the model of a general quadric (1) or (7). They can be formulated by constraints applied to the parameter vector β. Such constraints will be called "type constraints" in the following.

Plane: Restricting the general model (1) of a quadric to the case of a plane can be done by imposing the six linear type constraints

$$u_{xx} = 0, u_{xy} = 0, u_{xz} = 0, u_{yy} = 0, u_{yz} = 0, u_{zz} = 0 \tag{11}$$

such that (1) simplifies to

$$v^T q = w \tag{12}$$

We know that v≠0 is the normal vector of a plane with distance $|w|/|v|$ from the origin.

The nonuniqueness of the parametrization of the plane is expressed in the fact that the length of is not determined. (5b) selects the unit vector $|v|=1$. The minor problem that *v,w* and *–v,-w* describe the same plane, remains unsolved, but is practically marginal.

Since the range space of *U*=0 only contains the null-vector, a plane cannot be expressed in the form (7).

Sphere: Restricting the general model (1) of a quadric to the case of a sphere can be done by imposing the five linear type constraints

$$u_{xy}=0, u_{xz}=0, u_{yz}=0, u_{xx}=u_{yy}, u_{xx}=u_{zz} \tag{13}$$

If for some *r>0* we set *U=I*, i.e. the 3x3-unit matrix, and $\tilde{w}=r^2$, then (7) reads

$$\|q-\tilde{q}^2\| = r^2 \tag{14}$$

describing a sphere around center point $\tilde{q}$ with radius *r*. For the form (1) we find by (8) the relationships

$$v=-2\tilde{q},\ w=r^2-\|\tilde{q}\|^2 \tag{15}$$

With hindsight, *U,v,w* must be scaled to fulfill (5b) or (10) or some similar uniqueness constraint.

Principal axes transformation: If the quadric is neither a plane nor a sphere, and we want to get deeper insight into its geometric shape, it is necessary to perform a principal axes transformation [11]. For this purpose we have to make an eigenvalue decomposition of *U*, yielding

$$U=Q\Lambda Q^T \tag{16}$$

where *Q* is an orthogonal matrix of eigenvectors and Λ is a diagonal matrix of eigenvalues $\lambda_x, \lambda_y, \lambda_z$. Since *U* is symmetric, all three eigenvalues are real. Noticing that $QQ^T=I$, we can now rewrite (1) as

$$q^T Q\Lambda Q^T q + v^T QQ^T q = w \tag{17}$$

and with the principal axes transformation

$$q' := Q^T q,\ v' := Q^T v \tag{18}$$

we get

$$q'^T \Lambda q' + v'^T q' = \lambda_x q_x'^2 + \lambda_y q_y'^2 + \lambda_z q_z'^2 + v_x' q_x' + v_y' q_y' + v_z' q_z' = w \tag{19}$$

Similarly, applying the principal axes transformation to (7) with $\tilde{q}' := Q^T \tilde{q}$ we get

$$(q'-\tilde{q}')^T \Lambda (q'-\tilde{q}') = \lambda_x (q_x'-\tilde{q}_x')^2 + \lambda_y (q_y'-\tilde{q}_y')^2 + \lambda_z (q_z'-\tilde{q}_z')^2 = \tilde{w} \tag{20}$$

If $\det(Q)=1$ then *Q* and Q^T are rotation matrices, and the principal axes transformation is simply a rotation of the initial coordinate basis towards a basis defined by the eigenvectors of *U*. If on the contrary $\det(Q)=-1$ then an additional reflexion is necessary, because initial coordinate axes form a left handed cartesian basis, while the eigenvectors define a right handed cartesian basis or vice versa.

Ellipsoid or elliptic hyperboloid or cylinder: If $\tilde{w}>0$, then (7) describes an ellipsoid or elliptic hyperboloid or cylinder. Several cases need to be distinguished, depending on the signums of the eigenvalues $\lambda_x, \lambda_y, \lambda_z$. They are listed in Table 1, column 2. For example, in the case of $\lambda_x>0, \lambda_y>0, \lambda_z>0$ we get an ellipsoid with center point $\tilde{q}$ and semiaxes of length $\sqrt{\tilde{w}/\lambda_x}, \sqrt{\tilde{w}/\lambda_y}, \sqrt{\tilde{w}/\lambda_z}$ along the eigenvectors stored in *Q*.

Cone: For (20) to have a solution in the case $\tilde{w}=0$, there must be at least one negative and one positive eigenvalue. In this case, (20) describes an elliptic or spherical cone. The relevant cases are listed in Table 1, column 3.

Paraboloid: Like a plane, a paraboloid cannot be formulated by (7), but only by (1). It is obtained when one eigenvalue of *U* is zero, but not the corresponding element of v'.

Restricting the general model (1) of a quadric to any special case can again be done by adding type constraints.

eigenvalues of $\lambda_x, \lambda_y, \lambda_z$ of U	when $\tilde{w} > 0$	when $\tilde{w} = 0$
all positive and equal	sphere	not possible
all positive, two equal	spheroid	not possible
all positive, distinct	triaxial ellipsoid	not possible
one zero, two positive and equal	circular cylinder/ circular paraboloid	not possible
one zero, two positive and distinct	elliptic cylinder/ elliptic paraboloid	not possible
one negative, two positive and equal	circular hyperboloid of one sheet	circular cone
one negative, two positive and distinct	elliptic hyperboloid of one sheet	elliptic cone
two zero, one positive	two parallel planes	not possible
one negative, one zero, one positive	hyperbolic cylinder/ hyperbolic paraboloid	two intersecting planes
two negative, one positive and equal	circular hyperboloid of two sheets	circular cone
two negative, one positive and distinct	elliptic hyperboloid of two sheets	elliptic cone
all zero	not possible	degenerate
all negative	not possible	not possible

Table 1: Geometrical shapes of the quadrics described by (7)

Example 1: If the quadric is an elliptic or hyperbolic cylinder, U must be a singular matrix. This imposes the nonlinear type constraint:

$$\det(U) = 0 \tag{21}$$

Example 2: If the quadric should have prescribed pairwise orthogonal directions of principal axes, matrix Q is fixed. This means that $Q^T UQ$ is a diagonal matrix, which in turn means that the off-diagonal elements of $Q^T UQ$ must be zero. This can be enforced by three linear type constraints imposed on the parameters $u_{xx}, u_{xy}, u_{xz}, u_{yy}, u_{yz}, u_{zz}$:

$$\sum_{i,j=\{x,y,z\}} q_{xi} u_{ij} q_{jy} = \sum_{i,j=\{x,y,z\}} q_{xi} u_{ij} q_{jz} = \sum_{i,j=\{x,y,z\}} q_{yi} u_{ij} q_{jz} = 0 \tag{22}$$

Example 3: If the quadric should be an ellipsoid of prescribed lengths of the semiaxes , we find for the eigenvalues $\lambda_x, \lambda_y, \lambda_z$ of U the type constraints

$$a_x^2 \cdot \lambda_x = a_y^2 \cdot \lambda_y = a_z^2 \cdot \lambda_z = \tilde{w} \tag{23}$$

This means that the characteristic polynomial of $U / \tilde{w}$ is known, which in turn imposes three nonlinear type constraints on $u_{xx}, u_{xy}, u_{xz}, u_{yy}, u_{yz}, u_{zz}, \tilde{w}$. We here write down only one of them:

$$\det(U) \cdot a_x^2 \cdot a_y^2 \cdot a_z^2 = \tilde{w}^3 \tag{24}$$

Algebraic and geometric fitting

The problem is to determine the parameters of a quadric, best fitting p observed points. Each observed point induces an equation (1) or (7), e.g.

$$q_i^T U q_i + v^T q_i = w,\ i = 1, \ldots, p \tag{25}$$

and forms together with the uniqueness constraint and the m type constraints, if any, a nonlinear system of equations. The solvability of this set of equations for the 10 parameters is in general not trivial. Nevertheless, if $p + m + 1 = 10$, i.e. if the number of equations equals the number of parameters in vector β or $\tilde{\beta}$, we can hope for a unique solution, apart from special configurations and besides the sign indeterminacy mentioned in section 2.

Example 1 (cont'd): If an elliptic cylinder should be computed uniquely, we get $m=1$ type constraint (21), such that p=8 data points are required (excluding special configurations).

If we get more data points, we have to adjust some constraints. We consider three ways to deal with this problem: algebraic, geometric and general TLS fitting. The latter contains the first two as a special case. Note that these terms are not always used synonymously in the literature. We refer to the terminology used by [7] and others.

In algebraic fitting we adjust the constraint that the observed data points are located on the surface, by introducing a vector of residuals by

$$r_i := q_i^T U q_i + v^T q_i - w,\ i = 1, \ldots, p \tag{26}$$

and defining the objective function

$$\Omega(\beta) := \|r\|^2 \tag{27}$$

with some suitable vector norm. If the Euclidian norm is used, we arrive at a nonlinear least squares problem with constraints, for which the method of Lagrange multipliers is the standard method.

The algebraic fitting is the most common technique applied in CAD, reverse engineering and computer vision technology. Below we highlight some results in this field:

Lukacs *et al.* (1998) avoid constraints by eliminating m parameters from the vector β. This must be done for each type of surface (ellipsoid, cylinder, etc.) separately, but saves some computational costs [12].

Zhouchen Lin and Yameng Huang (2015) elegantly employ homogeneous coordinates to formulate the quadric fitting problem. The authors are concerned with the required positive semidefiniteness of U in ellipsoid/paraboloid-fitting. Here the Alternating Direction Method of Multipliers (ADMM) is prefered over Semidefinite Programs (SDP). In our paper we are not concerned with this part of the problem [13].

Reza and Sengupta AS (2017) develop a general algorithm for algebraic fitting ellipsoids of arbitrary shape and orientation. They use a type constraint to ensure that the resulting quadric is in fact an ellipsoid. Their method is based on iteratively improving the fit by changing the orientation of the coordinates to align along the axes of the ellipsoid using iterative random transformations [14].

Experiences show that algebraic fitting is biased and less suited for practial application [7]. The reason is that the algebraic distance (26) between point q_i and the quadric surface with parameters U,v,w is rarely equivalent to the geometric distance. As a remedy to this, Taubin's method is employed, it is also known as „gradient weighted algebraic fitting". The core idea is to introduce weights in (27) compensating for the defect of algebraic with respect to geometric fitting. This method is widely used, e.g. by Andrews and Séquin (2014) [4,15]. The advantage of algebraic fitting is its minimal computational costs.

Geometric fitting minimizes the distances between data points and the surface.

Example 4: Fitting a sphere to data points in the least squares sense means minimizing the objective function

$$\Omega(\tilde{q}, r) = \sum \left| \left\| q_i - \tilde{q} \right\| - r \right|^2 \tag{28}$$

Where symbols are used as in (14). Truly geometric fitting is computationally more costly, but can well be managed by the method of „orthogonal distance fitting "proposed by Sung Joon Ahn *et al.* (2002), Sung Joon Ahn (2004) [6]. This method is used by Chernov and Ma (2011) and others [7].

Total least squares fitting

Al-Subaihi and Watson GA (2005) use the term "algebraic fitting", but go beyond (26), (27) by re-formulating (25) as an operator equation [16].

$$H\beta = w \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \tag{29}$$

with the adjustment

$$(H + E)\beta = w \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} + r \tag{30}$$

minimizing a norm of the matrix [E r]. For special norms, this approach includes the approaches presented in the preceding section as special cases, but already goes beyond this into the direction of what is nowadays called total least squares (TLS) fitting: Also the operator H is adjusted.

Making the TLS approach more explicit, we allow for different observation errors in all $3p$ observed point coordinates. Given the observation vector

$$\left(x_1,\ldots,x_p,y_1,\ldots,y_p,z_1,\ldots,z_p\right)^T \tag{31}$$

and the corresponding $3p\times 3p$ covariance matrix

$$\Sigma=\begin{pmatrix}\sigma_{x_1}^2 & \cdots & \sigma_{x_1 z_p}\\ \vdots & \ddots & \vdots\\ \sigma_{x_1 z_p} & \cdots & \sigma_{z_p}^2\end{pmatrix} \tag{32}$$

we desire the TLS estimates of the parameters of a quadric (1) as well as of the true values of the coordinates of the observation points

$$\left(q_{x1},\ldots,q_{xp},q_{y1},\ldots,q_{yp},q_{z1},\ldots,q_{zp}\right)^T \tag{33}$$

The TLS objective function reads

$$\Omega\left(u_{xx},\ldots u_{zz},v_x,v_y,v_z,w,q_{x1},\ldots,q_{zp}\right)=\begin{pmatrix}x_1-q_{x1}\\ \vdots\\ z_p-q_{zp}\end{pmatrix}^T\Sigma^{-1}\begin{pmatrix}x_1-q_{x1}\\ \vdots\\ z_p-q_{zp}\end{pmatrix} \tag{34}$$

subject to the p quadratic point-on-quadric constraints (25) as well as the quadratic uniqueness constraint (5b). If the solution should be restricted to a special geometric shape like a plane, sphere etc., more linear and/or quadratic constraints must be added, like (21) … (24).

In some cases this model setup seems to be unnecessarily expensive. E.g. for a plane or sphere some parameters can be eliminated. This would reduce the TLS fitting to simple geometric fitting like in (28). But the proposed procedure is extremely general: All types of quadrics can be treated in a unified approach.

Example 1 (cont'd): If an elliptic cylinder should be fitted to *p=20* data points, we get
1. 60 known observation values (31)
2. 20 quadratic constraints (26) that the true points lie on the quadric
3. 1 cubic type constraint (21)
4. 1 quadratic uniqueness constraint (5b)
5. 10 parameters (4) of the quadric
6. 60 unknown true values of the coordinates (31) of the observation points,

This gives in total a redundancy (degrees of freedom) of 60 + 22 – 70 = 12.

Example 2 (cont'd): If an ellipsoid of prescribed lengths of the semiaxes should be fitted to *p=20* data points, we get three type-constraints. This gives in total a redundancy of 10.

We come up with a Gauss-Markov model with constraints [17]. The solution procedure is known as least squares estimation with constraints for parameters and takes advantage of the method of Lagrange multipliers. The extended objective function now reads

$$\Omega'\left(u_{xx},\ldots u_{zz},v_x,v_y,v_z,w,q_{x1},\ldots,q_{zp},k_0,\ldots,k_p,l_1,\ldots,l_m\right)=\begin{pmatrix}x_1-q_{x1}\\ \vdots\\ z_p-q_{zp}\end{pmatrix}^T\Sigma^{-1}\begin{pmatrix}x_1-q_{x1}\\ \vdots\\ z_p-q_{zp}\end{pmatrix}+ \tag{35}$$

$$k_0\left(u_{xx}^2+u_{xy}^2+u_{xz}^2+u_{yy}^2+u_{yz}^2+u_{zz}^2+v_x^2+v_y^2+v_z^2-1\right)+l^T B\left(\beta\right)+\sum_{i=1}^{p}k_i\left(q_i^T U q_i+v^T q_i-w\right)$$

where $k_0,\ldots,k_p,l_1,\ldots,l_m$ are the Lagrange multipliers and $B\left(\beta\right)=0$ denotes a system of m type-constraints, if any.
For the sake of simplicity, let us restrict to the case $\Sigma=\sigma^2 I$. The solution is found as a stationary point of Ω, where the necessary conditions read

$$
\begin{aligned}
&2k_0 u_{xx} + l^T \frac{\partial B}{\partial u_{xx}}(\beta) + \sum k_i q_{xi}^2 = 0 \\
&2k_0 u_{xy} + l^T \frac{\partial B}{\partial u_{xy}}(\beta) + 2\sum k_i q_{xi} q_{yi} = 0 \\
&\vdots \\
&2k_0 v_x + l^T \frac{\partial B}{\partial v_x}(\beta) + \sum k_i q_{xi} = 0 \\
&\vdots \\
&l^T \frac{\partial B}{\partial w}(\beta) - \sum k_i = 0 \\
&\frac{q_{xi} - x_i}{\sigma^2} + k_i \left(q_{xi} u_{xx} + q_{yi} u_{xy} + q_{zi} u_{xz} + v_x / 2 \right) = 0, \quad i = 1, \ldots, p \\
&\vdots \\
&u_{xx}^2 + u_{xy}^2 + u_{xz}^2 + u_{yy}^2 + u_{yz}^2 + u_{zz}^2 + v_x^2 + v_y^2 + v_z^2 - 1 = 0 \\
&q_i^T U q_i + v^T q_i - w = 0, \quad i = 1, \ldots, p \\
&B(\beta) = 0
\end{aligned}
\tag{36}
$$

This system of 11+4p+m cubic (with some possibly linear or quadratic) equations must be solved for the $11+4p+m$ unknowns.

Example 1 (cont'd): If the quadric should be an elliptic cylinder, the single type-constraint (21) and its derivatives read

$$
\begin{aligned}
&B(\beta) = u_{xx} u_{yy} u_{zz} + 2u_{xy} u_{xz} u_{yz} - u_{yz}^2 u_{xx} - u_{xz}^2 u_{yy} - u_{xy}^2 u_{zz} = 0 \\
&\frac{\partial B}{\partial u_{xx}} = u_{yy} u_{zz} - u_{yz}^2 \\
&\frac{\partial B}{\partial u_{xy}} = 2u_{xz} u_{yz} - 2u_{xy} u_{zz} \\
&\vdots \\
&\frac{\partial B}{\partial u_{zz}} = u_{xx} u_{yy} - u_{xy}^2
\end{aligned}
\tag{37}
$$

and the rest vanishing.

Initial guesses

Due to the nonlinearity of the system (36), we must start the procedure with good initial guesses for the unknowns. For this purpose the TLS fitting is best replaced by algebraic fitting. Uniqueness constraint (5b) is less convenient than (5a) because it is nonlinear. If some care is taken for the singularity mentioned above, (5a) is recommended here.

$$c^T \beta = 1 \tag{38a}$$

$$q_i^T U q_i + v^T q_i = w \tag{38b}$$

$$B(\beta) = 0 \tag{38c}$$

For $q_{x1},\dots,q_{zp}$ we can directly use the observed coordinates (31) as initial guesses. Note that (38a),(38b) are linear equations for β. Some type-constraints (38c) are fully linear equations for β, e.g. in the case of

1. plane, eq. (11)
2. sphere, eq. (13)
3. quadric with prescribed principal axes, eq. (22)

For the general quadric there is even no such constraint (38c). All those cases result in a fully linear overdetermined system of equations (38a)-(38c) for β, which can be solved by a standard least squares procedure. Later, we can take advantage of constraint (5b) by rescaling of the intial parameters, if desired.

In all other cases we can start with fitting a general quadric to all points as above and then we modify it slightly into the desired shape.

In Figure 1 a flow chart of the TLS fitting algorithm is displayed.

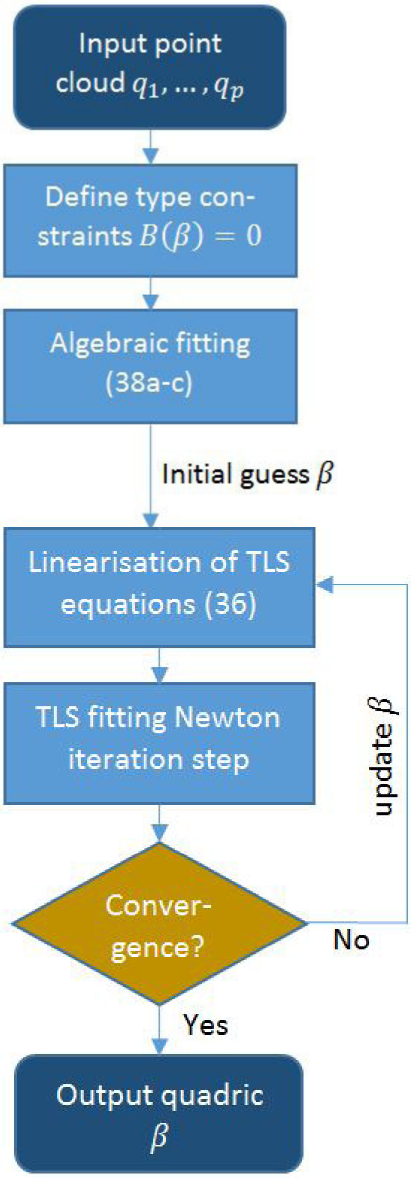

Figure 1: Flow chart of TLS fitting

Example 1 (cont'd): We modify the general quadric to a cylinder by replacing the least absolute eigenvalue of U by zero, etc.

Example 3 (cont'd): The matrix U of the general quadric should have eigenvalues approximately equal to $a_x^{-2}, a_y^{-2}, a_z^{-2}$. We modify the general quadric to an ellipsoid with prescribed semiaxes a_x, a_y, a_z by replacing U with

$$Q\begin{pmatrix} a_x^{-2} & 0 & 0 \\ 0 & a_y^{-2} & 0 \\ 0 & 0 & a_z^{-2} \end{pmatrix} Q^T$$

Inserting these initial guesses into the system of equations (36), it remains an over determined linear system of equations for the Lagrange multipliers $k_0,\ldots,k_p,l_1,\ldots,l_m$, which can be solved by a standard least squares procedure.

Application: Fitting a cylinder in oblique position

Given a cloud of p points on an elliptic cylinder in 3D space with oblique axis, the algebraic fitting as an extension of (27) for the type constraint (21) requires minimizing the following target function:

$$\Omega'\left(u_{xx},\ldots u_{zz},v_x,v_y,v_z,l\right)=l\cdot\det\left(U\right)+\sum\left(q_i^T U q_i+v^T q_i-1\right)^2 \tag{40}$$

with the choice $c=(0,\ldots,0,1)^T$ in (5a). (The latter means that w is set to unity because we know that the cylinder does not pass through the origin). l is the Lagrange multiplier for the type constraint (21). The necessary condition of a stationary point results in solving the following system of 10 nonlinear equations

$$\begin{gathered}
l\left(u_{yy}u_{zz}-u_{yz}^2\right)+2\sum q_{xi}^2\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
l\left(u_{xz}u_{yz}-u_{xy}u_{zz}\right)+2\sum q_{xi}q_{yi}\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
l\left(u_{xy}u_{yz}-u_{xz}u_{yy}\right)+2\sum q_{xi}q_{zi}\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
l\left(u_{xx}u_{zz}-u_{xz}^2\right)+2\sum q_{yi}^2\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
l\left(u_{xy}u_{xz}-u_{xx}u_{yz}\right)+2\sum q_{yi}q_{zi}\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
l\left(u_{xx}u_{yy}-u_{xy}^2\right)+2\sum q_{zi}^2\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
\sum q_{xi}\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
\sum q_{yi}\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
\sum q_{zi}\left(q_i^T U q_i+v^T q_i-1\right)=0 \\
u_{xx}u_{yy}u_{zz}+2u_{xy}u_{xz}u_{yz}-u_{yz}^2u_{xx}-u_{xz}^2u_{yy}-u_{xy}^2u_{zz}=0
\end{gathered} \tag{41}$$

For the TLS solution the system of $4p+12$ nonlinear equations as a specialization of (36) using (37) reads

$$\begin{gathered}
2k_0u_{xx}+l\left(u_{yy}u_{zz}-u_{yz}^2\right)+\sum k_i q_{xi}^2=0 \\
k_0u_{xy}+2l\left(u_{xz}u_{yz}-u_{xy}u_{zz}\right)+2\sum k_i q_{xi}q_{yi}=0 \\
k_0u_{xz}+2l\left(u_{xy}u_{yz}-u_{xz}u_{yy}\right)+2\sum k_i q_{xi}q_{zi}=0 \\
2k_0u_{yy}+l\left(u_{xx}u_{zz}-u_{xz}^2\right)+\sum k_i q_{yi}^2=0
\end{gathered} \tag{42}$$

$$k_0u_{yz}+2l\left(u_{xy}u_{xz}-u_{xx}u_{yz}\right)+2\sum k_iq_{yi}q_{zi}=0$$

$$2k_0u_{zz}+l\left(u_{xx}u_{yy}-u_{xy}^2\right)+\sum k_iq_{zi}^2=0$$

$$2k_0v_x+\sum k_iq_{xi}=0$$

$$2k_0v_y+\sum k_iq_{yi}=0$$

$$2k_0v_z+\sum k_iq_{zi}=0$$

$$\sum k_i=0$$

$$\frac{q_{xi}-x_i}{\sigma^2}+k_i\left(q_{xi}u_{xx}+q_{yi}u_{xy}+q_{zi}u_{xz}+\frac{v_x}{2}\right)=0,\quad i=1,\ldots,p$$

$$\frac{q_{yi}-y_i}{\sigma^2}+k_i\left(q_{xi}u_{xy}+q_{yi}u_{yy}+q_{zi}u_{yz}+\frac{v_y}{2}\right)=0,\quad i=1,\ldots,p$$

$$\frac{q_{zi}-z_i}{\sigma^2}+k_i\left(q_{xi}u_{xz}+q_{yi}u_{yz}+q_{zi}u_{zz}+\frac{v_z}{2}\right)=0,\quad i=1,\ldots,p$$

$$u_{xx}^2+u_{xy}^2+u_{xz}^2+u_{yy}^2+u_{yz}^2+u_{zz}^2+v_x^2+v_y^2+v_z^2-1=0$$

$$q_i^TUq_i+v^Tq_i-w=0,\quad i=1,\ldots,p$$

$$u_{xx}u_{yy}u_{zz}+2u_{xy}u_{xz}u_{yz}-u_{yz}^2u_{xx}-u_{xz}^2u_{yy}-u_{xy}^2u_{zz}=0$$

We set up a numerical experiment to test the performance of both fittings:
1. By MATLAB's pseudo random generator we generate p=20 points randomly distributed on an elliptic cylinder with semiaxes 1 and 0.6 of the ellipse. The axis points into the oblique direction of vector . The equation $(0.48\ 0.60\ 0.64)^T$ of the true cylinder reads

$$q^T\begin{pmatrix}0.7139 & -0.1078 & -0.4343\\ -0.1078 & 0.2395 & -0.1437\\ -0.4343 & -0.1437 & 0.4605\end{pmatrix}q=1$$

2. The observed coordinates are falsified by uncorrelated Gaussian noise, again generated by MATLAB's pseudo random generator. The chosen standard deviation is σ = 0.01.
3. The criterion of convergence of the iterative fitting is that the maximum change of all estimated U,v elements of two successive iteration steps is less than $10^{-6}\,w$.
4. As an initial guess we analytically fit a general quadric to these points, which is a perfect linear least squares problem. Later the matrix U is spectrally decomposed and the smallest eigenvalue of U is replaces by zero.
5. In the TLS fitting the observed coordinates x,y,z are used as initial guesses for $q_{x1},\ldots,q_{zp}$, and the Lagrange multipliers $k_0,\ldots,k_p,l$ are initially guessed as zero.
6. The common iterative Newton method is used to solve the nonlinear systems.

It is now interesting to see, if the iteration converges successfully. But it would not be good to compute this experiment only once because we could be lucky or unlucky with the results. It is better to perform multiple experiments in a Monte Carlo (MC) style approach. 1000 experiments have shown to give a realistic picture of the performance.

Figure 2 shows the convergence of the simple Newton method. The algebraic fitting (41) converges in only 81% of the MC experiments. Here between 11 and 16 iterations are required to meet the criterion of convergence. Here we should use some more elaborated nonlinear optimization method like Levenberg-Marquardt [18]. For TLS fitting (42) the simple Newton method always converges after 4 or 5 iterations. However, remember that the workload per iteration is much higher, because (42) has $4p+12$ = 92 equations and unknown quantities, while (41) has only 10 [19].

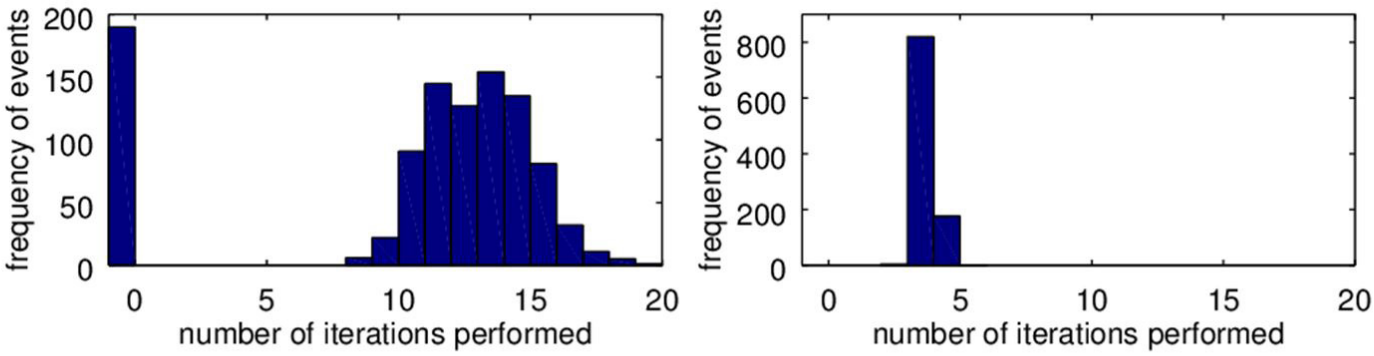

Figure 2: Results for convergence of the iteration. Left: algebraic fitting (Note: The bar at "0 iterations" shows the frequency of cases, where the iteration did not converge). Right: TLS fitting

Figure 3 shows the recovery of the true cylinder. Note that the left columns of Figure 3 shows only the 81% convergent experiments. In the first row the difference of the computed oblique axis of the cylinder from the true one in form of histograms of their spatial angle is displayed. The difference is about 1 degree. The performance of both fitting methods is almost identical.

The second and third row of Figure 3 shows the computed nonzero eigenvalues of U in form of histograms. Remember that the true eigenvalues are 1.0000 and $1/0.6^2$=2.7778, and this is where the peaks of all histograms are found. Although the difference is small, we see that the peaks of the left histograms are lower than of the right. From that we can conclude that algebraic fitting is slightly outperformed by the TLS fitting. We guess that once convergence is achieved also for the 19% divergent cases, they will contribute to the tails, rather than to the peaks of the left histograms of (Figure 3).

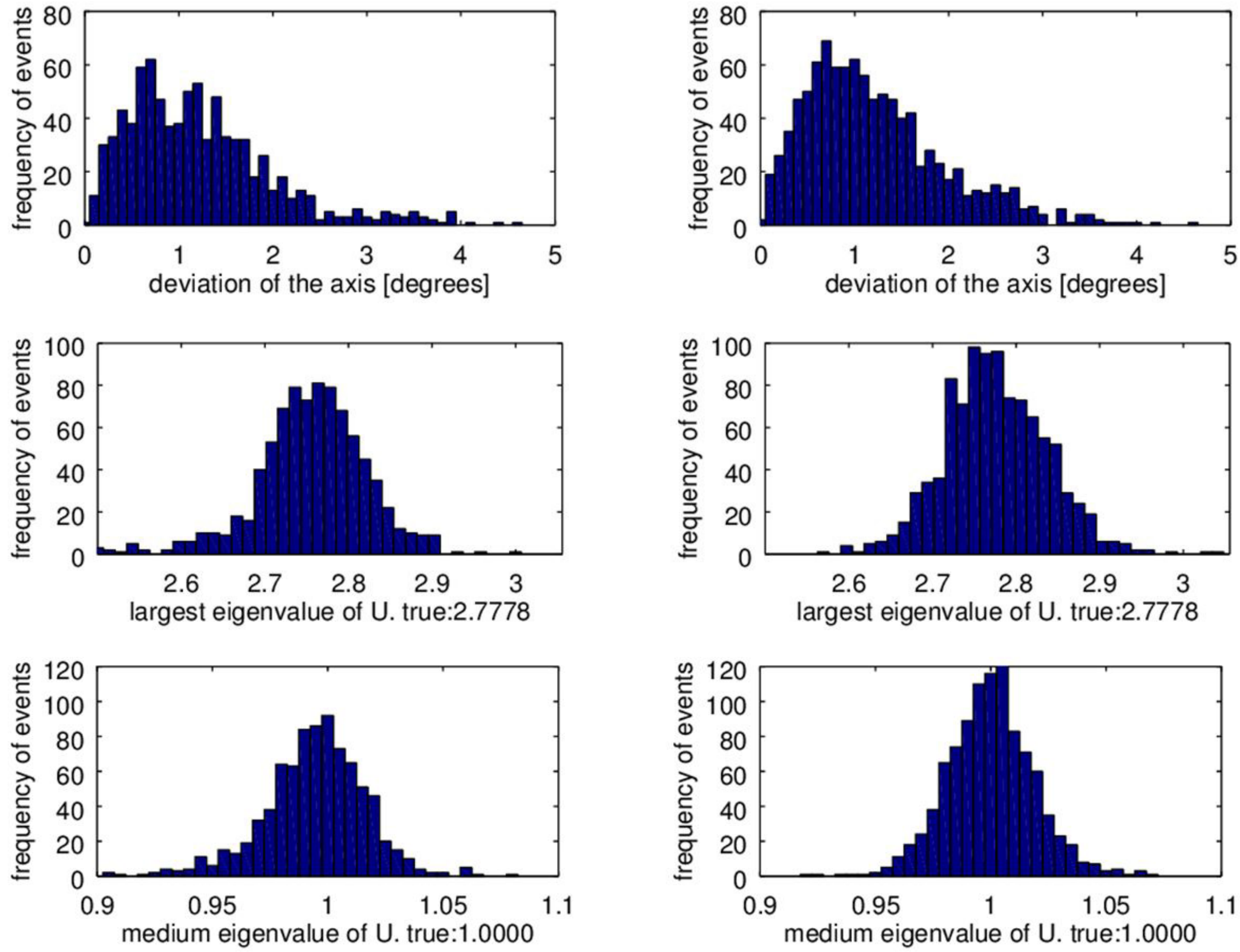

Figure 3: Deviations of the computed cylinder from the true one. Left: algebraic. Right: TLS fitting

Conclusion

We presented a unified approach to quadric surface fitting in the framework of TLS. It contains the geometric fitting as a special case and is different from the algebraic fitting. We discussed in detail the different parametrizations and the restriction to different special quadrics by type-constraints. Every conceivable quadric surface fitting problem can be formulated in this framework.

Numerically, the solution of the resulting system of equations is not simple, because this system can be quite large. It is much larger than for the algebraic solution. Moreover, the system is usually nonlinear and must be solved iteratively.

According to our research, we conclude that

1. It is possible to obtain good initial guesses, such that the iterative solution converges quickly,
2. Apart from illposed problems, the simple Newton method is sufficient to find the correct solution, and
3. Today's computers can manage the computational workload.

In our example we needed even much less iterations than for the algebraic solution, although the workload per iteration step is considerable heavier. Also the solution was mostly closer to the true one. Therefore, the approach can be generally recommended.

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